

Models for disorder in thiourea host/guest adducts
by James Francis Fait

A thesis submitted in partial fulfillment of the requirements for the degree of Doctor of Philosophy in Chemistry
Montana State University
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Abstract:
Thiourea host/guest adducts display a variety of types of disorder of the guest molecules. As these adducts also exhibit dramatic selectivity in the guest molecules included in the adduct, models that accurately describe the disorder of the guest are required to assess the principle forces involved in the formation of these adducts. Crystallographic structural studies for eight adducts of thiourea have been completed and disorder models for each adduct have been developed. Thermodynamic data on two adducts was collected for assessing the magnitude of the interactions involved in the formation and stabilization of these adducts. The principle interaction common to all of the adducts is coulombic interactions between localized partial charges on the guest and the dipole of thiourea. Six classifications of disorder are described. The disorder of each guest is described and categorized. Assessment of the interactions in these adducts allows predictions of other adducts that should form with thiourea.

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by

James Francis Fait

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APPROVAL

of a thesis submitted by

James Francis Fait

This thesis has been read by each member of the thesis committee and has been found to be satisfactory regarding content, English usage, format, citations, bibliographic style, and consistency, and is ready for submission to the College of Graduate Studies.

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Charles N. Caughlan — Chairperson, Graduate Committee

Approved for the Major Department

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Edwin H Abbott — Head, Major Department

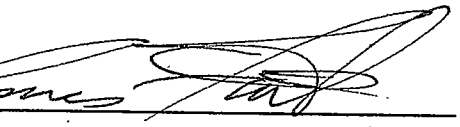
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ABSTRACT

Thiourea host/guest adducts display a variety of types of disorder of the guest molecules. As these adducts also exhibit dramatic selectivity in the guest molecules included in the adduct, models that accurately describe the disorder of the guest are required to assess the principle forces involved in the formation of these adducts. Crystallographic structural studies for eight adducts of thiourea have been completed and disorder models for each adduct have been developed. Thermodynamic data on two adducts was collected for assessing the magnitude of the interactions involved in the formation and stabilization of these adducts. The principle interaction common to all of the adducts is coulombic interactions between localized partial charges on the guest and the dipole of thiourea. Six classifications of disorder are described. The disorder of each guest is described and categorized. Assessment of the interactions in these adducts allows predictions of other adducts that should form with thiourea.

CHAPTER 1

INTRODUCTION

In molecular inclusion complexes, disorder is often observed because the interactions between the host lattice and the guest molecules are weak when compared to the stronger forces involved in other types of complexes.[26,58] One group of molecular complexes, based on urea and thiourea, consists of a open lattice of the urea forming continuous channels throughout the crystal.[25,28,58] In the thiourea adducts, the guest is located at particular positions along this channel, with the guest molecule disordered at these sites by any one of several mechanisms.[25] Thiourea forms host guest adducts with a wide variety of hydrocarbons, and the nature of the interactions involved in the formation of these adducts is of interest due to the selectivity of these adducts toward preferential inclusion of specific isomers in the host lattice.[3,4,9,17] These adducts are similar to the adducts formed by urea with some organic compounds, but show a striking difference in the type of guest molecules that are accommodated.[63] The urea adducts preferentially complex with straight chain hydrocarbons and derivatives. Hydrocarbon derivatives with bulky side groups and rings

destabilize the urea adducts.[64] More bulky ring systems and substituted guest molecules are preferred for adduct formation with thiourea,[3,17] with straight chain hydrocarbons included only when there are side chains or when the chain is long enough ($>C_{14}$) to form a helix with 5 carbons per turn in the channel.[34]

Historical

Discovery of the Urea Adducts

The discovery of the urea adducts in 1940 was made accidentally when Bengen, while studying the effect of urea on proteins in pasteurized milk, encountered foaming problems and an emulsion that led him to add a small amount of n-octanol as a defrothing agent.[10] Upon separation of the liquid, Bengen observed that long crystals had formed at the interface of the liquid layers. When Bengen attempted to reproduce the results, he observed that the crystals form when a saturated aqueous urea solution was mixed with n-octanol. Further investigations [46,53,55,64,68,69] showed that the urea adducts selectively complex with the straight chain hydrocarbons. Branched and/or cyclic compounds were not included in the crystal unless the straight portions of the complex were long enough to overcome the destabilizing effect of the bulky side groups.

Discovery of the Thiourea Adducts

The thiourea adducts were discovered independently by Angla in France (1947)[3,4,5] and Fetterly in the United States (1950).[17,18] Fetterly became aware of the urea adducts through the Technical Oil Mission reports in 1946. He was attempting to improve the octane rating of gasoline by complexing the low octane branched paraffins. Urea would not serve for this purpose, but it was soon discovered by Fetterly that thiourea did complex with isoparaffins as well as naphthenes, some polyhalogen hydrocarbons, and alcohols and ketones derived from these compounds.[45,56] Angla reported complexation of the terpene, camphene, cyclohexyl, and chloroparaffin classes (Figure 1).[5] Fetterly proposed that a "supported hydrogen bond" was responsible for the existence of these adducts.

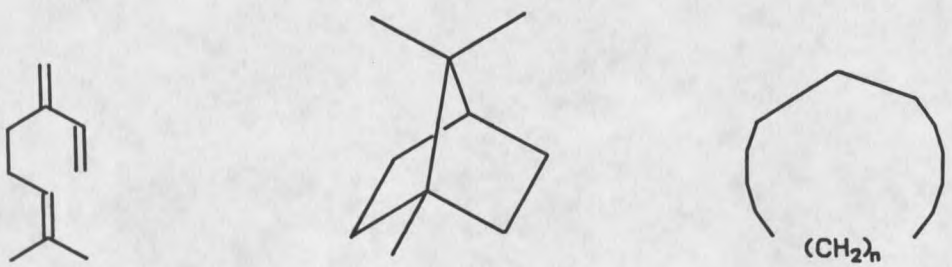


Figure 1. Examples of classes of compounds that form adducts with thiourea.

The supported hydrogen bond is defined as a hydrogen bond that is stabilized in a geometry that does not occur without the support of a channel or cavity by weak nonbonded interactions.[19] Fetterly also established complex formation with the related compounds selenourea and tellurourea.[18]

Induced Adduction

Induced adduct formation is defined as adduct formation by a guest that does not normally form a stable adduct with the host, but is induced to form an adduct by the presence of another guest that often forms a stable complex with the host. Both the urea and thiourea host/guest complexes show induced adduct formation.[21,55] Since the second guest, or inductor, initiates and stabilizes the host structure, otherwise unstable complexes can be formed. Application of induced adduction to the C_9 alkylbenzenes with thiourea by McCandless[29,30,31] gave a broader range of complexes for use in extractive crystallization.

Structural Studies on Adducts of Urea and Thiourea

Lenne, as part of his initial characterization of the thiourea adducts, reported some initial work on the crystal structure of the cyclohexane thiourea adduct.[28] He established the basic orientation of the thiourea in the

structure, and established the existence of a channel in which the guest molecules were disordered. He did not attempt to depict the guest disorder, but did locate the general location of the guest within the channel near the sulfurs of the thiourea. Subsequent x-ray analysis of a number of urea and thiourea adducts by Smith[58] and Schlenk[55] confirmed this, as well as investigating the structure of the urea adducts. All of these determinations indicated that the guest molecule was disordered, and the host lattice was nearly invariant with respect to the guest. Space group indications for the thiourea show it to be rhombohedral, space group R3c, with cell dimensions of a = b = 15.8Å, c = 12.5Å (hexagonal indexing). The urea adducts form in the hexagonal space group $P6_12$, with cell dimensions a = b = 8.230Å, c = 11.005Å.[58] The urea molecules form a spiral around the linear hydrocarbon guest located parallel to the c axis, with the environment of the guest quite uniform along the length of the channel.[58] The channel of the thiourea structure is also parallel to the c axis, however there are planes defined by three thioureas with the sulfurs directed into the channel, unlike the urea adducts.[56] Based on the strong dipole moment of thiourea and the observations of Lenne, Schlenk proposed that the guest should be located in this region of maximum interaction. These regions of maximum interaction

occur at c/2 intervals, giving an interplanar spacing of 6.25Å.

Other Properties

Redlich(1950)[45,46] contributed to the growing knowledge of the thiourea adducts by conducting a series of thermodynamic studies on several of the adducts. Using Gibbs free energy relationships and representing adduction by a chemical equilibrium, he reported that these adducts appear to form equilibrium systems much as in normal chemical reactions. Redlich reported the composition and equilibrium constants for the decomposition of the thiourea complexes of various isoparaffins, naphthenes, and carbon tetrachloride. The equilibrium constants for the adducts showed no trend with mole fraction of guest or with the size of guest.

Schiesser and Flitter(1952)[52] attempted to correlate the structure and the ability of a given guest to form a complex. Their work concentrated on a prediction of the channel size, and predicted adduct formation based only on guest size. This concept is in accordance with Fetterly's supported hydrogen bond,[19,52] but fails to predict the effect of inductors and the differences in selectivity between similar molecules when in adducts, especially those with conjugated systems and aromatic centers.

McLaughlin[33] compiled a comparison list of organic compounds of similar size and shape that either form or do not form complexes with thiourea. One example of this is benzene. Although the dimensions of the benzene ring are similar to those of cyclohexane, no adduct is formed. This suggests that more is involved in the adduct formation process than having a guest molecule of the right cross sectional dimensions. He also reported the formation of thiourea adducts with long chain ($>C_{14}$) n-paraffins, which form when the chain is long enough to form a helix in the thiourea channel with 5 methylene units per turn.

Extractive Crystallization

McCandless[29,30,31,32] developed extractive crystallization as one use for the thiourea adducts, and in his research on this process, concluded there was more involved in formation of these adducts than just having the right sized molecule to support the channel. Extractive crystallization, much like distillation, can be used to separate one compound from another. The utility is, however, that the equilibria governing adduct formation are not the same as those governing distillation, giving rise to a variety of new separations that are not feasible by distillation. This technique is enhanced by the use of inductors, chemicals that alter the selection rules for adduct formation utilizing induced adduction. This allows

the separation of isomers that might otherwise be extremely difficult to separate.

Related Substances

Gas Hydrates

Water forms host guest complexes of several types with a variety of gases and small molecules.[60] These hydrates form complexes with varying stoichiometry depending in part on the formation conditions, but also have a limiting value dependent on the size of the included molecule.[41] The hydrates have a significantly different structure from that of hexagonal ice,[12] and many of these complexes have melting points significantly above that of pure water,[60] indicating that the guest is stabilizing the lattice of the complex.

β-Quinol

Quinol forms stable adducts with many simple gases, including several of the noble gases.[38,39,40,42,43] The quinol structure, like that of the gas hydrates, is quite open, allowing for a variety of small molecules to be incorporated in the structure.[38] This system forms a cage around the guest, trapping it in a void in the lattice. Free rotation of the guest is often observed, indicating that the guest is not involved in any strong interactions with the quinol host lattice. Magnetic data on the O_2

quinol clathrate indicates that the guest molecules are isolated from each other, allowing investigations of properties that are inaccessible in the pure substance.[15]

Cyclodextrins and Amylose

The cyclodextrins complex with a wide variety of organic substances, principally by incorporation of hydrophobic sections of the molecule inside the cyclodextrin.[62] There is some channel character implicit in the cyclodextrin by nature of the molecular structure, and cyclodextrins exhibit host/guest interactions in solution as well as in the solid state.[54] The guest molecule in the cyclodextrin complexes is usually disordered, even at low temperature.[62] These complexes are selective only on geometric and hydrophobic bases. The cyclodextrins are related to the amylose complexes that form with nonpolar hydrocarbons and iodine. The familiar starch indicator for I_2 and the adducts formed by amylose with linear hydrocarbons are closely related, with the amylose forming a helix with six sugars per turn, and the guest molecule occupying the resulting channel in the crystal.[8,35,48,49,50,51]

Other Host Systems

Tri-o-thymotide

Tri-o-thymotide forms host/guest adducts with a variety of substances including alkanes and derivatives of

alkanes.[27,37,44] Two types of complex are formed, depending on the size of the guest molecule. For the smaller molecules, a cage type structure is formed that will accommodate molecules up to 9.5Å. If the molecule is longer than this, a channel structure is formed, where the ratio of host to guest need not be rational. Some of the channel forms of this host display one dimensional scattering characteristic of disorder in the guest region of the structure.[27]

Triphenylmethane

Triphenylmethane includes benzene, pyrrole, thiophen, or aniline as a molecule of crystallization.[23] 4,4'-Dihydroxytriphenylmethane and its derivatives, however, include a variety of hydrocarbons as guest molecules.[6] Based on the sizes of the guest molecules, the host lattice appears to have a diameter of at least 6.5Å. Aromatics also complex with the dihydroxytriphenylmethane derivatives, but form a different type of complex than the channel form observed with the aliphatic complexes.[6]

Cyclotriphospazenes

The related series of cyclotriphosphazenes, tris(1,8-naphthalenedioxy)cyclotriphosphazene, tris(2,3-naphthalenedioxy)cyclotriphosphazene, and tris(o-phenylenedioxy)cyclotriphosphazene, all form host guest adducts with a wide variety of compounds.[1,2] Some

of the host/guest systems exhibit preferential inclusion of one component of binary mixtures of guests.[2] Disorder is evident in several of these adducts, as is a nonstoichiometric ratio of host to guest.

N,N' Ditritrytlurea and Related Compounds

These hosts are characterized by a long molecular axis with rigid, bulky terminal groups.[22] These groups prevent close packing, resulting in open pockets in the structure that can entrap any molecule of an appropriate size to fit in the pocket. In the case of the N,N' ditritrytlurea, polar molecules can be accommodated, with hydrogen bonding occurring when possible to the urea moiety of the host molecule.

Zeolites

The zeolites are naturally occurring and synthetic aluminosilicates with cation exchange properties, and when dehydrated, molecular sieve and sorptive capabilities.[7] These properties arise because the dehydrated lattice of the zeolite is traversed by channels of molecular dimensions which are too narrow to accommodate some molecules, but narrow enough to contain others. This allows for the exchange of cations, as well as the molecular absorption character of these minerals.

Research Objectives

The objectives of this research are to determine the structures of a series of thiourea adducts, and to obtain crystallographic models of the disordered guests. Classification of the types of disorder, discerning some of the major interactions governing the host/guest interactions, and prediction of other guests that will form adducts with thiourea should follow from the models of the guest disorder.

CHAPTER 2

CARBON TETRACHLORIDE THIOUREA (1:3) ADDUCT

The first structure attempted in this project was that of the carbon tetrachloride thiourea adduct. In realization of the previous reports of serious disorder in these adducts, it was hoped that this simple molecule could be either ordered or be simple enough in its disorder to be easily characterized. In addition, the electron rich chlorine in the structure might enable a clearer picture of what was happening in the guest site than had been obtained to this point. To help minimize the effects of the adduct's instability and disorder, low temperature intensity data was collected at 170K.

Experimental

Crystal Preparation

Reagent grade thiourea, methanol, and carbon tetrachloride were purchased from the J. T. Baker Chemical Company. Carbon tetrachloride was allowed to diffuse into a saturated solution of thiourea in methanol at room temperature (≈25°C) and good quality crystals appeared in about 24 hours. An experimental density was obtained by flotation in chloroform/heptane solutions.

D_o = 1.42(2) gcm^{-3} (298K), D_c = 1.433 gcm^{-3} (170K), and M_r = 382.17. The adduct is unstable in air, as the crystals decompose through the loss of carbon tetrachloride through evaporation, resulting in a white microcrystalline powder. The crystal used for intensity data collection was mounted and sealed in a Lindemann glass capillary tube. Crystal dimensions were ≈0.5 x 0.5 x 1.0 mm^3.

Data Collection

Intensity data were collected on a Nicolet R3mE four circle diffractometer using the omega scan technique. The temperature of the crystal was maintained at 170K with a cold nitrogen stream supplied by a Nicolet LT-1 liquid nitrogen low temperature system. Three standard reflections were measured periodically throughout the course of the data collection to monitor crystal alignment and/or deterioration. There was no decrease in the standards over the course of the data collection; the maximum variation from the average was less than 3%. A total of 3531 reflections were collected, of which 1017 were unique and 640 were considered observed at the $6.0\sigma_F$ level (R_{merg} = 0.033). σ_F was calculated from counting statistics. Lattice parameters were obtained from the least squares fit to 12 reflections for which 8.5° < 2Θ < 25.5°. Unit cell dimensions, space group designation and

other details of the data collection, structure solution, and refinement are included in Table 1.

Table 1. Experimental Data for Carbon Tetrachloride Thiourea Adduct

Formula		$CCl_4 \cdot 3(SCN_2H_4)$
Cell Dimensions	a=b	15.539(4)Å
	c	12.529(9)Å
Space Group		$R\bar{3}$
Cell Volume		2620.0(20)Å^3
D_m		1.42(2) gcm^{-3}
D_c		1.433 gcm^{-3}
Crystal Dimensions		0.5 x 0.5 x 1.0 mm^3
$\sin\Theta / \lambda_{max}$		0.5944 Å^{-1}
Range	h	0 to ± 19
	k	0 to 19
	l	0 to ± 15
Total Reflections		3531
Unique Reflections		1017 R_{merg} = 0.033
Observed Reflections		640 6 σ_F cutoff
Number of parameters refined		83
$R = \frac{\Sigma(\lvert\lvert F_o\rvert - \lvert F_c\rvert\rvert)}{\Sigma\lvert F_o\rvert} =$		0.043
$R_w = \frac{\Sigma(\lvert\lvert F_o\rvert - \lvert F_c\rvert\rvert)w^{1/2}}{\Sigma\lvert F_o\rvert w^{1/2}} =$		0.033
$S = \frac{\Sigma(\lvert\lvert F_o\rvert - \lvert F_c\rvert\rvert)w^{1/2}}{(m-n)^{1/2}} =$		1.997

Data Reduction, Structure Solution, and Refinement

The data were reduced in the usual manner with appropriate Lorentz and polarization corrections. Scattering factors for S, Cl, N, C, H and anomalous scattering terms for S, Cl, N, and C were taken from the International Tables for X-ray Crystallography;[24] all atoms were assumed to be in the zero ionization state. No correction for absorption was made as the crystal was enclosed in a capillary preventing indexing of faces and the low temperature apparatus would not allow collection of psi scan data.

An initial model was obtained by direct methods utilizing the Nicolet program package,[57] the XTAL system of crystallographic programs,[61] and programs written locally. The S, C, and N atoms of the thiourea lattice structure were refined with anisotropic thermal parameters by full matrix least squares minimizing $\Sigma w(|F_o|-|F_c|)^2$ with all parameters refined in each full matrix block. Thiourea amino hydrogen position coordinates, determined from a difference Fourier electron density map at an intermediate stage of refinement, were refined along with isotropic thermal parameters. The weighting scheme used in the latter stages of refinement was $w = (\sigma_F)^{-2}$. A final difference Fourier electron density map showed maximum peak heights of $\simeq 0.30$ e/Å^3 in the vicinity of the chlorine atoms in the channel with the

most negative peak ≈ -0.25 e/Å^3. The largest shift over error value was less than 0.02 at convergence. The R for all of the data was 0.087, and the R for the observed data was 0.043. No corrections for secondary extinction were made or refined.

Disorder Model

Figure 2 illustrates the structure of the carbon tetrachloride thiourea adduct and the substantial disordering of the carbon tetrachloride molecule in the channel. The initial and final models for the carbon tetrachloride molecule are illustrated in Figure 3. Due to the substantial disorder of the system, obtaining a model for the carbon tetrachloride that made chemical sense was not a trivial problem. The initial model, derived by refining peaks located on difference Fourier electron density maps, suggested the final, simplified model with three anisotropic chlorine atoms representing the tetrahedral carbon tetrachloride. In the final model, the carbon tetrachloride is represented by an approximately tetrahedral carbon tetrachloride molecule with the carbon atom on the 3-fold axis and one of the molecular 2-fold axes normal to the 3-fold axis in the plane of the three thiourea sulfur atoms and approximately along a thiourea C-S vector. All atoms of the carbon tetrachloride were refined anisotropically with carbon to chlorine bond distances

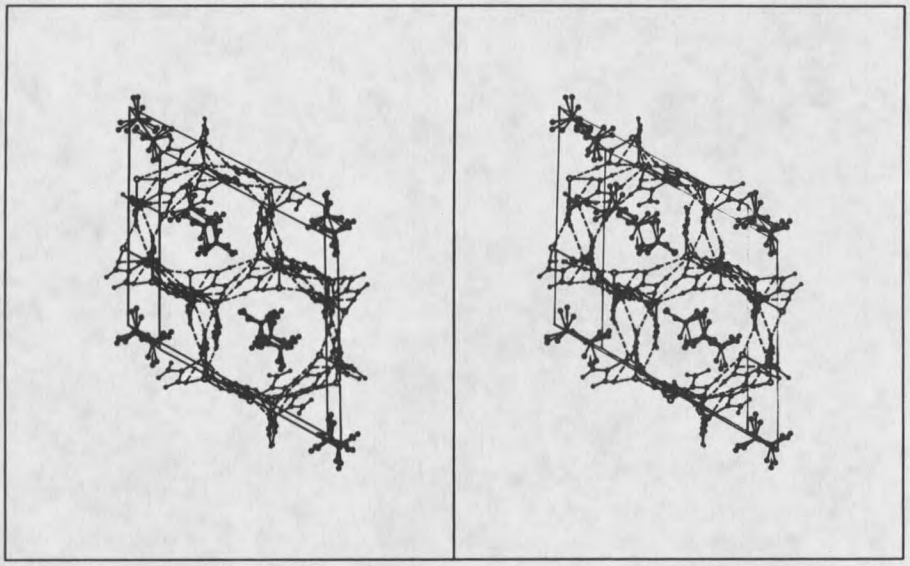


Figure 2. CCl_4 packing diagram view along c showing the hydrogen bonding of the thiourea host lattice and the disorder of the guest molecule.

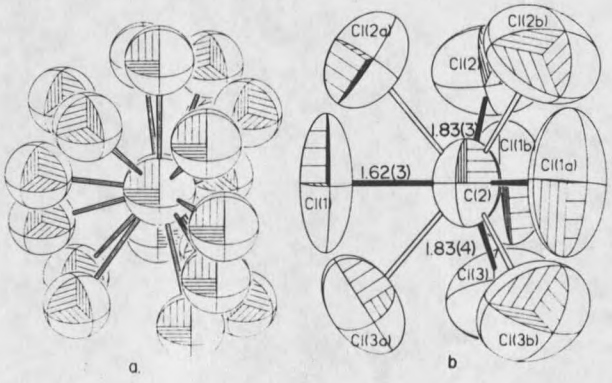


Figure 3. Initial and final disorder models for the CCl_4 guest. The initial model (a) suggested the final model (b).

ranging from 1.62Å to 1.83Å and the occupancy factors of the various chlorine atoms set at appropriate values such that the sum of the unique chlorine atom positions was 1.33. The occupancy of the chlorine atom in the plane of the thiourea sulfurs was set at 2/3, and the other two chlorine atom positions were assigned occupancies of 1/3 each, for a total occupancy of 1 1/3. This corresponds to a single carbon tetrachloride molecule disordered on the three fold special position. The bond lengths and angles are distorted from those expected for carbon tetrachloride, but fitting an idealized model to the observed chlorines resulted in a r.m.s. deviation of 0.0416Å on the chlorine positions, with the carbon displaced from the 3-fold axis by 0.184Å.

Results and Discussion

Derived Parameters

Tables 2 through 5 contain derived parameters for the carbon tetrachloride thiourea adduct. The bond lengths and angles for the thiourea molecule compare well with those previously observed for pure crystalline thiourea.[14,36]

Nature of the Bonding between Thiourea and the Guest Molecule

The structure as shown in Figure 4, and careful consideration of the disordered carbon tetrachloride

Table 2. Atomic Coordinates ($x10^4$) and Isotropic Thermal Parameters ($Å^2 x10^3$) for Carbon Tetrachloride Thiourea Adduct

	x	y	z	U
S(1)	2932(1)	-2(1)	7501(1)	31(1)*
C(1)	4043(3)	-4(3)	7499(3)	30(2)*
N(1)	4595(3)	234(3)	8371(3)	39(2)*
N(2)	4353(3)	-238(3)	6622(3)	38(2)*
C(2)	0	0	7508(9)	81(4)*
Cl(1)	1039(2)	1045(2)	7512(4)	138(2)*
Cl(2)	-57(6)	-793(5)	6399(5)	151(5)*
Cl(3)	53(6)	-728(5)	8626(5)	157(6)*
H(1)	5137(29)	106(30)	8384(38)	76(17)
H(2)	4458(25)	380(25)	8885(26)	22(12)
H(3)	4909(26)	-176(27)	6588(39)	59(16)
H(4)	3979(26)	-368(26)	5947(30)	62(14)

* Equivalent isotropic U defined as one third of the trace of the orthogonalised U_{ij} tensor.

Table 3. Bond Lengths (Å)

C(2)-Cl(1)	1.620(2)	C(2)-Cl(2)	1.830(11)
C(2)-Cl(3)	1.827(12)	C(2)-Cl(1a)	1.620(3)
C(2)-Cl(1b)	1.620(1)	C(2)-Cl(2a)	1.830(11)
C(2)-Cl(2b)	1.830(10)	C(2)-Cl(3a)	1.827(11)
C(2)-Cl(3b)	1.827(11)	S(1)-C(1)	1.727(5)
C(1)-N(1)	1.322(5)	C(1)-N(2)	1.322(6)
N(1)-H(1)	0.959(54)	N(1)-H(2)	0.748(37)
N(2)-H(3)	0.822(44)	N(2)-H(4)	0.987(39)

Table 4. Bond Angles (°)

CL(1)-C(2)-Cl(2)	111.5(5)	Cl(1)-C(2)-Cl(3)	106.7(5)
Cl(2)-C(2)-Cl(3)	99.6(3)	Cl(1)-C(2)-Cl(1a)	120.0(1)
Cl(2)-C(2)-Cl(1a)	106.7(5)	Cl(3)-C(2)-Cl(1a)	110.4(5)
Cl(1)-C(2)-Cl(1b)	120.0(1)	Cl(1)-C(2)-Cl(2b)	106.7(5)
Cl(1)-C(2)-Cl(3b)	110.4(5)	S(1)-C(1)-N(1)	120.5(4)
S(1)-C(1)-N(2)	120.2(3)	N(1)-C(1)-N(2)	119.3(4)
C(1)-N(1)-H(1)	118.1(28)	C(1)-N(1)-H(2)	123.6(31)
H(1)-N(1)-H(2)	117.4(43)	C(1)-N(2)-H(3)	121.2(33)
C(1)-N(2)-H(4)	120.7(26)	H(3)-N(2)-H(4)	117.2(42)

Table 5. Anisotropic Thermal Parameters ($Å^2 x 10^3$)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(2)	66(4)	66(4)	113(8)	0	0	33(2)
Cl(1)	57(2)	56(2)	265(4)	5(3)	-6(2)	0(1)
Cl(2)	226(7)	125(6)	133(7)	-44(4)	-16(6)	112(6)
Cl(3)	249(7)	134(6)	125(6)	23(5)	-9(6)	124(6)
S(1)	29(1)	36(1)	31(1)	-3(1)	-2(1)	18(1)
C(1)	31(2)	27(2)	28(2)	3(2)	2(2)	12(2)
N(1)	36(2)	54(2)	31(2)	-3(2)	-3(2)	26(2)
N(2)	38(2)	55(2)	33(2)	-3(2)	0(2)	31(2)

The anisotropic temperature factor exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$.

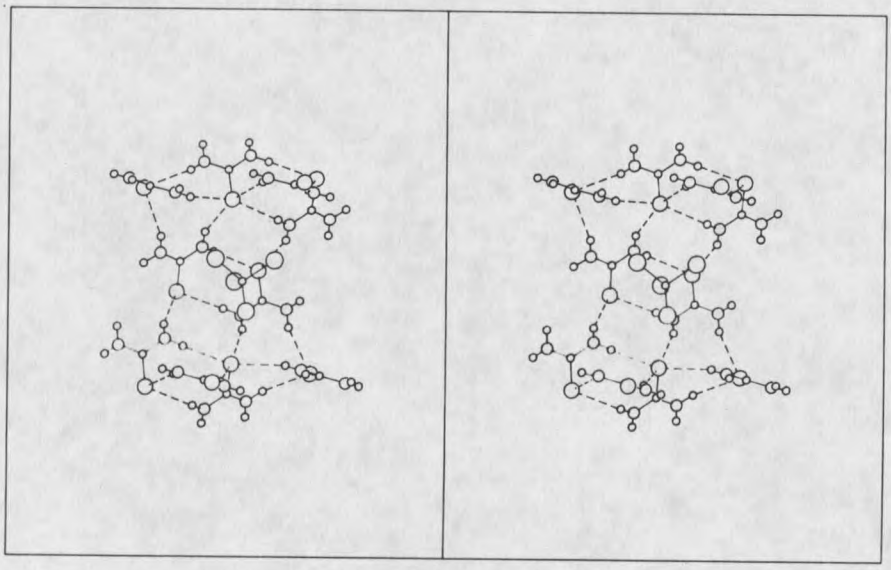


Figure 4. Cutaway view of carbon tetrachloride in the host lattice. Only one of three equivalent orientations of the carbon tetrachloride is shown.

molecule, suggests the qualitative nature of the bonding between the adducted organic molecule and the thiourea. There are three "open" areas of approach to the central carbon atom of the carbon tetrachloride molecule. These areas are 120° apart and the thiourea sulfur atoms point directly into them. The primary binding forces appear to involve coulombic interactions between the carbon in carbon tetrachloride and the sulfur of thiourea.

Figures 5 and 6 show the electron density distribution in the channel of the carbon tetrachloride adduct. Figure 5 is a view along the 3-fold axis, and shows the thiourea host in relation to the guest site, as well as the 3-fold symmetry imposed on the guest site. Figure 6 gives a closer view of the guest site, with the carbon and chlorine positions identifiable as regions of higher electron density.

The distance between the sulfur in the thiourea and the carbon in carbon tetrachloride is 4.59Å, which is substantially larger than the 3.50Å sum of the van der Waal radii.[11] Calculations[13] predict a +0.28 electron partial charge on the carbon of carbon tetrachloride, and a -0.52 electron partial charge on the sulfurs of thiourea. This indicates that the interactions appear to be between the positive carbon and the negative sulfur. All of the chlorines, which are also negative, are oriented so as to minimize the interactions with sulfur, as well as those

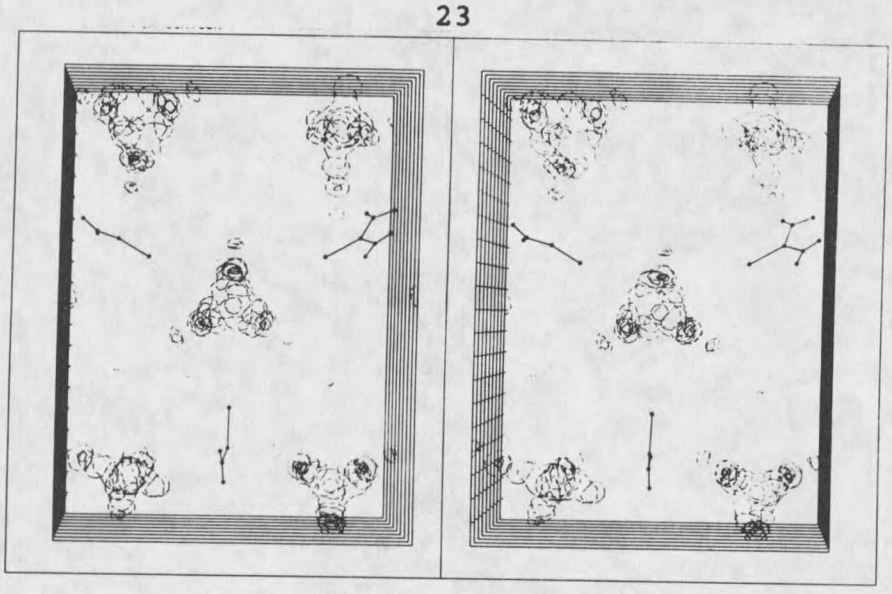


Figure 5. Stereo difference electron density contour map calculated from the final refinement without the guest molecule. View is along the 3-fold axis, with layers 0.5Å apart, solid contours at 3e/Å^3 and dotted contours at 1e/Å^3.

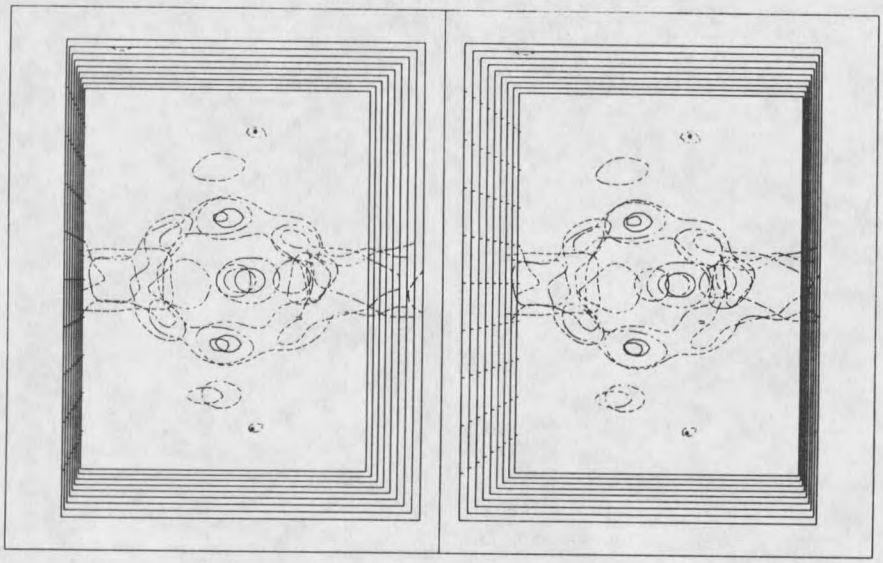


Figure 6. Stereo difference electron density contour map calculated from the final refinement without the guest molecule. View is normal to the 3-fold axis, with layers 0.5Å apart, solid contours at 3e/Å^3 and dotted contours at 1e/Å^3.

with the nitrogen, which is also negatively charged. None of the hydrogens appear to be involved with bonding with chlorine, therefore the primary positive interaction is that between the central carbon in carbon tetrachloride and the sulfur of thiourea, with this interaction being sufficiently large to overcome the negative contributions from the chlorine nitrogen and chlorine sulfur interactions.

CHAPTER 3

CYCLOHEXANE THIOUREA (1:3) ADDUCT

Some of the earliest crystal structure work on this class of compounds was concerned with the cyclohexane thiourea adduct.[25,28] This early work established the honeycomb type channel structure of the thiourea when adducted to an organic guest. Lenne[28] recognized that, for the cyclohexane adduct, the thiourea sulfur atoms pointed into the channel, and that the cyclohexane molecule appeared to be centered in the plane of the three sulfur atoms with the $\bar{3}$ axis normal to the plane of the cyclohexane molecule. Neither geometry nor orientation of the cyclohexane molecule were determined.

Experimental

Crystal Preparation

Reagent grade thiourea, cyclohexane, and ethanol were purchased from the J. T. Baker Chemical Company. Cyclohexane vapor was diffused into a saturated solution of thiourea at room temperature, with good crystals forming within about 24 hours. An experimental density was obtained by flotation in chloroform/heptane solutions. D_o = 1.14(3) gcm^{-3} and D_c = 1.187 gcm^{-3}. The adduct is

unstable in air, which is typical of many of the compounds in this series. The crystal used for intensity data collection had dimensions of 0.90 x 0.40 x 0.26 mm^3.

Data Collection

Intensity data were collected on a Nicolet R3m/E four circle diffractometer using the omega scan technique. Four standard reflections were measured periodically throughout the course of the data collection to monitor crystal alignment and/or deterioration. There was no decrease in the standards over the course of the data collection, with a maximum variation from the average of less than 3%. A total of 5855 reflections were collected of which 1768 were unique and 669 were considered observed at the $6\sigma_F$ level. Lattice parameters were obtained from least squares fit to 25 reflections for which $30.0° < 2\Theta < 35.0°$. Space group designation and other details of the data collection, structure solution and refinement are included in Table 6.

Data Reduction, Structure Solution, and Refinement

The data were reduced in the usual manner with appropriate Lorentz and polarization corrections. Scattering factors for S, N, C, H and anomalous scattering terms for S, N, and C were taken from the International Tables for X-ray Crystallography;[24] all atoms were assumed to be in the zero ionization state. No correction for absorption was made.

Table 6. Experimental Data for Cyclohexane Thiourea Adduct

Formula		$C_6H_{12}.3(SCN_2H_4)$
Cell Dimensions	a=b	15.856(2)
	c	12.461(2)
Space Group		R3
Cell Volume		2713.14(66)
D_m		1.14(3) gcm^{-3}
D_c		1.187 gcm^{-3}
Crystal Dimensions		.26 x .40 x .90 mm^3
$\sin\Theta / \lambda_{max}$		0.704 $Å^{-1}$
Range	h	0 to ± 23
	k	0 to 23
	l	0 to ± 18
Total Reflections		5855
Unique Reflections		1768 R_{merg} = 0.0068
Observed Reflections		669 6 σ_F cutoff
Number of parameters refined		Chair 60 / Boat 60
$R = \frac{\Sigma(\lvert\lvert F_o\rvert-\lvert F_c\rvert\rvert)}{\Sigma\lvert F_o\rvert} =$		0.062 / 0.063
$R_w = \frac{\Sigma(\lvert\lvert F_o\rvert-\lvert F_c\rvert\rvert)w^{1/2}}{\Sigma\lvert F_o\rvert w^{1/2}} =$		0.069 / 0.069
$S = \frac{\Sigma(\lvert\lvert F_o\rvert-\lvert F_c\rvert\rvert)w^{1/2}}{(m-n)^{1/2}} =$		1.890 / 1.813
$w = (\sigma_F^2 + gF^2)^{-1}$	where g =	0.00108

An initial model was obtained by direct methods. Subsequently, the atomic coordinates for the thiourea molecule from the carbon tetrachloride adduct were utilized as the compounds are isostructural. Computational work was done utilizing the Nicolet program package[57] and programs written locally. The S, C, and N atoms of the thiourea lattice structure were refined with anisotropic thermal parameters by full matrix least squares minimizing $\Sigma w(|F_o|-|F_c|)^2$ with all parameters refined in each full matrix block. Thiourea amino hydrogen position coordinates, determined from a difference Fourier electron density map at an intermediate stage of refinement, were refined along with isotropic thermal parameters. The weighting scheme used in the latter stages of refinement was $w = (\sigma_F^2 + gF^2)^{-1}$, where g was assigned a value of 0.00108 for both the chair model and the boat model. A final difference Fourier electron density map showed maximum peak heights $\approx$0.5 e/Å^3 in the vicinity of the adducted molecule in the channel, with the most negative peak of $\approx$0.35 e/Å^3 for both models. The largest shift over error value was less than 0.02 at convergence. No corrections for secondary extinction were made or refined.

Disorder Model

Figure 7 illustrates the structure of the cyclohexane adduct, and indicates the substantial disorder of the cyclohexane guest. The final model for the organic

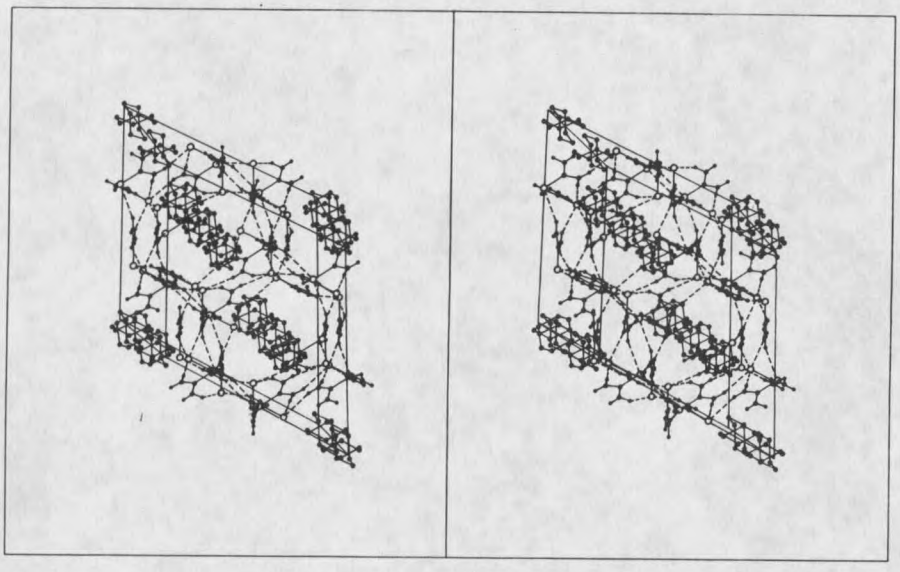


Figure 7. Cyclohexane packing diagram view along c showing the hydrogen bonding of the thiourea host lattice and the disorder of the guest molecule.

guest moiety involved one fully occupied adduct site as illustrated in Figures 8 and 9. All atoms of the cyclohexane were constrained in an idealized rigid group, with carbon - carbon bond distances of 1.540Å, tetrahedral angles, and carbon - hydrogen bond distances of 0.96Å. Both boat and chair conformations were considered, and refined independently. A single group thermal (U_g) was refined with the thermal parameters for the cyclohexane hydrogens of 1.2(U_g). Occupancies of the cyclohexane group atoms were set at 0.3333.

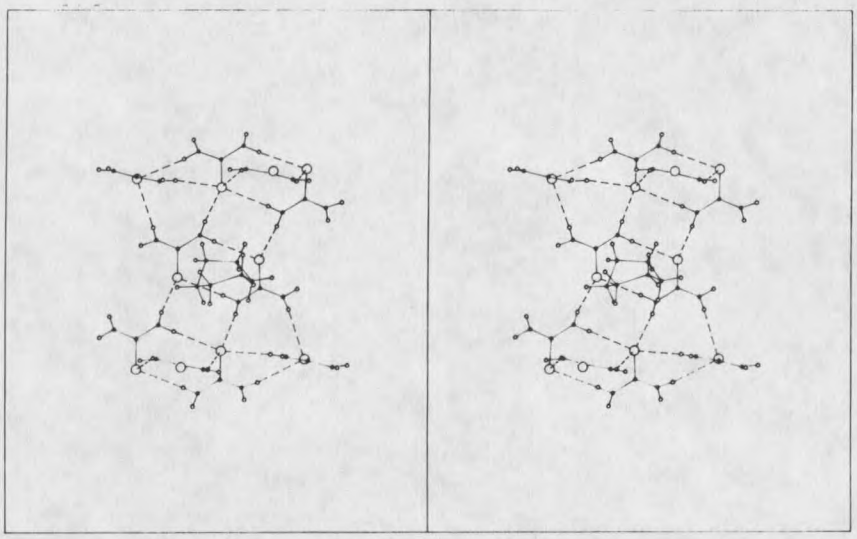


Figure 8. Cutaway view of cyclohexane boat conformation in the host lattice. Only one of the three equivalent orientations of the cyclohexane is shown.

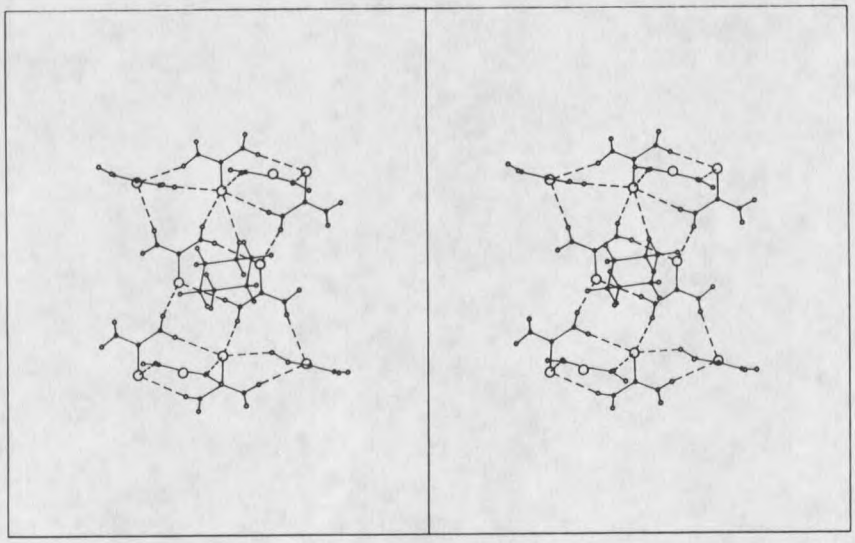


Figure 9. Cutaway view of cyclohexane chair conformation in the host lattice. Only one of the three equivalent orientations of the cyclohexane is shown.

Results and Discussion

Derived Parameters

Tables 7 through 14 contain derived parameters for the cyclohexane thiourea adduct. The bond lengths and angles for the thiourea molecule compare well with those previously observed for pure crystalline thiourea[14,36] and with the isostructural carbon tetrachloride adduct.

Table 7. Atomic Coordinates ($x10^4$) and Isotropic Thermal Parameters ($Å^2x10^3$) for Cyclohexane (boat) Thiourea Adduct

	x	y	z	U
S(1)	2998(1)	0(1)	2499(1)	62(1)*
C(1)	4078(4)	7(4)	2497(4)	56(3)*
N(1)	4582(4)	189(5)	3389(5)	74(3)*
N(2)	4400(5)	-183(5)	1612(5)	77(3)*
C(11)	-35(21)	398(18)	1389(8)	165(5)
C(12)	-818	-602	1866	165(5)
C(13)	-1028	-451	3038	165(5)
C(14)	-138	496	3488	165(5)
C(15)	830	540	3140	165(5)
C(16)	975	729	1923	165(5)
H(1)	5075(47)	191(45)	3514(57)	78(21)
H(2)	4157(41)	-153(38)	965(51)	65(17)
H(3)	4335(38)	290(35)	3989(45)	53(15)
H(4)	4879(45)	-141(46)	1516(56)	70(22)
H(11a)	17	328	630	197(6)
H(11b)	-226	886	1518	197(6)
H(12a)	-575	-1059	1844	197(6)
H(12b)	-1417	-862	1455	197(6)
H(13a)	-1610	-388	3065	197(6)
H(13b)	-1133	-1010	3460	197(6)
H(14a)	-175	489	4257	197(6)
H(14b)	-151	1066	3217	197(6)
H(15a)	1378	1067	3515	197(6)
H(15b)	796	-78	3306	197(6)
H(16a)	1411	1422	1794	197(6)
H(16b)	1259	359	1625	197(6)

* Equivalent isotropic U defined as one third of the trace of the orthogonalised U_{ij} tensor.

Table 8. Atomic Coordinates ($x10^4$) and Isotropic Thermal Parameters ($Å^2x10^3$) for Cyclohexane (chair) Thiourea Adduct

	x	y	z	U
S(1)	2998(1)	1(1)	2500(1)	62(1)*
C(1)	4079(4)	6(4)	2495(5)	57(3)*
N(1)	4584(5)	186(5)	3389(5)	75(3)*
N(2)	4401(5)	-184(5)	1612(5)	76(3)*
C(11)	86(25)	-418(19)	1483(12)	179(6)
C(12)	-848	-354	1736	179(6)
C(13)	-983	-360	2961	179(6)
C(14)	-71	536	3459	179(6)
C(15)	862	472	3207	179(6)
C(16)	997	478	1982	179(6)
H(1)	5031(45)	178(45)	3428(53)	56(19)
H(2)	4081(38)	-224(35)	986(45)	50(15)
H(3)	4439(50)	506(46)	4008(57)	91(22)
H(4)	4926(42)	-131(41)	1535(49)	56(18)
H(11a)	15	-1019	1779	215(7)
H(11b)	169	-415	720	215(7)
H(12a)	-777	247	1441	215(7)
H(12b)	-1417	-912	1425	215(7)
H(13a)	-1566	-321	3119	215(7)
H(13b)	-1054	-961	3256	215(7)
H(14a)	-155	533	4223	215(7)
H(14b)	0	1137	3164	215(7)
H(15a)	1431	1030	3518	215(7)
H(15b)	791	-129	3502	215(7)
H(16a)	1067	1078	1687	215(7)
H(16b)	1579	439	1824	215(7)

* Equivalent isotropic U defined as one third of the trace of the orthogonalised U_{ij} tensor.

Table 9. Bond Lengths (Å)(boat)

S(1)-C(1)	1.679(7)	C(1)-N(1)	1.307(8)
C(1)-N(2)	1.306(9)	N(1)-H(1)	0.782(81)
N(1)-H(3)	0.891(60)	N(2)-H(2)	0.902(66)
N(2)-H(4)	0.726(78)		

Table 10. Bond Lengths (Å)(chair)

S(1)-C(1)	1.681(8)	C(1)-N(1)	1.310(9)
C(1)-N(2)	1.303(10)	N(1)-H(1)	0.704(80)
N(1)-H(3)	1.005(79)	N(2)-H(2)	0.910(59)
N(2)-H(4)	0.787(72)		

Table 11. Bond Angles (°)(boat)

S(1)-C(1)-N(1)	119.5(5)	S(1)-C(1)-N(2)	119.9(5)
N(1)-C(1)-N(2)	120.6(7)	C(1)-N(1)-H(1)	130.8(55)
C(1)-N(1)-H(3)	119.1(39)	H(1)-N(1)-H(3)	110.0(67)
C(1)-N(2)-H(2)	121.5(46)	C(1)-N(2)-H(4)	127.9(53)
H(2)-N(2)-H(4)	106.7(69)		

Table 12. Bond Angles (°)(chair)

S(1)-C(1)-N(1)	119.4(6)	S(1)-C(1)-N(2)	120.0(5)
N(1)-C(1)-N(2)	120.5(7)	C(1)-N(1)-H(1)	123.3(55)
C(1)-N(1)-H(3)	119.9(48)	H(1)-N(1)-H(3)	115.1(69)
C(1)-N(2)-H(2)	118.6(41)	C(1)-N(2)-H(4)	125.3(43)
H(2)-N(2)-H(4)	114.1(59)		

Table 13. Anisotropic Thermal Parameters ($Å^2x10^3$)(boat)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S(1)	64(1)	79(1)	48(1)	-5(1)	-4(1)	40(1)
C(1)	54(3)	59(3)	55(3)	3(2)	1(2)	28(3)
N(1)	60(4)	106(4)	63(3)	-0(3)	-6(3)	47(3)
N(2)	73(4)	113(5)	63(4)	1(3)	6(3)	58(4)

The anisotropic temperature factor exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$

Table 14. Anisotropic Thermal Parameters ($Å^2x10^3$)(chair)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S(1)	64(1)	79(1)	48(1)	-6(1)	-4(1)	40(1)
C(1)	56(3)	59(3)	56(3)	6(2)	3(3)	28(3)
N(1)	59(4)	103(4)	69(4)	-1(3)	-10(3)	45(3)
N(2)	74(4)	110(5)	62(4)	1(3)	7(3)	59(4)

The anisotropic temperature factor exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$

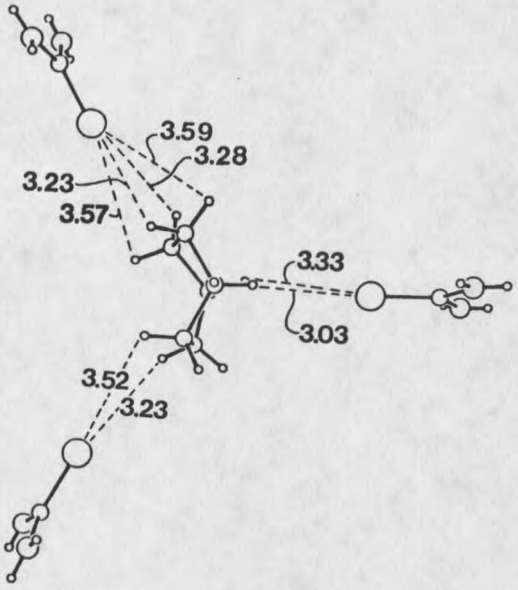


Figure 10. Cyclohexane boat conformer shown looking down the c axis. Only one of the three equivalent orientations of the cyclohexane is shown, with close interactions with sulfur illustrated.

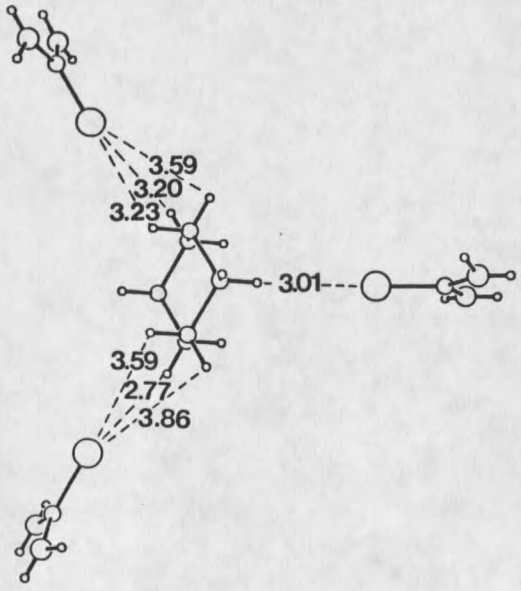


Figure 11. Cyclohexane chair conformer shown looking down the c axis. Only one of the three equivalent orientations of the cyclohexane is shown, with close interactions with sulfur illustrated.

Nature of the Bonding between Thiourea and the Guest Molecule

The structure of the cyclohexane thiourea adduct, as shown in Figures 10 and 11, suggests the qualitative nature of the principle interactions between the adducted organic molecule and the thiourea. This apparently involves coulombic interactions between some of the cyclohexane hydrogen atoms, which would be very slightly positive, and the three coplanar sulfur atoms protruding into the channel, which are partially negative. Figures 10 and 11 illustrate this, as well as showing some of the close interactions between the sulfurs and the cyclohexane guest.

MNDO[13] calculations on thiourea as found in this structure and on cyclohexane in both the boat and chair conformations agree with weak coulombic interactions to account for the formation and stability of these adducts. The calculated charge on the thiourea sulfur is -0.516 electrons and the average charge on the cyclohexane hydrogens is +0.0064 electrons (boat form) or +0.0066 electrons (chair form).

CHAPTER 4

BICYCLO[2.2.2]OCTANE THIOUREA (1:3) ADDUCT

Based on the observations and conclusions arrived at in the study of the carbon tetrachloride thiourea adduct and cyclohexane thiourea adduct structures, it was predicted that a) bicyclo[2.2.2]octane would form an extremely stable complex with thiourea, and, b) due to the potential three-fold symmetry of the molecule we hoped to see a reduction of the disorder problems that have been observed in all of the thiourea host/guest adducts studied to this point.

Experimental

Crystal Preparation

Reagent grade thiourea and ethanol were purchased from the J. T. Baker Chemical Company. Bicyclo[2.2.2]octane (reagent grade) was purchased from Wiley Organics. A saturated solution of thiourea in ethanol was set up to allow slow liquid diffusion of the organic molecule into it at room temperature, with good crystals forming in about one week. An experimental density was obtained by flotation in chloroform/heptane solutions. D_o = 1.21(2) gcm^{-3} and D_c = 1.219 gcm^{-3}. As expected, the adduct is

stable in air, which is atypical when compared to prior adducts that have been studied in this series. The crystal used for intensity data collection had dimensions of 0.69 x 0.34 x 0.36 mm^3.

Data Collection

Intensity data were collected on a Nicolet R3m/E four circle diffractometer using the omega scan technique. Three standard reflections were measured periodically throughout the course of the data collection to monitor crystal alignment and/or deterioration. There was no decrease in the standards over the course of the data collection, with a maximum variation from the average of less than 3%. A total of 10471 reflections were collected of which 3252 were unique and 1427 were considered observed at the $6\sigma_F$ level. Lattice parameters were obtained from least squares fit to 25 reflections for which $25.0° < 2\Theta < 30.0°$. Space group designation and other details of the data collection, structure solution and refinement are included in Table 15.

Data Reduction, Structure Solution, and Refinement

The data were reduced in the usual manner with appropriate Lorentz and polarization corrections. Scattering factors for S, N, C, H and anomalous scattering terms for S, N, and C were taken from the International

Table 15. Experimental Data for Bicyclo[2.2.2]octane Thiourea Adduct

Formula		$C_8H_{12}\cdot 3(SCN_2H_4)$
Cell Dimensions	a=b	16.001(2)
	c	12.484(2)
Space Group		$R\bar{3}$
Cell Volume		2768.01(66)
D_m		1.21(2) gcm^{-3}
D_c		1.219 gcm^{-3}
Crystal Dimensions		0.69 x 0.34 x 0.36 mm^3
$\sin\Theta / \lambda_{max}$		0.856 $Å^{-1}$
Range	h	0 to ± 28
	k	0 to 28
	l	0 to ± 22
Total Reflections		10471
Unique Reflections		3252 R_{merg} = 0.0085
Observed Reflections		1427 6 σ_F cutoff
Number of parameters refined		60

$$R = \frac{\Sigma(||F_o|-|F_c||)}{\Sigma|F_o|} = 0.065$$

$$R_w = \frac{\Sigma(||F_o|-|F_c||)w^{\frac{1}{2}}}{\Sigma|F_o|w^{\frac{1}{2}}} = 0.077$$

$$S = \frac{\Sigma(||F_o|-|F_c||)w^{\frac{1}{2}}}{(m-n)^{\frac{1}{2}}} = 1.486$$

$w = (\sigma_F^2 + gF^2)^{-1}$ where g = 0.00365

Tables for X-ray Crystallography;[24] all atoms were assumed to be in the zero ionization state. No correction for absorption was made.

An initial model was obtained by utilizing the atomic coordinates for the thiourea molecule from the carbon tetrachloride adduct as the compounds are isostructural. Computational work was done utilizing the Nicolet program package,[57] the XTAL system of programs,[61] and programs written locally. The S, C, and N atoms of the thiourea lattice structure were refined with anisotropic thermal parameters by full matrix least squares minimizing $\Sigma w(|F_o|-|F_c|)^2$ with all parameters refined in each full matrix block. Thiourea amino hydrogen position coordinates, determined from a difference Fourier electron density map at an intermediate stage of refinement, were refined along with isotropic thermal parameters. The weighting scheme used in the latter stages of refinement was $w = (\sigma_F^2 + gF^2)^{-1}$, where g was refined and converged to a value of 0.00365. A final difference Fourier electron density map showed maximum peak heights $\approx$0.47 e/Å^3 in the vicinity of the adducted molecule in the channel. The largest shift over error value was less than 0.003 at convergence. The R for all unique data was 0.147, and the R for the observed data was 0.065. No corrections for secondary extinction were made or refined.

Disorder Model

Figure 12 illustrates the structure of the bicyclo[2.2.2]octane adduct. The final model for the organic guest moiety involved one fully occupied adduct site. All atoms of the bicyclo[2.2.2]octane were constrained in an idealized rigid group, with carbon-carbon bond distances of 1.540Å, tetrahedral angles, and carbon - hydrogen bond distances of 0.96Å. A single group thermal (U_g) was refined with the thermal parameters for the bicyclo[2.2.2]octane hydrogens of 1.2(U_g). Occupancies of the bicyclo[2.2.2]octane group atoms were set at 0.3333, which corresponds to a fully occupied guest site, illustrated in Figure 13.

Results and Discussion

Derived Parameters

Tables 16 through 19 contain derived parameters for the bicyclo[2.2.2]octane thiourea adduct. The bond lengths and angles for the thiourea molecule compare well with those previously observed for pure crystalline thiourea[14,36] and with the isostructural carbon tetrachloride and cyclohexane adducts. While it is clear that the adduct is extremely stable as expected, the hoped for improvement in terms of disorder did not occur due to the tilting of the bicyclo[2.2.2]octane molecule relative

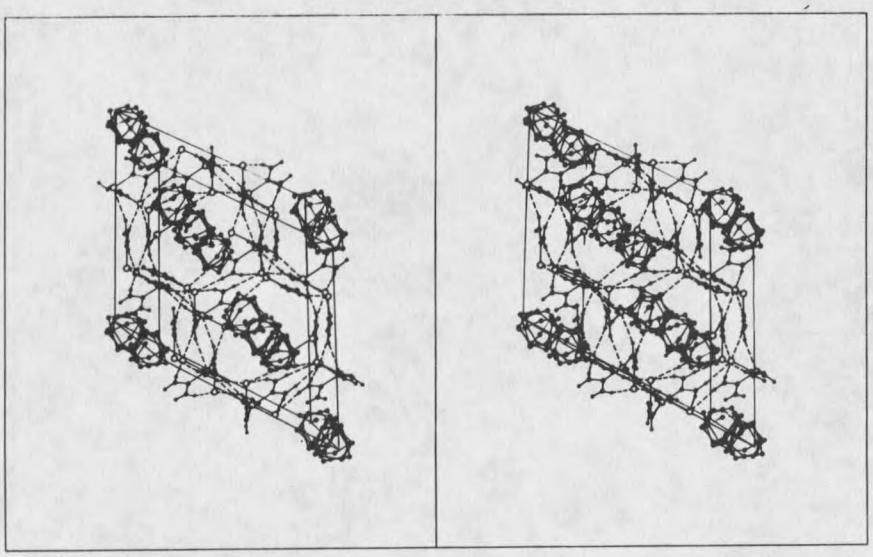


Figure 12. Bicyclo[2.2.2]octane packing diagram view along c showing the hydrogen bonding of the thiourea host lattice and the disorder of the guest molecule.

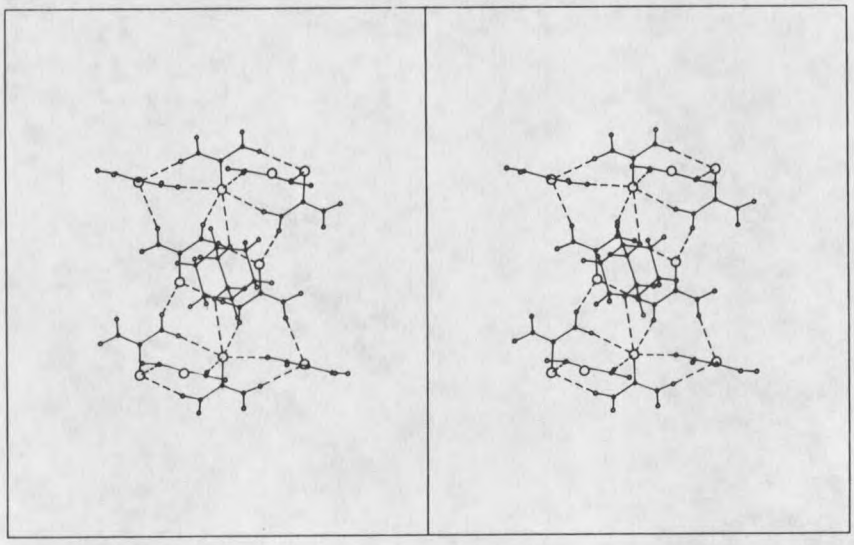


Figure 13. Cutaway view of bicyclo[2.2.2]octane in the host lattice. Only one of the three equivalent orientations of the guest is shown.

to the three-fold axis. A line through the bridgehead carbons makes an angle of 76.3° with the crystallographic three-fold axis. This is illustrated in Figure 14.

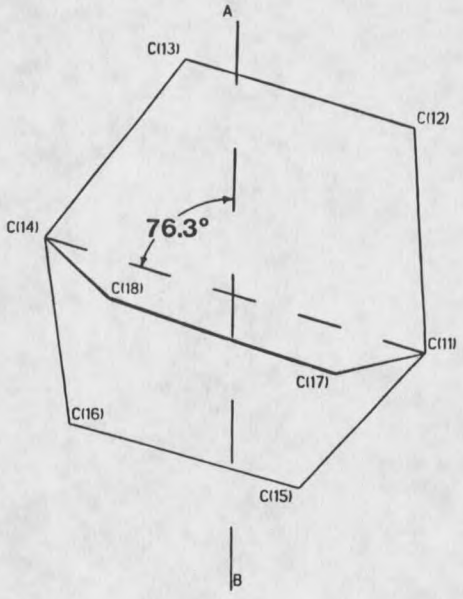


Figure 14. View of the bicyclo[2.2.2]octane normal to the 3-fold axis. The dashed line A--B is the crystallographic 3-fold, and the dashed line from C11 to C14 is the 3-fold axis of the bicyclo[2.2.2]octane.

Table 16. Atomic Coordinates ($x10^4$) and Isotropic Thermal Parameters ($Å^2x10^3$) for Bicyclo[2.2.2]octane Thiourea Adduct

	x	y	z	U
S(1)	3015(1)	1(1)	2500(1)	45(1)*
C(1)	4091(2)	1(2)	2500(2)	43(1)*
N(1)	4601(2)	194(2)	3391(3)	59(1)*
N(2)	4406(2)	-197(2)	1614(3)	58(1)*
C(11)	-573(10)	313(10)	2233(8)	141(3)
C(12)	-951	-159	3335	141(3)
C(13)	-432	-711	3671	141(3)
C(14)	333	-557	2825	141(3)
C(15)	-739	-471	1407	141(3)
C(16)	-168	-969	1743	141(3)

Table 16. Continued.

	x	y	z	U
C(17)	515	1048	2313	141(3)
C(18)	1045	531	2705	141(3)
H(1)	4384(29)	297(32)	4070(43)	71(12)
H(2)	5123(32)	111(31)	3465(36)	70(12)
H(3)	4179(38)	-272(38)	913(50)	94(16)
H(4)	4974(36)	-173(34)	1624(37)	80(15)
H(11)	-911	639	2012	169(3)
H(12a)	-827	332	3855	169(3)
H(12b)	-1633	-601	3291	169(3)
H(13a)	-895	-1387	3728	169(3)
H(13b)	-123	-474	4351	169(3)
H(14)	671	-882	3046	169(3)
H(15a)	-1415	-940	1375	169(3)
H(15b)	-523	-179	716	169(3)
H(16a)	311	-853	1209	169(3)
H(16b)	-601	-1651	1811	169(3)
H(17a)	756	1326	1621	169(3)
H(17b)	618	1548	2809	169(3)
H(18a)	1349	793	3385	169(3)
H(18b)	1543	626	2195	169(3)

* Equivalent isotropic U defined as one third of the trace of the orthogonalised U_{ij} tensor.

Table 17. Bond Lengths (Å)

S(1)-C(1)	1.721(4)	C(1)-N(1)	1.323(4)
C(1)-N(2)	1.319(5)	N(1)-H(1)	0.960(54)
N(1)-H(2)	0.914(59)	N(2)-H(3)	0.932(63)
N(2)-H(4)	0.890(64)		

Table 18. Bond Angles (°)

S(1)-C(1)-N(1)	120.0(3)	S(1)-C(1)-N(2)	120.2(3)
N(1)-C(1)-N(2)	119.7(4)	C(1)-N(1)-H(1)	123.3(30)
C(1)-N(1)-H(2)	123.6(29)	H(1)-N(1)-H(2)	111.8(43)
C(1)-N(2)-H(3)	130.2(42)	C(1)-N(2)-H(4)	118.9(30)
H(3)-N(2)-H(4)	110.1(50)		

Table 19. Anisotropic Thermal Parameters ($Å^2x10^3$)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S(1)	41(1)	52(1)	45(1)	-3(1)	-2(1)	26(1)
C(1)	41(1)	40(1)	48(1)	3(1)	0(1)	19(1)
N(1)	49(1)	79(2)	53(2)	-1(1)	-8(1)	36(1)
N(2)	54(2)	72(2)	56(2)	0(1)	6(1)	38(1)

The anisotropic temperature factor exponent takes the form: $-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$

Nature of the Bonding between Thiourea and the Guest Molecule

As shown in figure 15, the bonding apparently involves interactions between the bicyclo[2.2.2]octane hydrogens and the three coplanar sulfur atoms protruding into the channel. MNDO[13] calculations carried out for thiourea as it found in this structure and for the bicyclo[2.2.2]octane. These results suggest reasonably strong interactions between the thiourea sulfur and several of the bicyclo[2.2.2]octane hydrogens, particularly the bridgehead hydrogen, which calculates to have a +0.023 electron charge on it. It appears that the combination of interactions of the bridgehead hydrogens with the sulfurs and the size of the bicyclo[2.2.2]octane molecule (≈6.9Å long if one includes the van der Waal radii[11] and the expected values for bond distances and angles[24] have forced the bicyclo[2.2.2]octane away from the predicted orientation relative to the three-fold axis. This tilt is a result of the c/2 spacing of the thiourea interaction

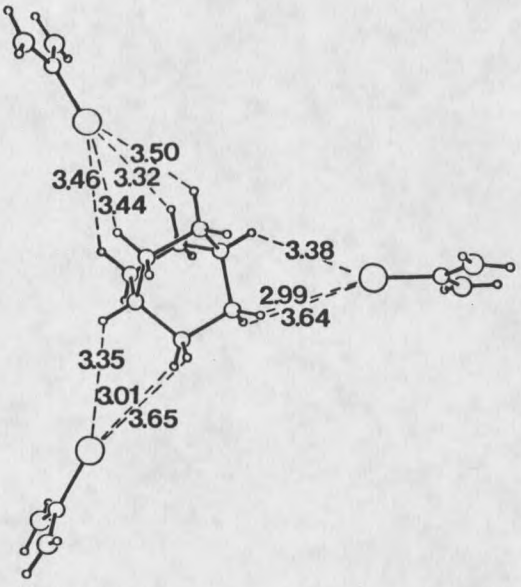


Figure 15. Bicyclo[2.2.2]octane shown looking down the c axis. Only one of the three equivalent orientations of the bicyclo[2.2.2]octane is shown, with close interactions with sulfur illustrated.

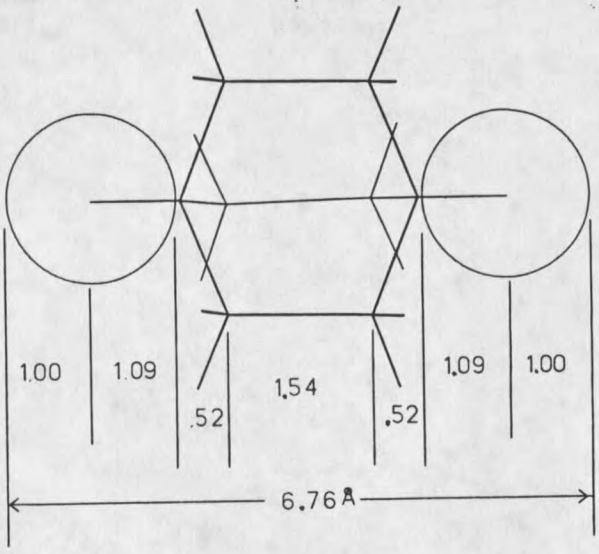


Figure 16. Size calculation for Bicyclo[2.2.2]octane. C-C bond lengths of 1.54Å, C-H bond lengths of 1.09Å, tetrahedral angles, and a 1.00Å Van der Waal's radius for hydrogen were used. Overall length of the molecule is 6.76Å.

site. This distance is ≈6.25Å, which is significantly less than the 6.8Å length of the bicyclo[2.2.2]octane molecule.(Figure 16)

CHAPTER 5

CIS-PARA-MENTHANE THIOUREA (1:3) ADDUCT

The isomers of 1-isopropyl-4-methyl-cyclohexane (para-menthane) both form adducts with thiourea. When a mixture of these two isomers is used as the guest, the resulting adduct is enriched in the cis isomer. Because of this known selectivity of this pair of compounds, the cis isomer was chosen for structural work to examine the potential reasons for the selectivity of the adduct, and to explore further the interactions in the thiourea adducts. Mark Spinti, a Master of Science candidate in Chemical Engineering at Montana State University, collected intensity data and initially modelled the disorder of the guest molecule as part of his thesis work.[59] Upon subsequent analysis of his results, it was decided to expand the refinement of the disorder model in hopes of improving the understanding of the disorder and elucidating the possible reasons for the disorder. As indications of a superlattice were seen in the preliminary crystallographic investigation, a subsequent data set was collected at low temperature on the supercell.

Experimental

Crystal Preparation

Reagent grade thiourea and ethanol were purchased from the J. T. Baker Chemical Company. Cis-para-menthane was obtained from the Glidden Company. An experimental density was obtained by flotation in chloroform/heptane solutions. D_o = 1.16(3) gcm^{-3} and D_c = 1.13 gcm^{-3}. The crystal used for intensity data collection on the subcell had dimensions of 0.69 x 0.34 x 0.36 mm^3, and the one used for the supercell data had dimensions of 0.36 x 0.42 x 0.58 mm^3.

Data Collection

Intensity data were collected on a Nicolet R3m/E four circle diffractometer using the omega scan technique. The temperature was maintained at -120°C using the Nicolet LT-1 low temperature apparatus. Four standard reflections were measured periodically throughout the course of the data collection to monitor crystal alignment and/or deterioration. There was no decrease in the standards over the course of the data collection, with a maximum variation from the average of less than 3%. A total of 7219 reflections were collected on the subcell of which 2623 were unique and 1472 were considered observed at the $6\sigma_F$ level. A total of 23754 reflections were collected on the supercell, with the two data sets merged together for structure solution and refinement. This gave 6128 unique

and 1646 observed reflections at $6\sigma_F$ for the supercell refinement. Lattice parameters were obtained from least squares fit to 25 reflections for which $25.0° < 2\Theta < 30.0°$. Space group designation and other details of the data collection, structure solution and refinement are included in Tables 16 and 17.

Data Reduction, Structure Solution, and Refinement

The data were reduced in the usual manner with appropriate Lorentz and polarization corrections. Scattering factors for S, N, C, H and anomalous scattering terms for S, N, and C were taken from the International Tables for X-ray Crystallography;[24] all atoms were assumed to be in the zero ionization state. No correction for absorption was made.

An initial model for the subcell was obtained by utilizing the atomic coordinates for the thiourea molecule from the carbon tetrachloride adduct as the compounds are isostructural. Computational work was done utilizing the Nicolet program package[5,7] and programs written locally. The S, C, and N atoms of the thiourea lattice structure were refined with anisotropic thermal parameters by block cascade full matrix least squares minimizing $\Sigma w(|F_o|-|F_c|)^2$. Thiourea amino hydrogen position coordinates were calculated at an intermediate stage of refinement, and were refined with a fixed isotropic thermal

Table 20. Experimental Data for Cis-p-Menthane Thiourea Adduct.

Formula		$2(C10H20)\cdot 9(SCN_2H_4)$
Cell Dimensions	a	15.764(3)Å
	c	12.428(3)Å
Space Group		R3
Cell Volume		2674.62(97)$Å^3$
D_m		1.16(3) gcm^{-3}
D_c		1.13 gcm^{-3}
Crystal Dimensions		0.58 x 0.74 x 0.92 mm^3
$\sin\Theta / \lambda_{max}$		0.807 $Å^{-1}$
Range	h	0 to ±26
	k	0 to 26
	l	0 to ±21
Total Reflections		7219
Unique Reflections		2623 R_{merg} = 0.0189
Observed Reflections		1472 6 σ_F cutoff
Number of parameters refined		67
$R = \frac{\Sigma(\lvert\lvert F_o\rvert-\lvert F_c\rvert\rvert)}{\Sigma\lvert F_o\rvert} =$		0.075
$R_w = \frac{\Sigma(\lvert\lvert F_o\rvert-\lvert F_c\rvert\rvert)w^{1/2}}{\Sigma\lvert F_o\rvert w^{1/2}} =$		0.090
$S = \frac{\Sigma(\lvert\lvert F_o\rvert-\lvert F_c\rvert\rvert)w^{1/2}}{(m-n)^{1/2}} =$		1.303
$w = (\sigma_F^2 + gF^2)^{-1}$	where g =	0.00926

Table 21. Experimental Data for Cis-p-Menthane Thiourea Adduct Supercell.

Formula		$5(C10H20)\cdot 24(SCN_2H_4)$
Cell Dimensions	a	15.786(2)Å
	c	49.712(8)Å
Space Group		R3
Cell Volume		10728.4(44)$Å^3$
D_m		1.16(3) gcm^{-3}
D_c		1.174 gcm^{-3}
Crystal Dimensions		0.36 x 0.42 x 0.58 mm^3
$\sin\Theta / \lambda_{max}$		0.807 $Å^{-1}$
Range	h	0 to ±26
	k	0 to 26
	l	0 to ±84
Total Reflections		23754
Unique Reflections		6128 R_{merg} = 0.025
Observed Reflections		1646 6 σ_F cutoff
Number of parameters refined		134

$$R = \frac{\Sigma(||F_o|-|F_c||)}{\Sigma|F_o|} = 0.066$$

$$R_w = \frac{\Sigma(||F_o|-|F_c||)w^{\frac{1}{2}}}{\Sigma|F_o|w^{\frac{1}{2}}} = 0.072$$

$$S = \frac{\Sigma(||F_o|-|F_c||)w^{\frac{1}{2}}}{(m-n)^{\frac{1}{2}}} = 2.896$$

$w = (\sigma_F^2 + gF^2)^{-1}$ where g = 0.00041

factor 1.2 times the equivalent isotropic thermal factor for the atom to which they were connected. The weighting scheme used in the latter stages of refinement was $w = (\sigma_F^2 + gF^2)^{-1}$, where g was refined and converged to a value of 0.00926. A final difference Fourier electron density map showed maximum peak heights $\simeq 0.40$ e/Å^3 in the vicinity of the adducted molecule in the channel. The average shift over error value was 0.012 at convergence. No corrections for secondary extinction were made or refined.

Disorder Model

Figure 17 illustrates the subcell structure of the cis-para-menthane adduct. The final model for the organic guest moiety involves three partially occupied adduct sites represented by two cis-para-menthane molecules. All atoms of the cis-para-menthane were constrained in an idealized rigid group, with carbon - carbon bond distances of 1.540Å, tetrahedral angles, and carbon - hydrogen bond distances of 0.96Å. A single group thermal (U_g) was refined with the thermal parameters for the cis-para-menthane hydrogens of $1.2(U_g)$. Occupancies of the cis-para-menthane group atoms were tied to a free variable so that the sum of the occupancies was constrained to 0.222, which corresponds to two thirds occupancy for a given adduct site. The disorder model consists of a dimer generated from a single rigid

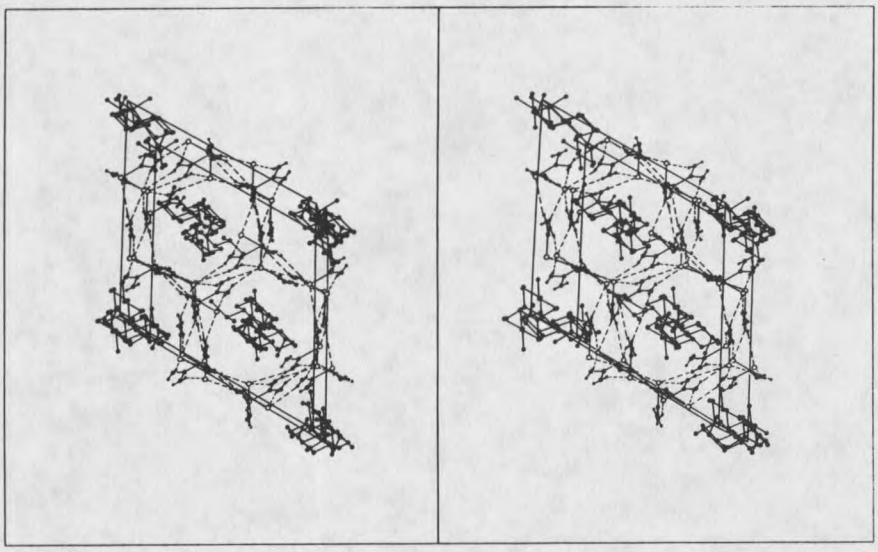


Figure 17. Cis-p-menthane adduct subcell packing diagram view along c showing the hydrogen bonding of the thiourea host lattice and the disorder of the guest molecule. Only one of three guest positions are shown for clarity.

group by a pseudocenter symmetry operation that operates only on the guest molecule. This additional symmetry site lies on the three-fold axis and has a z coordinate of approximately 0.67. Figure 18 shows the two independent molecules separated in space for visual clarity.

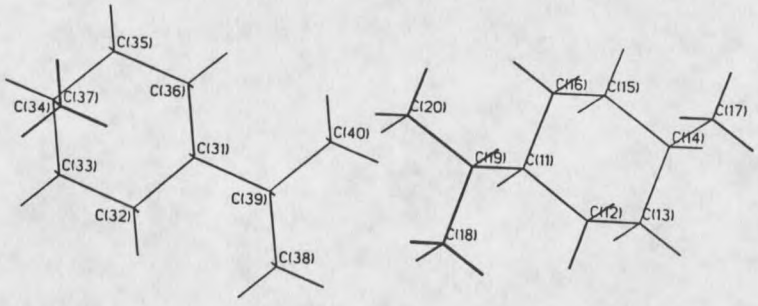


Figure 18. Disorder model for Cis-p-menthane subcell guest molecules.

Supercell Structure Determination

The supercell structure, as illustrated in Figure 19, was determined by direct methods, with thiourea positions found in the E-map. Idealized thioureas based on the thiourea from the refined subcell structure were generated for each of the four unique thioureas in the asymmetric unit, with calculated hydrogen positions. These thioureas were treated as rigid groups, and had independent anisotropic thermal parameters for the nonhydrogen atoms, and fixed isotropic U of 0.06 for the hydrogens. The

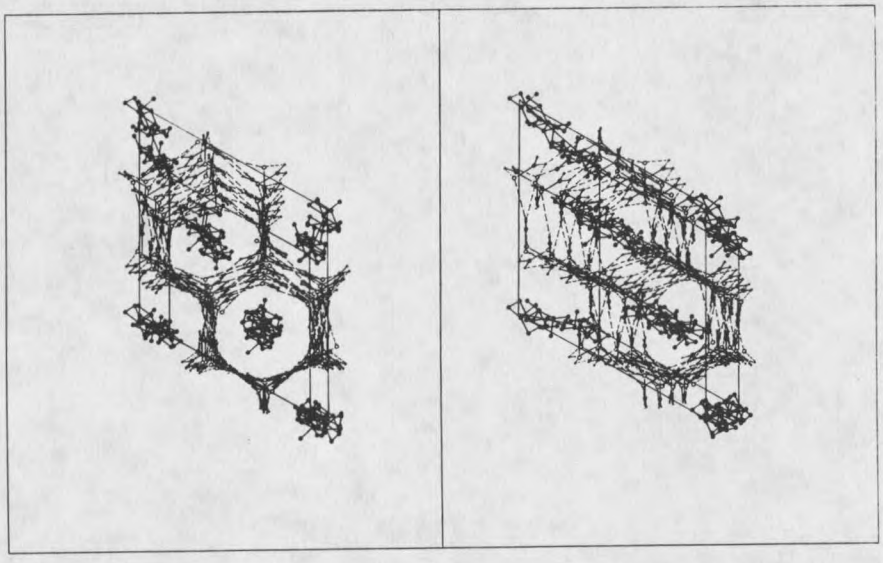


Figure 19. Cis-p-menthane supercell packing diagram view along c showing the hydrogen bonding of the thiourea host lattice and the disorder of the guest molecule.

channel showed indications for 3 cis-p-menthane positions, with one at half occupancy and two at full occupancy. The model for the cis-p-menthane was the same conformation used for the subcell, and the centroids of each model fixed relative to the three fold axis. Figure 20 illustrates the model used in the supercell refinement. No corrections for absorption or extinction were applied.

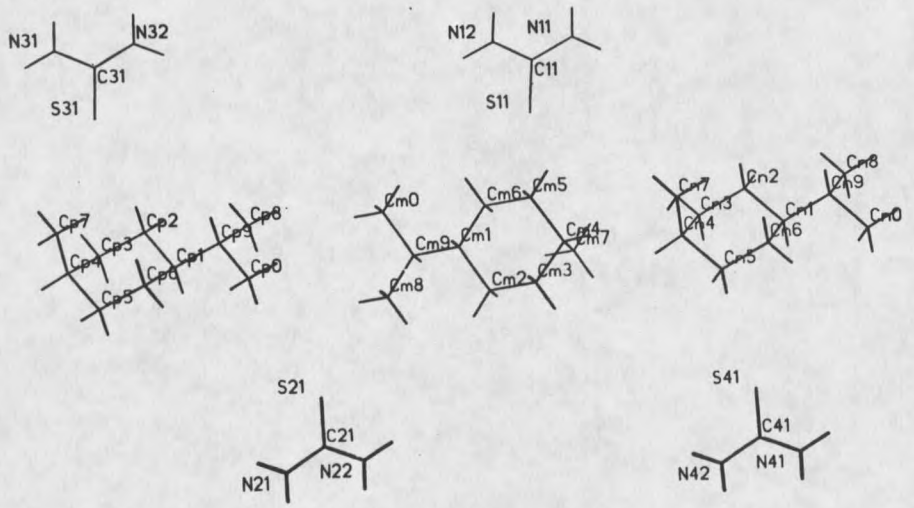


Figure 20. Cis-p-menthane supercell refinement model showing numbering scheme and the seven rigid groups used for the refinement.

Results and Discussion

Derived Parameters

Tables 22 through 25 contain derived parameters for the cis-para-menthane thiourea adduct, and Tables 26 and 27 contain the derived parameters for the supercell data. The bond lengths and angles for the thiourea molecule compare well with those previously observed for pure crystalline thiourea,[14,36] and with the isostructural rhombohedral thiourea adducts. The supercell data set has only 174 more unique observed reflections than in the subcell, but contributes significantly to the understanding of the disorder of the guest molecule.

Table 22. Atomic Coordinates ($x10^4$) and Isotropic Thermal Parameters ($Å^2x10^3$) for Cis-p-menthane subcell.

	x	y	z	U
S(1)	-1(1)	2974(1)	2500(1)	41(1)*
C(1)	2(2)	4052(2)	2500(2)	40(1)*
N(1)	147(3)	4554(2)	1595(2)	53(1)*
N(2)	-149(3)	4408(3)	3403(2)	52(1)*
C(11)	135(15)	-65(18)	4343(19)	139(4)
C(12)	623	-124	3298	139(4)
C(13)	-143	-898	2554	139(4)
C(14)	-918	-626	2285	139(4)
C(15)	-1407	-569	3324	139(4)
C(16)	-641	205	4067	139(4)
C(17)	-439	365	1720	139(4)
C(18)	1677	435	5349	139(4)
C(19)	901	707	5079	139(4)
C(20)	412	764	6118	139(4)
C(31)	-214(20)	-920(24)	9120(15)	139(4)
C(32)	556	-884	9900	139(4)
C(33)	190	-970	11051	139(4)
C(34)	11	-125	11292	139(4)
C(35)	-753	-161	10512	139(4)
C(36)	-386	-75	9361	139(4)
C(37)	963	842	11156	139(4)
C(38)	339	-1679	7722	139(4)
C(39)	160	-834	7963	139(4)
C(40)	-604	-870	7183	139(4)
H(1)	-41(26)	4799(28)	1634(29)	43(5)
H(2)	-159(27)	4774(27)	3333(29)	42(5)
H(3)	-66(26)	4191(25)	3928(30)	43(5)
H(4)	60(29)	4298(27)	905(32)	67(5)
H(11)	-164	-684	4689	166(5)
H(12a)	1106	-295	3466	166(5)
H(12b)	922	493	2946	166(5)
H(13a)	162	-933	1906	166(5)
H(13b)	-441	-1516	2906	166(5)
H(14)	-1395	-1108	1821	166(5)
H(15a)	-1707	-1185	3676	166(5)
H(15b)	-1891	-398	3156	166(5)
H(16a)	-342	822	3715	166(5)
H(16b)	-946	240	4715	166(5)
H(17a)	-134	331	1072	166(5)
H(17b)	39	847	2184	166(5)
H(17c)	-922	535	1552	166(5)

Table 22 (cont.).

	x	y	z	U
H(18a)	2154	918	5812	166(5)
H(18b)	1981	400	4701	166(5)
H(18c)	1378	-183	5701	166(5)
H(19)	1200	1324	4727	166(5)
H(20a)	889	1247	6582	166(5)
H(20b)	113	147	6471	166(5)
H(20c)	-72	934	5950	166(5)
H(31)	-801	-1523	9204	166(5)
H(32a)	667	-1411	9750	166(5)
H(32b)	1150	-282	9814	166(5)
H(33a)	666	-947	11538	166(5)
H(33b)	-404	-1573	11136	166(5)
H(34)	-217	-178	12014	166(5)
H(35a)	-1346	-763	10597	166(5)
H(35b)	-864	366	10662	166(5)
H(36a)	208	528	9276	166(5)
H(36b)	-863	-98	8875	166(5)
H(37a)	1440	866	11642	166(5)
H(37b)	1191	895	10434	166(5)
H(37c)	852	1369	11306	166(5)
H(38a)	568	-1625	7001	166(5)
H(38b)	815	-1656	8209	166(5)
H(38c)	-255	-2282	7807	166(5)
H(39)	754	-232	7879	166(5)
H(40a)	-375	-817	6461	166(5)
H(40b)	-1198	-1473	7267	166(5)
H(40c)	-715	-343	7333	166(5)

* Equivalent isotropic U defined as one third of the trace of the orthogonalised U_{ij} tensor.

Table 23. Bond Lengths (Å) for Cis-p-menthane subcell.

S(1)-C(1)	1.700(4)	C(1)-N(11)	1.483(6)
C(1)-N(12)	1.378(6)	N(11)-H(1)	0.502(5)
N(11)-H(4)	0.894(4)	N(12)-H(2)	0.583(5)
N(12)-H(3)	0.688(4)		

Table 24. Bond Angles (°) for Cis-p-menthane subcell.

S(1)-C(1)-N(11)	122.3(3)	S(1)-C(1)-N(12)	133.9(3)
C(1)-N(11)-H(1)	90.9(51)	C(1)-N(11)-H(4)	118.5(29)
C(1)-N(12)-H(2)	106.5(44)	C(1)-N(12)-H(3)	122.8(35)
N(11)-C(1)-N(12)	123.7(4)	H(1)-N(11)-H(4)	128.6(42)
H(2)-N(12)-H(3)	127.6(49)		

Table 25. Anisotropic Thermal Parameters ($Å^2x10^3$) for Cis-p-menthane subcell.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S(1)	58(1)	48(1)	20(1)	2(1)	4(1)	29(1)
C(1)	43(1)	49(1)	26(1)	0(1)	-1(1)	21(1)
N(1)	84(2)	53(2)	31(1)	2(1)	-1(1)	42(1)
N(2)	85(2)	57(2)	29(1)	-3(1)	0(1)	45(2)

The anisotropic temperature factor exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$

Table 26. Atomic coordinates ($x10^4$) and isotropic thermal parameters ($Å^2x10^3$) for Cis-p-menthane supercell.

	x	y	z	U
S(11)	6648(4)	407(3)	223(1)	40(2)*
C(11)	6684	-649	208	56(4)*
N(11)	6828	-972	-24	40(3)*
N(12)	6578	-1166	429	45(3)*
H(11)	6853	-1566	-30	60
H(12)	6906	-611	-186	60
H(13)	6606	-1759	419	60
H(14)	6473	-948	600	60
S(21)	3691(4)	406(4)	1461(1)	32(2)*
C(21)	2605	-658	1454	30(3)*
N(21)	2238	-1186	1676	81(4)*
N(22)	2098	-976	1227	57(4)*
H(21)	1621	-1783	1670	60
H(22)	2591	-971	1842	60
H(23)	1482	-1574	1226	60
H(24)	2348	-607	1064	60
S(31)	3056(4)	7(4)	624(1)	58(2)*
C(31)	4132	8	629	39(3)*
N(31)	4510	-111	403	42(3)*
N(32)	4618	137	857	55(3)*
H(31)	5122	-102	407	60
H(32)	4173	-205	236	60
H(33)	5228	143	857	60
H(34)	4359	225	1023	60
S(41)	6299(4)	-305(5)	1032(1)	40(2)*
C(41)	7383	761	1043	39(3)*
N(41)	7864	1083	1274	67(4)*
N(42)	7772	1285	822	45(3)*
H(41)	8479	1683	1278	60
H(42)	7597	717	1436	60
H(43)	8388	1882	831	60

Table 26. (cont.).

	x	y	z	U
H(44)	7438	1067	653	60
Centroid p	0	0	938(3)	
Cp(1)	-91	-77	1055	110(3)
Hp(1)	-629	-702	1097	110(3)
Cp(2)	661	-212	892	110(3)
Hp(2A)	880	-569	997	110(3)
Hp(2B)	1201	410	848	110(3)
Cp(3)	192	-773	634	110(3)
Hp(3A)	660	-855	533	110(3)
Hp(3B)	-348	-1396	678	110(3)
Cp(4)	-139	-198	453	110(3)
Hp(4)	-453	-552	304	110(3)
Cp(5)	-912	-70	627	110(3)
Hp(5A)	-1453	-692	671	110(3)
Hp(5B)	-1132	287	522	110(3)
Cp(6)	-443	491	886	110(3)
Hp(6A)	98	1114	842	110(3)
Hp(6B)	-911	573	986	110(3)
Cp(7)	705	798	395	110(3)
Hp(7A)	1174	716	294	110(3)
Hp(7B)	997	1147	556	110(3)
Hp(7C)	485	1153	291	110(3)
Cp(9)	381	483	1312	110(3)
Cp(8)	735	-88	1480	110(3)
Hp(8A)	1027	262	1641	110(3)
Hp(8B)	1202	-170	1379	110(3)
Hp(8C)	194	-711	1524	110(3)
Hp(9)	921	1105	1268	110(3)
Cp(0)	-369	616	1474	110(3)
Hp(0A)	-76	966	1635	110(3)
Hp(0B)	-910	-7	1518	110(3)
Hp(0C)	-589	971	1369	110(3)
Centroid m	0	0	2798(3)	
Cm(1)	142	118	2684	110(3)
Hm(1)	272	761	2644	110(3)
Cm(2)	-789	-404	2855	110(3)
Hm(2A)	-1322	-436	2758	110(3)
Hm(2B)	-924	-1047	2897	110(3)
Cm(3)	-647	160	3117	110(3)
Hm(3A)	-1226	-166	3224	110(3)
Hm(3B)	-514	803	3076	110(3)
Cm(4)	188	193	3286	110(3)
Hm(4)	296	563	3436	110(3)
Cm(5)	1136	734	3102	110(3)
Hm(5A)	1271	1378	3062	110(3)
Hm(5B)	1670	767	3199	110(3)
Cm(6)	994	171	2841	110(3)

Table 26. (cont.).

	x	y	z	U
Hm(6A)	861	-473	2882	110(3)
Hm(6B)	1572	496	2734	110(3)
Cm(7)	-5	-820	3339	110(3)
Hm(7A)	-584	-1146	3445	110(3)
Hm(7B)	-94	-1171	3175	110(3)
Hm(7C)	528	-787	3436	110(3)
Cm(9)	-4	-447	2424	110(3)
Cm(8)	-860	-500	2267	110(3)
Hm(8A)	-949	-851	2104	110(3)
Hm(8B)	-1438	-825	2374	110(3)
Hm(8C)	-726	144	2226	110(3)
Hm(9)	-138	-1090	2464	110(3)
Cm(0)	924	75	2253	110(3)
Hm(0A)	836	-277	2090	110(3)
Hm(0B)	1059	718	2212	110(3)
Hm(0C)	1457	107	2350	110(3)
Centroid n	0	0	4440(5)	
Cn(1)	458	336	4545	110(3)
Hn(1)	-58	-321	4565	110(3)
Cn(2)	1172	372	4329	110(3)
Hn(2A)	1435	-26	4385	110(3)
Hn(2B)	1688	1027	4307	110(3)
Cn(3)	638	-7	4062	110(3)
Hn(3A)	1084	17	3929	110(3)
Hn(3B)	123	-663	4084	110(3)
Cn(4)	235	645	3960	110(3)
Hn(4)	-117	394	3807	110(3)
Cn(5)	-500	592	4187	110(3)
Hn(5A)	-1015	-63	4209	110(3)
Hn(5B)	-763	990	4131	110(3)
Cn(6)	34	971	4454	110(3)
Hn(6A)	550	1627	4432	110(3)
Hn(6B)	-412	947	4587	110(3)
Cn(7)	1041	1683	3938	110(3)
Hn(7A)	1487	1707	3805	110(3)
Hn(7B)	1374	1918	4105	110(3)
Hn(7C)	778	2079	3883	110(3)
Cn(9)	993	714	4810	110(3)
Cn(8)	1415	77	4899	110(3)
Hn(8A)	1749	313	5066	110(3)
Hn(8B)	1861	101	4766	110(3)
Hn(8C)	900	-579	4922	110(3)
Hn(9)	1508	1369	4788	110(3)

Table 26. (cont.).

	x	y	z	U
Cn(0)	278	676	5024	110(3)
Hn(0A)	611	912	5191	110(3)
Hn(0B)	-238	20	5046	110(3)
Hn(0C)	14	1073	4969	110(3)

* Equivalent isotropic U defined as one third of the trace of the orthogonalised U_{ij} tensor

Table 27. Anisotropic thermal parameters ($Å^2x10^3$) for Cis-p-menthane supercell.

	U11	U22	U33	U23	U13	U12
S(11)	42(2)	45(2)	32(2)	-4(2)	-1(2)	21(2)
C(11)	54(5)	47(5)	50(5)	15(4)	1(5)	14(4)
N(11)	64(4)	32(3)	30(4)	-12(3)	-9(4)	29(3)
N(12)	87(5)	51(4)	25(4)	-5(3)	-3(4)	55(3)
S(21)	45(2)	36(2)	5(1)	7(1)	-1(1)	13(2)
C(21)	49(4)	29(4)	13(3)	4(3)	9(3)	21(3)
N(21)	98(5)	65(5)	50(5)	-8(5)	-25(5)	19(5)
N(22)	69(5)	47(4)	58(5)	0(4)	-0(4)	31(4)
S(31)	75(3)	81(3)	25(2)	10(2)	7(2)	46(2)
C(31)	38(4)	49(4)	27(4)	-9(4)	2(3)	19(3)
N(31)	48(3)	65(4)	26(3)	3(3)	3(3)	37(3)
N(32)	54(4)	113(5)	31(3)	9(4)	-6(3)	67(3)
S(41)	42(2)	30(2)	32(2)	11(1)	-9(2)	6(2)
C(41)	45(4)	41(4)	32(4)	5(4)	14(4)	22(4)
N(41)	53(4)	105(5)	24(4)	-9(4)	-20(4)	24(4)
N(42)	76(5)	35(4)	18(3)	6(3)	-3(4)	22(3)

The anisotropic temperature factor exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11}+...+2hka^*b^*U_{12})$

Nature of the Bonding between Thiourea and the Guest Molecule

As shown in Figures 21 and 22, the bonding apparently involves interactions between the cis-para-menthane hydrogens and the three coplanar sulfur atoms

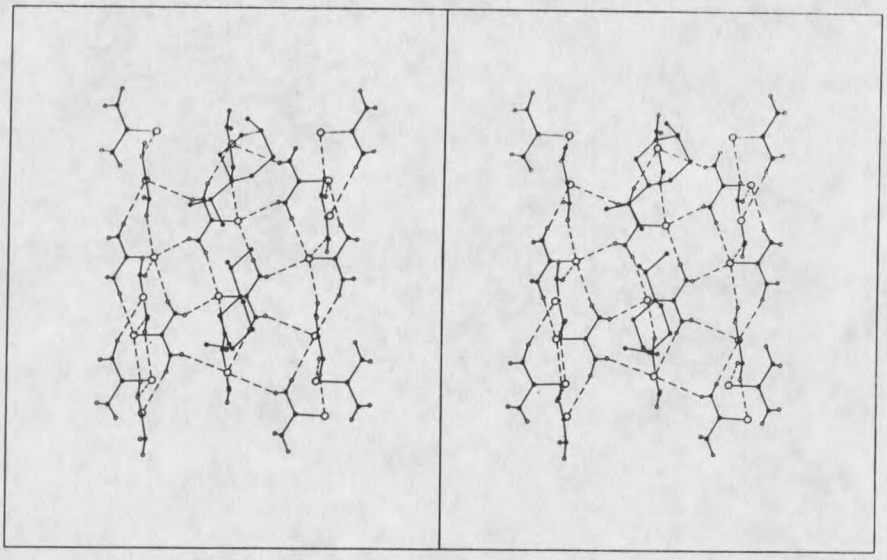


Figure 21. Cutaway view of the Cis-p-menthane subcell illustrating some of the close interactions of the guest and the hydrogen bonding network. Only one of each of the guest model orientations is illustrated.

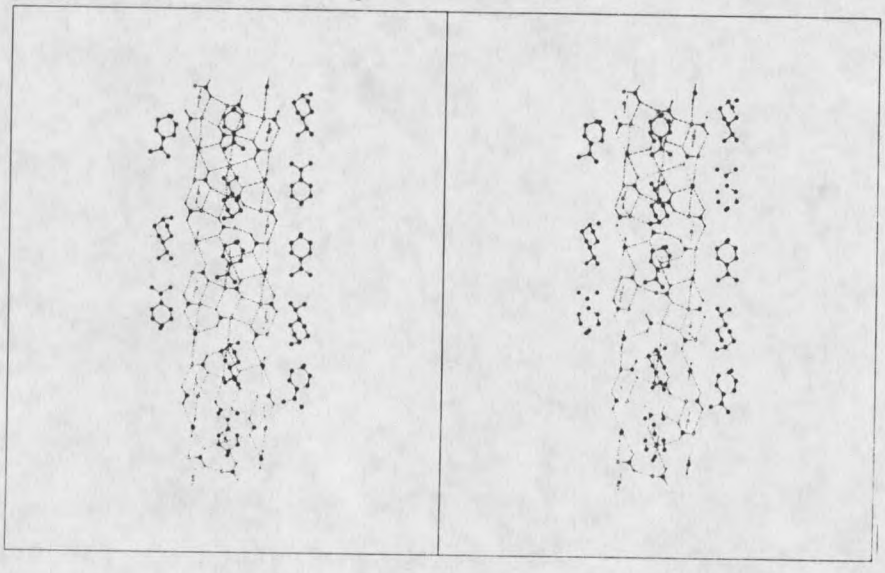


Figure 22. Cutaway view of the Cis-p-menthane supercell illustrating some of the close interactions of the guest and the hydrogen bonding network. Only one of each of the guest model orientations is illustrated.

protruding into the channel. The isopropyl group appears to serve as one possible site for binding, allowing a single cis-p-menthane to partially occupy two sites in the guest. This suggests some interaction between the sulfur and the methyl and methylene groups of the guest. The supercell model, while disordered, suggests that the guest attempts to pack as efficiently as possible, with isopropyl groups on two molecules sharing a single site.

The supercell resolves some of the disorder seen in the subcell, but the model is still disordered due to the three fold axis still present in this structure. The methyl group in the axial conformation forces the channel to remain roughly circular, which results in the retention of the three fold symmetry for the thiourea lattice. This is the major contribution to the scattering, and allows other rotationally related positions for the guest. This disorder could conceivably be resolved in the isopropyl cyclohexane adduct, which would be expected to be monoclinic at low temperature.

CHAPTER 6

ADAMANTANE THIOUREA ADDUCT

The adamantane adduct was initially prepared and initial structural work done by B. E. Robertson, J. S. Rutherford, and R. Gopal.[47] This initial work was incomplete, and a new data set was collected to improve our understanding of this adduct. It was hoped that this adduct, with the highly symmetrical adamatane as the guest molecule, would not be disordered in the same way as the other adducts studied to this point.

Experimental

Crystal Preparation

Reagent grade thiourea and ethanol were purchased from the J. T. Baker Chemical Company. Adamantane (reagent grade) was purchased from Aldrich Chemical Co. Adamantane dissolved in heptane was added to a saturated solution of thiourea in ethanol, and the resulting white flocculent precipitate recrystallized by heating to ~60°C in water and then slowly cooling the crystals in a dewar flask filled with heated water. Good quality crystals formed in about 24 hours, and were stable to exposure to air for several months without any sign of deterioration. This stability

is comparable to that of the bicyclo[2.2.2]octane adduct. An experimental density was obtained by flotation in chloroform/heptane solutions. D_o = 1.21(2) gcm^{-3} and D_c = 1.219 gcm^{-3}. The crystal used for intensity data collection had dimensions of 0.69 x 0.34 x 0.36 mm^3.

Data Collection

Intensity data were collected on a Nicolet R3m/E four circle diffractometer using the omega scan technique. Three standard reflections were measured periodically throughout the course of the data collection to monitor crystal alignment and/or deterioration. There was no decrease in the standards over the course of the data collection, with a maximum variation from the average of less than 3%. A total of 8945 reflections were collected of which 1389 were unique and 766 were considered observed at the $6\sigma_F$ level. Lattice parameters were obtained from least squares fit to 25 reflections for which 25.0° < 2Θ < 30.0°. Space group designation and other details of the data collection, structure solution and refinement are included in Table 28.

Data Reduction, Structure Solution, and Refinement

The data were reduced in the usual manner with appropriate Lorentz and polarization corrections. Scattering factors for S, N, C, H and anomalous scattering terms for S, N, and

Table 28. Experimental Data for Adamantane Thiourea Adduct

Formula		$C_{10}H_{14} \cdot 3(SCN_2H_4)$
Cell Dimensions	a	16.160(1)Å
	c	12.530(2)Å
Space Group		R3c
Cell Volume		2833.90Å^3
D_m		1.25(2) gcm^{-3}
D_c		1.2373 gcm^{-3}
Crystal Dimensions		0.42 x 0.37 x 0.46 mm^3
$\sin \Theta / \lambda_{max}$		0.807 Å^{-1}
Range	h	0 to ±27
	k	0 to 27
	l	0 to ±21
Total Reflections		8945
Unique Reflections		1389 R_{merg} = 0.0084
Observed Reflections		766 6 σ_F cutoff
Number of parameters refined		41
$R = \frac{\Sigma(\lvert\lvert F_o\rvert - \lvert F_c\rvert\rvert)}{\Sigma\lvert F_o\rvert} =$		0.068
$R_w = \frac{\Sigma(\lvert\lvert F_o\rvert - \lvert F_c\rvert\rvert)w^{1/2}}{\Sigma\lvert F_o\rvert w^{1/2}} =$		0.069
$S = \frac{\Sigma(\lvert\lvert F_o\rvert - \lvert F_c\rvert\rvert)w^{1/2}}{(m-n)^{1/2}} =$		1.927
$w = (\sigma_F^2 + gF^2)^{-1}$	where g =	0.000735

C were taken from the International Tables for X-ray Crystallography;[24] all atoms were assumed to be in the zero ionization state. No correction for absorption was made.

An initial model was obtained by utilizing the atomic coordinates for the thiourea molecule from the carbon tetrachloride adduct as the compounds are isostructural. Computational work was done utilizing the Nicolet program package,[57] the XTAL system of programs,[61] and programs written locally. The S, C, and N atoms of the thiourea lattice structure were refined with anisotropic thermal parameters by full matrix least squares minimizing $\Sigma w(|F_o|-|F_c|)^2$ with all parameters refined in each full matrix block. Thiourea amino hydrogen position coordinates, determined from a difference Fourier electron density map at an intermediate stage of refinement, were refined along with isotropic thermal parameters. The weighting scheme used in the latter stages of refinement was $w = (\sigma_F^2 + gF^2)^{-1}$, where g was refined and converged to a value of 0.000735. A final difference Fourier electron density map showed maximum peak heights ≈ 0.5 e/Å^3 in the vicinity of the adducted molecule in the channel. The largest shift over error value was less than 0.003 at convergence. No corrections for secondary extinction were made or refined. The -1 2 0 and -1 3 2 reflections exhibited extinction and were removed from the data set.

Figure 23 illustrates the structure of the adamantane adduct. The final model for the organic guest moiety involved one fully occupied adduct site, which is represented by three anisotropic carbons. The apical carbon is on the 3 axis, with an occupancy of 1/12. The two other atoms have their occupancies set at 3/4. The resulting set of atoms through symmetry sets for a fully occupied adduct site.(Figure 24)

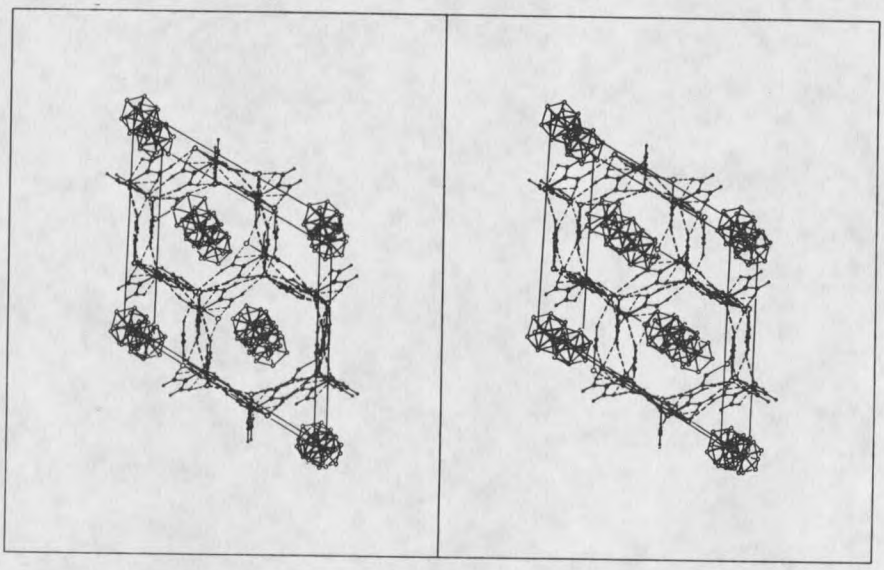


Figure 23. Adamantane adduct packing diagram view along c showing the hydrogen bonding of the thiourea host lattice and the disorder of the guest molecule.

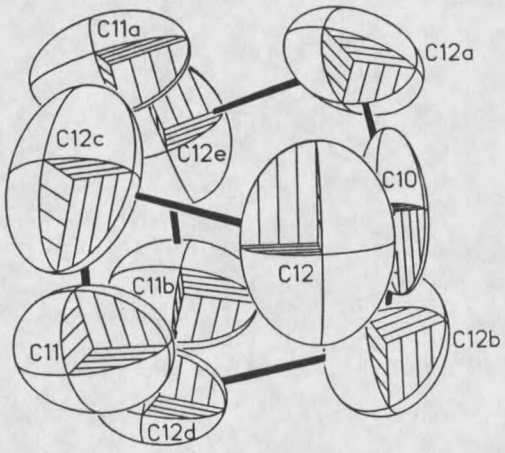


Figure 24. Thermal ellipsoid plot of Adamantane disorder model. Generated atoms C11a, C11b, C12a, and C12b are generated by the three fold symmetry, and atoms C12c, C12d, and C12e are generated by the two fold symmetry operation.

Results and Discussion

Derived Parameters

Tables 29 through 32 contain derived parameters for the adamantane thiourea adduct. The bond lengths and angles for the thiourea molecule compare well with those previously observed for pure crystalline thiourea,[14,36] and with the isostructural carbon tetrachloride, cyclohexane and bicyclo[2.2.2]octane adducts.

Table 29. Atomic Coordinates ($x10^4$) and Isotropic Thermal Parameters ($Å^2x10^3$) for Adamantane Thiourea Adduct.

	x	y	z	U
S(1)	0	3043(1)	2500	38(1)*
C(1)	0	4103(2)	2500	37(1)*
N(1)	176(2)	4603(2)	1613(2)	49(1)*
C(10)	0	0	1499(12)	138(11)*
C(11)	998(7)	693(8)	1737(10)	128(6)*
C(12)	232(13)	960(7)	1759(9)	151(8)*
H(1a)	175	5196	1617	61
H(1b)	305	4373	963	61

* Equivalent isotropic U defined as one third of the trace of the orthogonalised U_{ij} tensor.

Table 30. Bond Lengths (Å)

S(1)-C(1)	1.713(4)	C(1)-N(1)	1.318(3)
C(1)-N(1a)	1.318(3)	C(10)-C(11)	1.462(9)
C(10)-C(12)	1.440(13)	C(10)-C(11b)	1.462(15)
C(10)-C(11d)	1.462(9)	C(10)-C(12b)	1.440(11)
C(10)-C(12d)	1.439(7)	C(11)-C(12)	1.500(26)
C(11)-C(12d)	1.333(20)	C(12)-C(11b)	1.333(18)
C(12)-C(12a)	1.967(25)		

Table 31. Bond Angles (°)

S(1)-C(1)-N(1)	120.3(2)	S(1)-C(1)-N(1a)	120.3(2)
N(1)-C(1)-N(1a)	119.4(4)	C(11)-C(10)-C(12)	62.2(10)
C(11)-C(10)-C(11b)	115.9(6)	C(12)-C(10)-C(11b)	54.7(9)
C(11)-C(10)-C(11d)	115.9(7)	C(12)-C(10)-C(11d)	154.8(13)
C(11)-C(10)-C(12b)	154.8(13)	C(12)-C(10)-C(12b)	115.0(6)
C(11)-C(10)-C(12d)	54.7(10)	C(12)-C(10)-C(12d)	115.0(6)
C(10)-C(11)-C(12)	58.1(6)	C(10)-C(11)-C(12d)	61.8(7)
C(12)-C(11)-C(12d)	117.9(8)	C(10)-C(12)-C(11)	59.6(8)
C(10)-C(12)-C(11b)	63.5(7)	C(11)-C(12)-C(11b)	122.0(13)
C(10)-C(12)-C(12a)	98.0(9)	C(11)-C(12)-C(12a)	104.7(11)

Table 32. Anisotropic Thermal Parameters ($Å^2x10^3$)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S(1)	45(1)	33(1)	40(1)	1(1)	2(1)	22(1)
C(1)	31(2)	31(1)	49(2)	-1(1)	-2(2)	16(1)
N(1)	64(2)	41(1)	46(1)	8(1)	3(1)	31(1)
C(10)	193(17)	193(17)	26(9)	0	0	97(8)
C(11)	81(6)	105(7)	189(10)	7(7)	26(6)	39(5)
C(12)	233(13)	77(6)	132(8)	22(5)	19(9)	69(8)

The anisotropic temperature factor exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$

Disorder Analysis

While it is clear that the adduct is extremely stable, the hoped for improvement in terms of disorder did not occur due to site symmetry that the adamantane molecule does not have, as well as what appears to be rapid interconversion of various rotamers of the adamatane relative to the three thiourea binding site. The model used for refinement consisted of an apex carbon of adamantane and two other carbons representing the other carbons of the adamatane.(Figure 24) All of these atoms were refined anisotropically, and the resulting derived distances are unreasonable upon initial inspection. However, this model represents the electron density found in the active site, as shown in Figure 25. Upon further investigation, it was shown that the two non-apical carbons mentioned above are actually the centroid of three atoms superimposed upon each other by the site symmetry. This

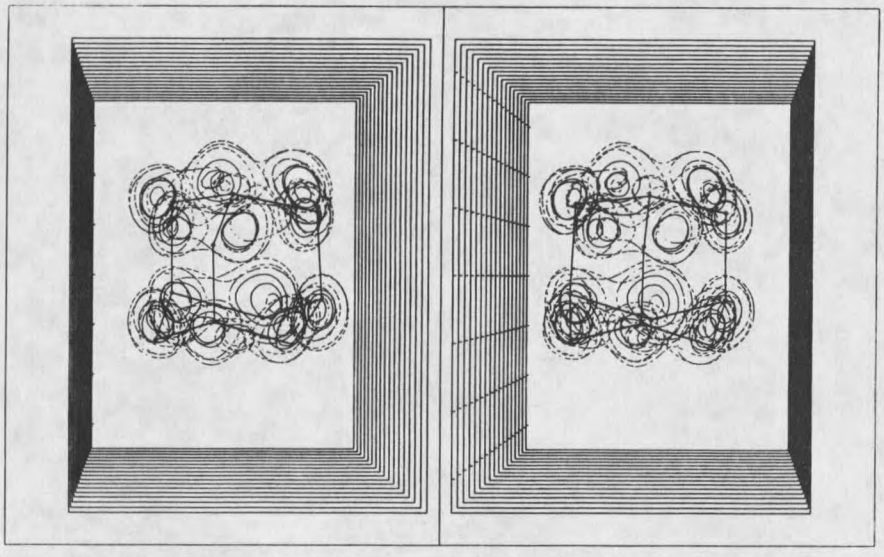


Figure 25. Stereo difference electron density contour map calculated from the final refinement without the guest molecule. View is normal to the three fold axis, with layers 0.5Å apart, and contours at $1e/Å^3$(dotted) and $2e/Å^3$(solid).

results from both a 60° rotation about the three fold axis, and from the 2 fold axis normal to the three fold at the site. When tetrahedral angles and normal carbon-carbon bond lengths are used, a calculation assuming that the apical carbons are in their correct positions and that the molecule is approximately aligned with a local three fold axis coincident with the crystallographic three fold axis, the above operations gives two centroids with 3 carbons within ~0.5Å of each other, spaced about 1.9Å apart in the z direction.(Figure 26) This is within the error of this

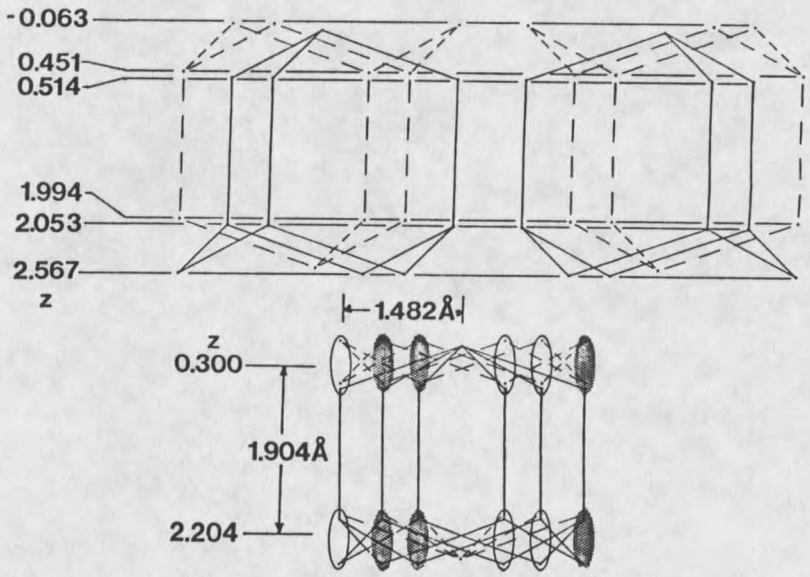


Figure 26. Disorder analysis for the adamantane. The top figure gives the z coordinate in angstroms, with the origin on a three fold axis at the apical carbon and the distance between apical carbons on the three fold axis set to that found in the refined structure. The lower figure gives the average z coordinates for three fold related carbons, and shows with shading the two independent anisotropic carbons that make up the disorder model.

calculation for the observed carbon-carbon distance in this structure.

Nature of the Bonding between Thiourea and the Guest Molecule

As shown in Figure 27, the bonding apparently involves interactions between the adamantane hydrogens and the three coplanar sulfur atoms protruding into the channel. These interactions are not very strong, as solid

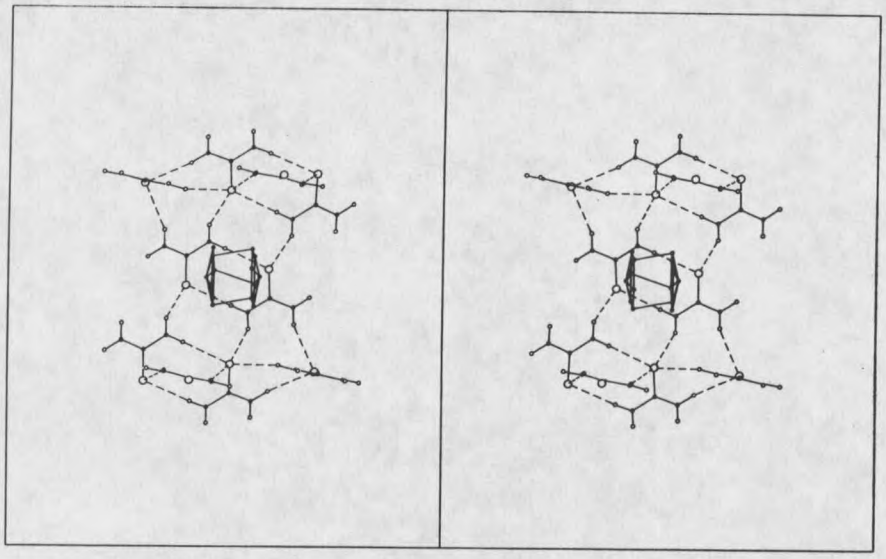


Figure 27. Cutaway view of the adamantane in the host lattice. View is normal to the 3-fold axis. Interactions that dominate appear to be the sulfur interacting with 3 hydrogens on the adamatane, giving rise to disorder positions every 60° about the c axis.

state NMR indicates that the adamantane is dynamically disordered on the NMR time scale at room temperature, with rapid interchange of the adamantane orientations in the channel. This would not necessarily disrupt all of the interactions, as the molecule has a high level of symmetry, allowing for interconversion of sites with only a rotation of about 60° around 3 of the 4 three fold axes of the adamantane, with a number of other possible rotations giving the same effect.

CHAPTER 7

1,2,4 TRICHLOROBENZENE ADDUCT

The isomers of trichlorobenzene all form adducts with thiourea. When a mixture of these isomers is used as the guest, the resulting adduct is enriched in the 1,2,4 isomer. Because of this known selectivity, and also the induced selectivity in other aromatic systems when the 1,2,4 isomer is included in the guest feedstock, investigation of this adduct was initiated Rebecca Welling.[65] No structural data was available at that point on any aromatic adduct of thiourea, and preliminary photographic investigations indicated that there was a significant difference between the aromatic adducts and the rhombohedral adducts. Tom Wick collected initial intensity data on the 1,2,4 trichlorobenzene adduct, and worked on an initial model of the thiourea lattice and the disorder of the guest molecule.[66] Upon subsequent analysis of his results, it was decided to recollect the data and expand the refinement of the disorder model in hopes of improving the understanding of the disorder and elucidating the possible reasons for the disorder.

Experimental

Crystal Preparation

Reagent grade thiourea and ethanol were purchased from the J. T. Baker Chemical Company. 1,2,4 trichlorobenzene was obtained from Aldrich Chemical Corp. An experimental density was obtained by flotation in chloroform/heptane solutions. D_o = 1.32(2) gcm^{-3} and D_c = 1.2995 gcm^{-3}. The crystal used for intensity data collection had dimensions of 0.6 x 0.6 x 0.9 mm^3.

Data Collection

Intensity data were collected on a Nicolet R3m/E four circle diffractometer using the omega scan technique. Three standard reflections were measured periodically throughout the course of the data collection to monitor crystal alignment and/or deterioration. There was no decrease in the standards over the course of the data collection, with a maximum variation from the average of less than 3%. A total of 4968 reflections were collected of which 4169 were unique and 1754 were considered observed at the $6\sigma_F$ level. Lattice parameters were obtained from least squares fit to 25 reflections for which $25.0° < 2\Theta < 35.0°$. Space group designation and other details of the data collection, structure solution and refinement are included in Table 33.

Table 33. Experimental Data for Trichlorobenzene Thiourea Adduct

Formula		$2(C_6H_3Cl_3)\cdot 9(SCN_2H_4)$
Cell Dimensions	a	9.778(1)
	b	15.345(3)
	c	12.292(1)
	β	111.87(1)
Space Group		$P2_1/a$
Cell Volume		1711.52(39)
D_m		1.32(2) gcm^{-3}
D_c		1.2995 gcm^{-3}
Crystal Dimensions		0.65 x 0.65 x 1.2 mm^3
$\sin\Theta / \lambda_{max}$		0.704 $Å^{-1}$
Range	h	0 to 11
	k	0 to 22
	l	0 to ±18
Total Reflections		4968
Unique Reflections		4169 R_{merg} = 0.0057
Observed Reflections		1754 6 σ_F cutoff
Number of parameters refined		134
$R = \frac{\Sigma(\lvert\lvert F_o\rvert-\lvert F_c\rvert\rvert)}{\Sigma\lvert F_o\rvert} =$		0.091
$R_w = \frac{\Sigma(\lvert\lvert F_o\rvert-\lvert F_c\rvert\rvert)w^{\frac{1}{2}}}{\Sigma\lvert F_o\rvert w^{\frac{1}{2}}} =$		0.105
$S = \frac{\Sigma(\lvert\lvert F_o\rvert-\lvert F_c\rvert\rvert)w^{\frac{1}{2}}}{(m-n)^{\frac{1}{2}}} =$		1.717
$w = (\sigma_F^2 + gF^2)^{-1}$	where g =	0.00535

Data Reduction, Structure Solution, and Refinement

The data were reduced in the usual manner with appropriate Lorentz and polarization corrections. Scattering factors for S, Cl, N, C, H and anomalous scattering terms for S, Cl, N, and C were taken from the International Tables for X-ray Crystallography;[24] all atoms were assumed to be in the zero ionization state. No correction for absorption was made, as the crystal was mounted such that the beam was nearly normal to the long axis of the crystal. Psi scan data for this crystal showed only slight effects of absorption.

The initial model for the thiourea was obtained by direct methods. The three unique thioureas were all located from the E map. Attempts to refine a model for the guest based on peaks located in the difference map failed to converge or make chemical sense. Upon reexamining the density measurements and molecular weight considerations, as well as size calculations for the trichlorobenzene, a rigid group model was constructed using idealized trichlorobenzenes that were fit to the 6 highest peaks in the difference map in four orientations, as illustrated in Figure 28. The positional parameters of the group were allowed to refine as an idealized group, with a common isotropic group thermal for all of the atoms. Computational work was done utilizing the Nicolet program package,[57] and programs written locally. The S, C, and N

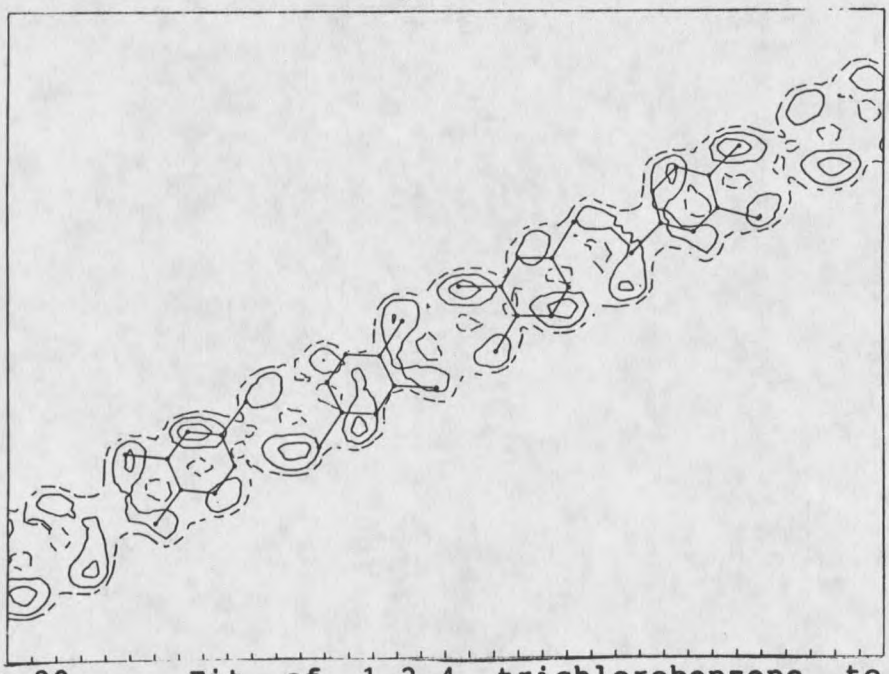


Figure 28. Fit of 1,2,4 trichlorobenzene to the 6 maxima of the electron density. Contours are at arbitrary levels.

atoms of the thiourea lattice structure were refined with anisotropic thermal parameters by full matrix least squares minimizing $\Sigma w(|F_o|-|F_c|)^2$ with all parameters refined in each full matrix block. The weighting scheme used in the latter stages of refinement was $w = (\sigma_F^2 + gF^2)^{-1}$, where g was refined and converged to a value of 0.00535. A final difference Fourier electron density map showed maximum peak heights $\approx$0.73 e/Å^3 in the vicinity of the adducted molecule in the channel, and the most negative peak height was $\approx$0.39 e/Å^3. The maximum shift over error value was less than 0.08 at convergence. No corrections for secondary extinction were made or refined. The 1 1 2 and -2 2 3

reflections exhibited extinction, and were removed from the data set.

Disorder Model

Figure 29 illustrates the structure of the 1,2,4 trichlorobenzene adduct. The final model for the organic guest moiety involved six partially occupied adduct sites. All atoms of the 1,2,4 trichlorobenzene were constrained in an idealized rigid group, with carbon - carbon bond distances of 1.350Å, carbon - chlorine bond distances of 1.740Å, and 120° angles. A single group thermal (U_g) was

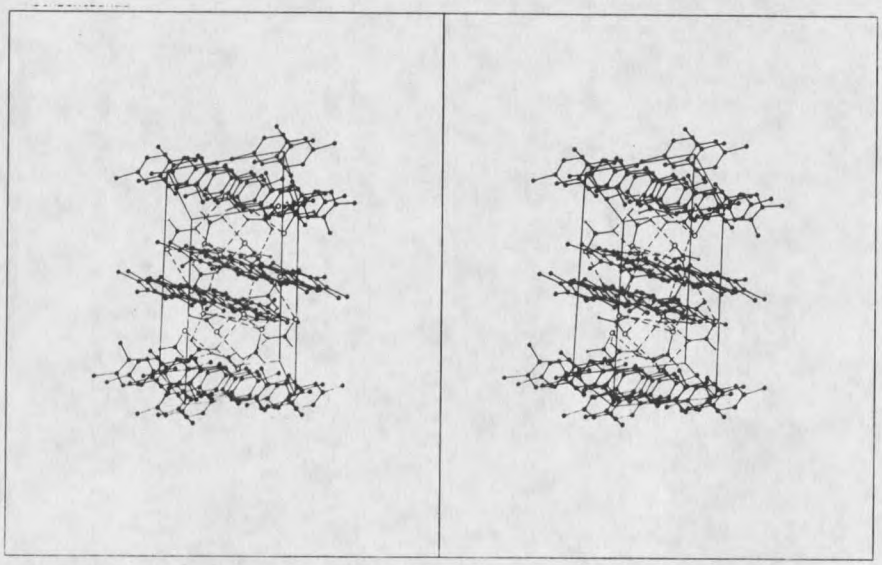


Figure 29. 1,2,4 Trichlorobenzene adduct packing diagram illustrating the hydrogen bonding and disorder model.

refined with the thermal parameters for the 1,2,4 trichlorobenzene chlorines of 1.2(U_g). Occupancies of the 1,2,4 trichlorobenzene group atoms were set at 0.16667. Figure 30 shows the four independent molecule separated in space for visual clarity.

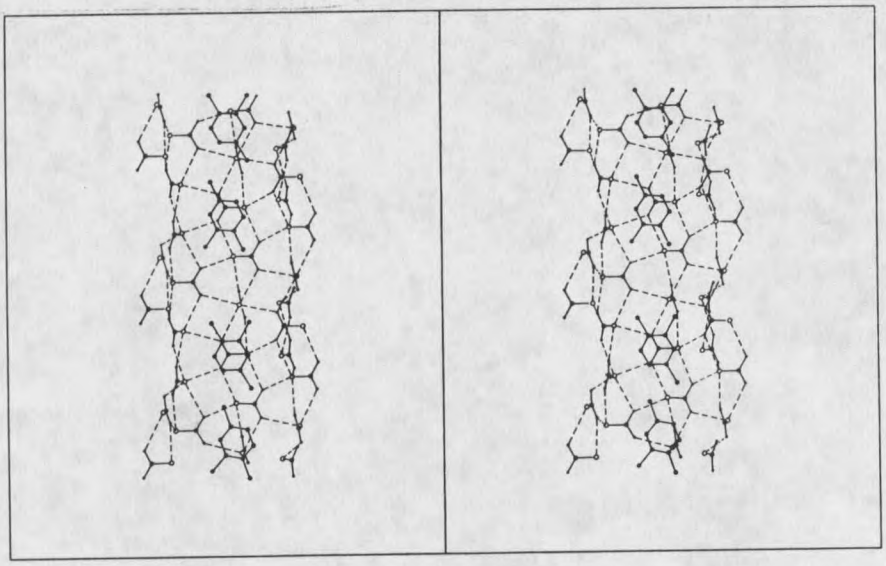


Figure 30. Cutaway view of the trichlorobenzene in the host lattice. View is normal to the channel, with 5 binding sites shown.

Results and Discussion

Derived Parameters

Tables 34 through 37 contain derived parameters for the 1,2,4 trichlorobenzene thiourea adduct. The bond lengths and angles for the thiourea molecule compare well with those previously observed for pure crystalline thiourea,[14,36] and with the rhombohedral thiourea adducts.

Table 34. Atomic Coordinates ($x10^4$) and Isotropic Thermal Parameters ($Å^2x10^3$) for 1,2,4 Trichlorobenzene Thiourea Adduct

	x	y	z	U
S(1)	-1025(2)	8531(1)	4396(2)	71(1)*
C(1)	-2237(8)	8108(5)	4955(2)	68(2)*
N(11)	-3650(7)	8053(5)	4311(6)	85(2)*
N(12)	-1767(8)	7845(5)	6058(6)	89(2)*
S(2)	4912(2)	8627(1)	1412(2)	65(1)*
C(2)	5898(8)	7906(5)	931(6)	63(2)*
N(21)	7302(8)	7741(5)	1583(6)	90(2)*
N(22)	5293(8)	7505(4)	-83(5)	83(2)*
S(3)	3182(2)	13030(1)	2024(2)	66(1)*
C(3)	2718(9)	14088(5)	2205(6)	69(2)*
N(31)	1760(8)	14527(5)	1325(6)	85(2)*
N(32)	3326(8)	14450(5)	3266(6)	88(2)*
Cl(1)	4671(16)	10533(10)	3535(14)	162(2)
Cl(2)	2433	9154	3786	162(2)
Cl(3)	-1201	9766	-699	162(2)
C(11)	3059	10296	2348	135(2)
C(12)	2009	9745	2495	135(2)
C(13)	663	9616	1574	135(2)
C(14)	373	10031	503	135(2)
C(15)	1406	10600	367	135(2)
C(16)	2763	10716	1281	135(2)
Cl(4)	-7244(17)	9367	-5883(13)	162(2)
Cl(5)	-5510	10703	-6797	162(2)
Cl(6)	-1138	10769	-2501	162(2)
C(21)	-5551	9763	-4938	135(2)
C(22)	-4772	10351	-5349	135(2)
C(23)	-3348	10597	-4632	135(2)
C(24)	-2740	10296	-3481	135(2)
C(25)	-3503	9690	-3080	135(2)
C(26)	-4923	9438	-3800	135(2)
Cl(7)	-2236(16)	-10617(11)	-1081(12)	162(2)
Cl(8)	-361	-9293	-1898	162(2)
Cl(9)	3846	-9299	2472	162(2)
C(31)	-566	-10266	-87	135(2)
C(32)	323	-9704	-476	135(2)
C(33)	1716	-9454	298	135(2)
C(34)	2215	-9722	1465	135(2)
C(35)	1343	-10264	1847	135(2)
C(36)	-62	-10500	1078	135(2)
Cl(A)	9490(15)	-9443(9)	8473(12)	162(2)
Cl(B)	7479	-10739	9158	162(2)
Cl(C)	3603	-10755	4656	162(2)

Table 34 (cont.).

	x	y	z	U
C(41)	7858	-9815	7408	135(2)
C(42)	6956	-10385	7716	135(2)
C(43)	5576	-10610	6895	135(2)
C(44)	5138	-10306	5746	135(2)
C(45)	6024	-9718	5446	135(2)
C(46)	7399	-9487	6270	135(2)

* Equivalent isotropic U defined as one third of the trace of the orthogonalised U_{ij} tensor.

Table 35. Bond Lengths (Å)

S(1)-C(1)	1.704(9)	C(1)-N(11)	1.314(9)
C(1)-N(12)	1.323(10)	S(2)-C(2)	1.711(9)
C(2)-N(21)	1.331(9)	C(2)-N(22)	1.317(9)
S(3)-C(3)	1.723(8)	C(3)-N(31)	1.322(9)
C(3)-N(32)	1.355(10)		

Table 36. Bond Angles (°)

S(1)-C(1)-N(11)	121.0(6)	S(1)-C(1)-N(12)	120.1(6)
N(11)-C(1)-N(12)	119.0(8)	S(2)-C(2)-N(21)	120.2(6)
S(2)-C(2)-N(22)	121.2(6)	N(21)-C(2)-N(22)	118.7(8)
S(3)-C(3)-N931)	121.0(6)	S(3)-C(3)-N(32)	118.2(5)
N(31)-C(3)-N(32)	120.8(7)		

Table 37. Anisotropic Thermal Parameters ($Å^2 x 10^3$)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S(1)	58(1)	90(1)	59(1)	12(1)	16(1)	-3(1)
C(1)	68(3)	74(3)	60(3)	6(3)	22(2)	1(3)
N(11)	64(3)	108(3)	82(3)	-8(3)	28(2)	-20(3)
N(12)	85(3)	105(3)	79(3)	13(3)	34(2)	2(3)
S(2)	59(1)	71(1)	60(1)	-9(1)	18(1)	1(1)
C(2)	64(3)	66(3)	63(3)	5(2)	29(2)	3(3)
N(21)	66(3)	117(3)	82(3)	-2(3)	22(2)	20(3)
N(22)	109(3)	78(3)	63(2)	-17(2)	34(2)	-3(3)

Table 37. (cont.)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S(3)	77(1)	65(1)	51(1)	-2(1)	19(1)	10(1)
C(3)	78(3)	65(3)	74(3)	-10(3)	39(2)	-2(3)
N(31)	82(3)	79(3)	74(3)	15(2)	5(3)	15(3)
N(32)	87(3)	93(3)	68(3)	-17(3)	11(3)	0(3)

The anisotropic temperature factor exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$

Nature of the Bonding between Thiourea and the Guest Molecule

As shown in Figure 30, the bonding apparently involves interactions between the 1,2,4 trichlorobenzene and the three coplanar sulfur atoms protruding into the channel. These planes intersect the trichlorobenzne near the carbons attached to chlorine. Due to the several different orientations that are available to the trichlorobenzne, this gives the effect of a dimer of dimers type disorder model which stretches four trichlorobenzene molecules over six binding sites in the crystal. This effectively gives an occupancy of 2/3 for the trichlorobenzne compared to the stoichiometric 1:3 adducts studied earlier. This preferred interaction can be inferred from the electron withdrawing effect of chlorine, which would then make the carbons attached to chlorine somewhat positive. These positive carbons are ideally situated to form a good coulombic interaction with the partially negative sulfur of each of the three thioureas.

CHAPTER 8

1,2,4 TRIMETHYLBENZENE ADDUCT

The 1,2,4 isomer of trimethylbenzene forms an adduct with thiourea when present above a certain critical concentration.[31] When a mixture of isomers of C_9 alkylbenzenes is incorporated in the thiourea host as the guest, the resulting adduct is enriched in the 1,2,4 trimethylbenzene. Because of this known selectivity, and also the induced selectivity in other aromatic systems when 1,2,4 trimethylbenzene is included in the guest feedstock, investigation of this adduct was initiated Rebecca Welling at Montana State University.[65] No structural data was available at that point on any aromatic adduct of thiourea, and preliminary photographic investigations indicated that there was a significant difference between the aromatic adducts and the rhombohedral adducts. An initial intensity data set was obtained by the Molecular Structure Corporation, and while the thiourea positions were well defined, the guest could not be modelled successfully. Subsequently, a second data set was obtained, and Tom Wick worked on an initial model of the thiourea lattice and the disorder of the guest molecule.[66] Upon subsequent analysis of his results, it was decided expand the refinement of the

disorder model in hopes of improving the understanding of the disorder and elucidating the possible reasons for the disorder.

Experimental

Crystal Preparation

Reagent grade thiourea and ethanol were purchased from the J. T. Baker Chemical Company. 1,2,4 trimethylbenzene was obtained from Aldrich Chemical Corp. Crystals were prepared by adding 5 ml of trimethylbenzene to 5ml of ethanol saturated with thiourea at room temperature, and then heating the mixture until the precipitate dissolved. The solution was then place in a dewar flask of hot water, and slowly allowed to cool. Good crystals often appeared after 24 to 48 hours. An experimental density was obtained by flotation in chloroform/heptane solutions. D_o = 1.08(5) gcm^{-3} and D_c = 1.1821 gcm^{-3}. The crystal used for intensity data collection had dimensions of 0.6 x 0.6 x 0.8 mm^3.

Data Collection

Intensity data were collected on a Nicolet R3m/E four circle diffractometer using the omega scan technique. Three standard reflections were measured periodically throughout the course of the data collection to monitor crystal alignment and/or deterioration. There was no decrease in the standards over the course of the data

collection, with a maximum variation from the average of less than 3%. A total of 5330 reflections were collected of which 3985 were unique and 1163 were considered observed at the $6\sigma_F$ level. Lattice parameters were obtained from least squares fit to 25 reflections for which $28° < 2\Theta < 31°$. Space group designation and other details of the data collection, structure solution and refinement are included in Table 38.

Data Reduction, Structure Solution, and Refinement

The data were reduced in the usual manner with appropriate Lorentz and polarization corrections. Scattering factors for S, Cl, N, C, H and anomalous scattering terms for S, Cl, N, and C were taken from the International Tables for X-ray Crystallography;[24] all atoms were assumed to be in the zero ionization state. No correction for absorption was made.

The initial model for the thiourea was obtained by direct methods. The three unique thioureas were all located from the E map. Attempts to refine a model based on peaks located in the difference map failed to converge or make chemical sense. Upon reexamining the density measurements and molecular weight considerations, as well as size calculations for the trimethylbenzene, a rigid group model was constructed using idealized trimethylbenzenes that were fit to the 6 highest peaks in

Table 38. Experimental Data for Trimethylbenzene Thiourea Adduct

Formula		$2(C_9H_{12})\cdot 9(SCN_2H_4)$
Cell Dimensions	a	10.037(5)
	b	15.155(4)
	c	12.354(4)
	β	112.77(3)
Space Group		$P2_1/a$
Cell Volume		1732.84
D_m		1.08(5) gcm^{-3}
D_c		1.182 gcm^{-3}
Crystal Dimensions		0.6 x 0.6 x 0.8 mm^3
$\sin\Theta / \lambda_{max}$		0.650 $Å^{-1}$
Range	h	0 to 14
	k	0 to 20
	l	0 to ±16
Total Reflections		5330
Unique Reflections		3985 R_{merg} = 0.0290
Observed Reflections		1163 6 σ_F cutoff
Number of parameters refined		134
$R = \frac{\Sigma(\lvert\lvert F_o\rvert-\lvert F_c\rvert\rvert)}{\Sigma\lvert F_o\rvert} =$		0.088
$R_w = \frac{\Sigma(\lvert\lvert F_o\rvert-\lvert F_c\rvert\rvert)w^{\frac{1}{2}}}{\Sigma\lvert F_o\rvert w^{\frac{1}{2}}} =$		0.093
$S = \frac{\Sigma(\lvert\lvert F_o\rvert-\lvert F_c\rvert\rvert)w^{\frac{1}{2}}}{(m-n)^{\frac{1}{2}}} =$		1.506
$w = (\sigma_F^2 + gF^2)^{-1}$	where g =	0.00419

the difference map in four orientations, as in the trichlorobenzene adduct. The positional parameters of the group were allowed to refine as an idealized group, with a common isotropic group thermal for all of the atoms. Computational work was done utilizing the Nicolet program package,[57] and programs written locally. The S, C, and N atoms of the thiourea lattice structure were refined with anisotropic thermal parameters by full matrix least squares minimizing $\Sigma w(|F_o|-|F_c|)^2$ with all parameters refined in each full matrix block. The weighting scheme used in the latter stages of refinement was $w = (\sigma_F^2 + gF^2)^{-1}$, where g was refined and converged to a value of 0.00419. A final difference Fourier electron density map showed maximum peak heights $\approx$0.50 e/Å^3 in the vicinity of the adducted molecule in the channel. The maximum shift over error value was less than 0.2 at convergence. No corrections for secondary extinction were made or refined.

Disorder Model

Figure 31 illustrates the structure of the 1,2,4 trimethylbenzene adduct, showing the disordered guest and the host lattice. The final model for the organic guest moiety involved six partially occupied adduct sites. All atoms of the 1,2,4 trimethylbenzene were constrained in an idealized rigid group, with aromatic carbon - carbon bond distances of 1.350Å, carbon - methyl carbon bond distances of 1.540Å, and 120° angles. A single group thermal (U_g)

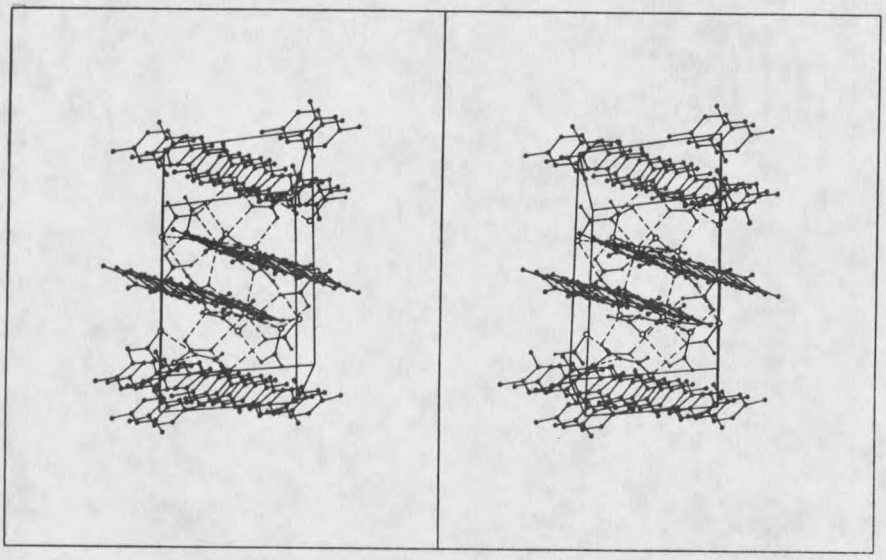


Figure 31. 1,2,4-Trimethylbenzene adduct packing diagram view along a showing the hydrogen bonding of the thiourea host lattice and the disorder of the guest molecule.

was refined with the thermal parameters for the 1,2,4 trimethylbenzene methyl groups of 1.2(U_g). Occupancies of the 1,2,4 trimethylbenzene group atoms were set at 0.16667. Figure 32 shows the four independent molecule separated in space for visual clarity.

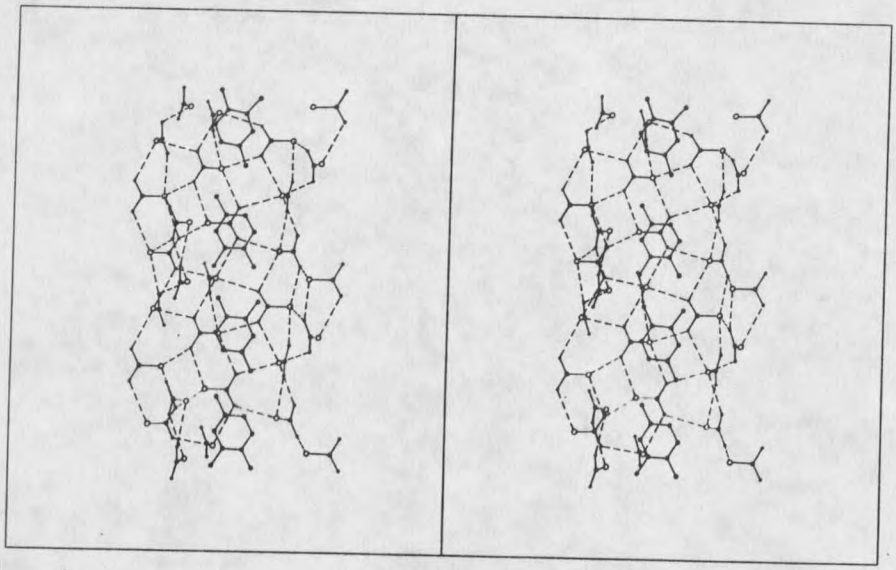


Figure 32. Cutaway view of the trimethylbenzene in the host lattice. View is normal to the channel, with 5 binding sites shown.

Results and Discussion

Derived Parameters

Tables 39 through 42 contain derived parameters for the 1,2,4 trimethylbenzene thiourea adduct. The bond lengths and angles for the thiourea molecule compare well with those previously observed for pure crystalline thiourea,[14,36] and with the rhombohedral thiourea adducts.

Table 39. Atomic Coordinates ($x10^4$) and Isotropic Thermal Parameters ($Å^2x10^3$) for 1,2,4 Trimethylbenzene Thiourea Adduct

	x	y	z	U
S(1)	-1004(3)	8493(2)	4392(2)	71(1)*
C(1)	-2194(11)	8094(6)	4984(8)	65(3)*
N(11)	-1707(10)	7848(7)	6096(7)	81(3)*
N(12)	-3600(9)	8043(6)	4396(8)	78(3)*
S(2)	4972(3)	8596(2)	1402(2)	65(1)*
C(2)	5938(11)	7891(7)	911(9)	65(3)*
N(21)	5329(10)	7490(6)	-140(7)	80(3)*
N(22)	7333(9)	7730(6)	1553(8)	84(3)*
S(3)	3129(3)	13003(2)	2035(2)	68(1)*
C(3)	2724(11)	14064(7)	2219(9)	73(3)*
N(31)	1758(10)	14530(6)	1335(7)	86(3)*
N(32)	3289(10)	14445(6)	3253(7)	87(3)*
Cc(1)	24308(29)	10546(22)	23232(28)	98(3)
Cc(2)	22208	9381	23633	98(3)
Cc(3)	18842	9702	19376	98(3)
C(11)	22899	10295	22215	98(3)
C(12)	21853	9803	22429	98(3)
C(13)	20512	9654	21526	98(3)
C(14)	20249	9951	20393	98(3)
C(15)	21298	10438	20177	98(3)
C(16)	22633	10594	21082	98(3)
Cc(4)	12486(29)	9514(23)	13689(25)	98(3)
Cc(5)	14258	10689	12923	98(3)
Cc(6)	18214	10577	16995	98(3)
C(21)	13989	9785	14551	98(3)
C(22)	14839	10340	14183	98(3)
C(23)	16227	10568	14960	98(3)
C(24)	16750	10258	16112	98(3)
C(25)	15911	9690	16473	98(3)
C(26)	14521	9464	15698	98(3)
Cc(7)	12159(31)	10515(22)	11080(25)	98(3)
Cc(8)	10316	9283	11707	98(3)
Cc(9)	6534	9475	7579	98(3)
C(31)	10711	10210	10153	98(3)
C(32)	9786	9689	10478	98(3)
C(33)	8403	9496	9665	98(3)
C(34)	7983	9774	8504	98(3)
C(35)	8915	10288	8175	98(3)
C(36)	10290	10491	8994	98(3)
Cc(A)	860(30)	9462(23)	2047(29)	98(3)
Cc(B)	2709	10696	1450	98(3)
Cc(C)	6458	10482	5601	98(3)

Table 39. (cont.)

	x	y	z	U
C(41)	2340	9713	2968	98(3)
C(42)	3226	10296	2681	98(3)
C(43)	4586	10513	3516	98(3)
C(44)	5042	10166	4648	98(3)
C(45)	4172	9565	4925	98(3)
C(46)	2812	9348	4090	98(3)

* Equivalent isotropic U defined as one third of the trace of the orthogonalised U_{ij} tensor.

Table 40. Bond Lengths (Å)

S(1)-C(1)	1.733(13)	C(1)-N(11)	1.322(13)
C(1)-N(12)	1.339(12)	S(2)-C(2)	1.705(12)
C(2)-N(21)	1.346(13)	C(2)-N(22)	1.337(12)
S(3)-C(3)	1.695(12)	C(3)-N(31)	1.346(12)
C(3)-N(32)	1.314(13)		

Table 41. Bond Angles (°)

S(1)-C(1)-N(11)	119.9(8)	S(1)-C(1)-N(12)	118.8(8)
N(11)-C(1)-N(12)	121.3(11)	S(2)-C(2)-N(21)	121.1(8)
S(2)-C(2)-N(22)	120.8(8)	N(21)-C(2)-N(22)	118.1(11)
S(3)-C(3)-N(31)	121.6(8)	S(3)-C(3)-N(32)	120.8(8)
N(31)-C(3)-N(32)	117.6(10)		

Table 42. Anisotropic Thermal Parameters ($Å^2 \times 10^3$)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S(1)	57(2)	84(2)	59(1)	12(1)	9(1)	-4(2)
C(1)	67(4)	62(4)	66(4)	-4(4)	24(4)	-4(2)
N(11)	80(4)	97(4)	56(4)	24(4)	16(3)	2(4)
N(12)	47(4)	93(4)	88(4)	-3(4)	18(3)	-9(4)
S(2)	55(2)	66(2)	61(1)	-10(1)	8(1)	1(1)
C(2)	60(4)	68(4)	70(4)	0(4)	31(4)	0(4)
N(21)	98(4)	78(4)	67(4)	-14(4)	34(4)	0(4)
N(22)	62(4)	98(4)	85(4)	-2(4)	21(4)	16(4)
S(3)	79(2)	63(2)	50(1)	-3(1)	11(1)	10(2)
C(3)	76(4)	64(4)	74(4)	-17(4)	23(4)	1(4)
N(31)	90(4)	72(4)	69(4)	7(4)	1(4)	17(4)
N(32)	103(4)	73(4)	68(4)	-15(4)	14(4)	9(4)

The anisotropic temperature factor exponent takes the form: $-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$

Nature of the Bonding between Thiourea and the Guest Molecule

As shown in Figure 32, the bonding apparently involves interactions between the 1,2,4 trimethylbenzene and the three coplanar sulfur atoms protruding into the channel. Due to the several different orientations that are available to the trimethylbenzene, this gives the effect of a dimer of dimers type disorder model which stretches four trimethylbenzene molecules over six binding sites in the crystal. This effectively gives an occupancy of 2/3 for the trimethylbenzene compared to the stoichiometric 1:3 adducts studied earlier. The dominant interactions appear to be with the sulfur of thiourea and the carbon of the methyl group. The methyl hydrogens may be somewhat more positive than otherwise, giving rise to a coulombic stabilization of the guest in the lattice.

CHAPTER 9

1,2,4-TRIMETHYLBENZENE 1,2,4-TRICHLOROBENZENE MIXED THIOUREA ADDUCT

The separations of the C_9 alkylbenzenes using induced adduction studied by McCandless,[30] and the structural studies on these adducts made it desirable to investigate the mixed adduct of 1,2,4-trichlorobenzene and 1,2,4-trimethylbenzene. Initial structural determination work was done by Mark Spinti.[59] Upon examination of his results, it was decided to continue the refinement using a model derived from that used in the 1,2,4-trichlorobenzene adduct refinement.

Experimental

Crystal Preparation

Reagent grade thiourea and ethanol were purchased from the J. T. Baker Chemical Company. 1,2,4 trimethylbenzene and 1,2,4 trichlorobenzene were obtained from the Aldrich Chemical Corp. An experimental density was obtained by flotation in chloroform/heptane solutions. D_o = 1.28(5) gcm^{-3} and D_c = 1.253 gcm^{-3}. The crystal used for intensity data collection had dimensions of 0.7 x 0.7 x 0.8 mm^3.

Data Collection

Intensity data were collected on a Nicolet R3m/E four circle diffractometer using the omega scan technique. Three standard reflections were measured periodically throughout the course of the data collection to monitor crystal alignment and/or deterioration. There was no decrease in the standards over the course of the data collection, with a maximum variation from the average of less than 3%. A total of 3462 reflections were collected of which 2925 were unique and 1145 were considered observed at the $6\sigma_F$ level. Lattice parameters were obtained from least squares fit to 25 reflections for which $22° < 2\Theta < 28°$. Space group designation and other details of the data collection, structure solution and refinement are included in Table 43.

Data Reduction, Structure Solution, and Refinement

The data were reduced in the usual manner with appropriate Lorentz and polarization corrections. Scattering factors for S, Cl, N, C, H and anomalous scattering terms for S, Cl, N, and C were taken from the International Tables for X-ray Crystallography;[24] all atoms were assumed to be in the zero ionization state. No correction for absorption was made.

Table 43. Experimental Data for Mixed TMB/TCB Thiourea Adduct

Formula		$C_9H_{12}\cdot C_6H_3Cl_3\cdot 9(SCN_2H_4)$
Cell Dimensions	a	9.886(7)
	b	15.245(8)
	c	12.313(6)
	β	112.48(4)
Space Group		$P2_1/a$
Cell Volume		1716.27(206)
D_m		1.28(5) gcm^{-3}
D_C		1.253 gcm^{-3}
Crystal Dimensions		0.7 x 0.7 x 0.8 mm^3
$\sin\Theta / \lambda_{max}$		0.595 $Å^{-1}$
Range	h	0 to 12
	k	0 to 19
	l	0 to ±15
Total Reflections		3462
Unique Reflections		2925 R_{merg} = 0.0046
Observed Reflections		1145 6 σ_F cutoff
Number of parameters refined		135
$R = \frac{\Sigma(\lvert\lvert F_o\rvert-\lvert F_c\rvert\rvert)}{\Sigma\lvert F_o\rvert} =$		0.086
$R_w = \frac{\Sigma(\lvert\lvert F_o\rvert-\lvert F_c\rvert\rvert)w^{1/2}}{\Sigma\lvert F_o\rvert w^{1/2}} =$		0.096
$S = \frac{\Sigma(\lvert\lvert F_o\rvert-\lvert F_c\rvert\rvert)w^{1/2}}{(m-n)^{1/2}} =$		1.613
$w = (\sigma_F^2 + gF^2)^{-1}$	where g =	0.00407

The initial model for the thiourea was obtained by using the thiourea positions from the isostructural trichlorobenzene adduct. Attempts to refine a model based on peaks located in the difference map failed to converge or make chemical sense. A rigid group model based on the trichlorobenzene refinement but with both chlorine and methyl groups at the 1,2 and 4 positions on the benzene ring. The model was fit to the 6 highest peaks in the difference map in the channel in 4 orientations, as with the trichlorobenzene and trimethylbenzene refinements. These groups were refined with a common isotropic group thermal for all of the atoms. Computational work was done utilizing the Nicolet program package[57] and programs written locally. The S, C, and N atoms of the thiourea lattice structure were refined with anisotropic thermal parameters by full matrix least squares minimizing $\Sigma w(|F_o|-|F_c|)^2$ with all parameters refined in each full matrix block. The weighting scheme used in the latter stages of refinement was $w = (\sigma_F^2 + gF^2)^{-1}$, where g was refined and converged to a value of 0.00407. A final difference Fourier electron density map showed maximum peak heights $\approx$0.50 e/Å^3 in the vicinity of the adducted molecule in the channel. The maximum shift over error value was less than 0.2 at convergence. No corrections for secondary extinction were made or refined. The 0 2 0 and -1 1 1

reflections exhibited extinction and were removed form the data set.

Disorder Model

Figure 33 illustrates the structure of the mixed 1,2,4-trichlorobenzene/1,2,4-trimethylbenzene adduct. The final model for the organic guest moiety involved six partially occupied adduct sites. All atoms of the 1,2,4 trisubstituted benzene were constrained in an idealized rigid group, with aromatic carbon - carbon bond distances of 1.350Å, carbon - chlorine bond distances of 1.7Å, carbon - methyl carbon bond distances of 1.540Å, and 120° angles. A single group thermal (U_g) was refined with the thermal parameters for the groups at the 1,2 and 4 positions of $1.2(U_g)$. Occupancies of the 1,2,4 trisubstituted benzene group atoms were set at 0.16667. Figure 34 shows the four independent molecule separated in space for visual clarity.

Results and Discussion

Derived Parameters

Tables 44 through 47 contain derived parameters for the 1,2,4 trimethylbenzene thiourea adduct. The bond lengths and angles for the thiourea molecule compare well with those previously observed for pure crystalline thiourea[14,36] and with the rhombohedral thiourea adducts.

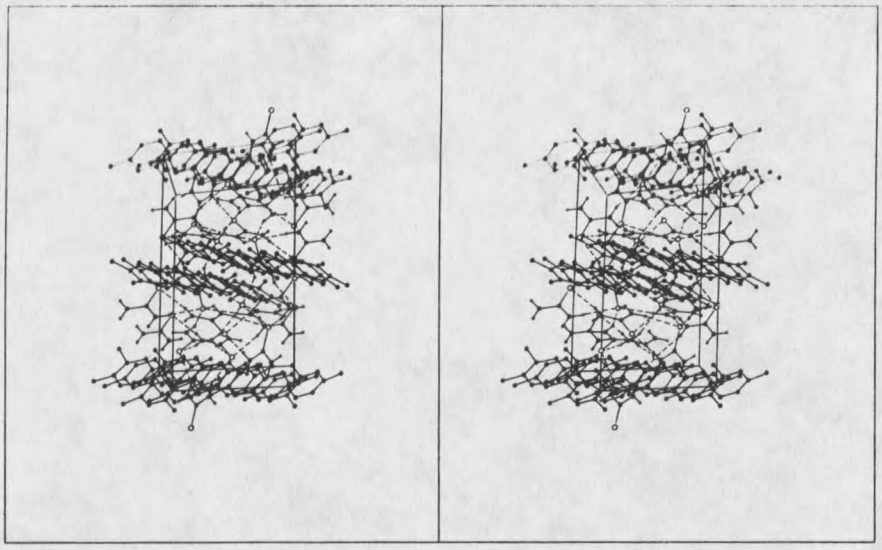


Figure 33. Mixed TMB/TCB thiourea adduct packing diagram view along a showing the hydrogen bonding of the thiourea host lattice and the disorder of the guest molecule.

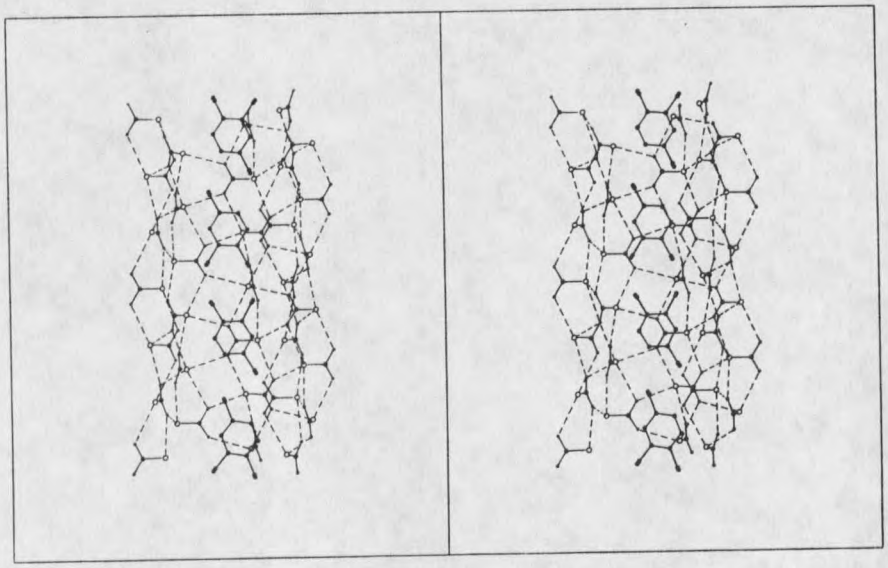


Figure 34. Cutaway view of the trisubstituted aromatic in the host lattice. Both methyl carbons and chlorines are shown at the 1,2 and 4 positions of each model. View is normal to the channel, with 5 binding sites shown.

Table 44. Atomic Coordinates ($x10^4$) and Isotropic Thermal Parameters ($Å^2x10^3$) for Mixed TMB/TCB Thiourea Adduct

	x	y	z	U
S(1)	-54(3)	6386(2)	1395(2)	72(1)*
C(1)	924(11)	7087(6)	908(8)	75(3)*
N(11)	334(9)	7476(6)	-119(7)	92(3)*
N(12)	2336(8)	7239(6)	1563(7)	94(3)*
S(2)	3991(3)	6492(2)	4385(2)	79(1)*
C(2)	2802(9)	6903(6)	4969(8)	70(3)*
N(21)	3275(9)	7171(6)	6053(7)	93(3)*
N(22)	1410(9)	6942(6)	4318(7)	91(3)*
S(3)	3157(3)	3011(2)	2046(2)	74(1)*
C(3)	2725(10)	4070(6)	2228(7)	70(3)*
N(31)	3327(9)	4468(6)	3254(7)	95(3)*
N(32)	1802(9)	4529(6)	1369(7)	92(3)*
Cc(1)	4498(26)	10612(16)	3479(20)	167(3)
Cl(1)	4788	10539	3577	167(3)
Cc(2)	2549	9297	3868	167(3)
Cl(2)	2524	9336	4979	167(3)
Cc(3)	-930	9605	-365	167(3)
CI(3)	-1233	9679	-461	167(3)
C(11)	3127	10287	2451	92(3)
C(12)	2089	9790	2690	92(3)
C(13)	771	9572	1781	92(3)
C(14)	410	9950	674	92(3)
C(15)	1414	10488	453	92(3)
C(16)	2776	10652	1339	92(3)
Cc(4)	-7225(20)	9299(14)	-5969(18)	167(3)
Cl(4)	-7520	9342	-6031	167(3)
Cc(5)	-5635	10536	-6825	167(3)
Cl(5)	-5802	10677	-6951	167(3)
Cc(6)	-1656	10719	-2763	167(3)
Cl(6)	-1353	10683	-2681	167(3)
C(21)	-5806	9713	-5095	92(3)
C(22)	-5034	10302	-5509	92(3)
C(23)	-3588	10513	-4810	92(3)
C(24)	-2985	10229	-3645	92(3)
C(25)	-3768	9655	-3224	92(3)
C(26)	-5136	9349	-3977	92(3)
Cc(7)	-1772(25)	-10518(16)	-915(19)	167(3)
Cc(8)	-100	-9165	-1568	167(3)
Cl(7)	-2063	-10465	-1001	167(3)
Cl(8)	-96	-9211	-1785	167(3)
Cc(9)	3788	-9249	2543	167(3)
Cl(9)	4080	-9301	2629	167(3)

Table 44. (cont.)

	x	y	z	U
C(31)	-373	-10125	14	92(3)
C(32)	535	-9604	-350	92(3)
C(33)	1876	-9317	469	92(3)
C(34)	2392	-9645	1613	92(3)
C(35)	1487	-10168	1976	92(3)
C(36)	145	-10455	1157	92(3)
Cc(A)	9120(25)	-9485(16)	8285(19)	167(3)
Cl(A)	9413	-9537	8364	167(3)
Cc(B)	7243	-10679	8894	167(3)
Cl(B)	7386	-10826	9023	167(3)
Cc(C)	3680	-10716	4662	167(3)
Cl(C)	3382	-10670	4558	167(3)
C(41)	7740	-9853	7302	92(3)
C(42)	6829	-10420	7598	92(3)
C(43)	5412	-10583	6792	92(3)
C(44)	4978	-10274	5642	92(3)
C(45)	5902	-9723	5338	92(3)
C(46)	7239	-9464	6192	92(3)
H(11a)	913	7860	-386	111
H(11b)	-677	7376	-603	111
H(12a)	2896	7625	1280	110
H(12b)	2789	6961	2316	110
H(21a)	2599	7398	6373	107
H(21b)	4301	7143	6534	107
H(22a)	735	7168	4638	103
H(22b)	1059	6744	3519	103
H(31a)	3080	5066	3340	115
H(31b)	4012	4159	3915	115
H(32a)	1592	5125	1500	107
H(32b)	1335	4270	605	107

* Equivalent isotropic U defined as one third of the trace of the orthogonalised U_{ij} tensor.

Table 45. Bond Lengths (Å)

S(1)-C(1)	1.697(12)	C(1)-N(11)	1.315(12)
C(1)-N(12)	1.332(12)	S(2)-C(2)	1.714(12)
C(2)-N(21)	1.302(12)	C(2)-N(22)	1.302(11)
S(3)-C(3)	1.706(10)	C(3)-N(31)	1.320(11)
C(3)-N(32)	1.305(11)		

Table 46. Bond Angles (°)

S(1)-C(1)-N(11)	121.4(8)	S(1)-C(1)-N(12)	121.1(7)
N(11)-C(1)-N(12)	117.5(10)	S(2)-C(2)-N(21)	120.7(7)
S(2)-C(2)-N(22)	119.5(8)	N(21)-C(2)-N(22)	119.8(10)
S(3)-C(3)-N(31)	121.1(6)	S(3)-C(3)-N(32)	122.2(7)
N(31)-C(3)-N(32)	116.7(9)		

Table 47. Anisotropic Thermal Parameters ($Å^2 x 10^3$)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S(1)	63(1)	84(2)	63(1)	10(1)	18(1)	-1(1)
C(1)	87(4)	75(4)	71(4)	-5(4)	39(3)	3(4)
N(11)	90(4)	120(4)	71(3)	25(3)	36(3)	-11(4)
N(12)	59(3)	126(4)	90(4)	16(4)	18(3)	-16(4)
S(2)	64(1)	102(2)	64(1)	-15(1)	19(1)	2(1)
C(2)	56(4)	73(4)	72(4)	-1(3)	14(3)	0(3)
N(21)	74(4)	133(4)	70(3)	-27(3)	23(3)	9(4)
N(22)	75(4)	122(4)	74(3)	-7(3)	27(3)	7(4)
S(3)	81(2)	79(2)	57(1)	-1(1)	20(1)	11(1)
C(3)	62(4)	83(4)	60(4)	-20(3)	17(3)	-9(3)
N(31)	101(4)	92(4)	73(4)	-11(3)	10(3)	9(4)
N(32)	91(4)	85(4)	76(4)	-6(3)	3(3)	9(3)

The anisotropic temperature factor exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$

Nature of the Bonding between Thiourea and the Guest Molecule

As shown in Figure 34, the bonding apparently involves interactions between the 1,2,4 trimethylbenzene and the three coplanar sulfur atoms protruding into the channel. Due to the several different orientations that are available to the aromatic, this gives the effect of a dimer of dimers type disorder model which stretches four trisubstituted aromatic molecules over six binding sites in the crystal. This effectively gives an occupancy of 2/3

for the trisubstituted aromatic, as in the other aromatic adducts. The principle interactions appear to be a compromise between those seen in the trimethylbenzene adduct, where the sulfur interacts with the methyl group, and those seen in the trichlorobenzene adduct, where the sulfur interacts with the carbon attached to chlorine. As resolution of the disorder is necessarily incomplete, this averaging is expected, thereby not giving a great deal of added insight into the nature of the interactions between the host and the guest.

CHAPTER 10

THERMODYNAMICS OF HOST/GUEST ADDUCTS

An estimation of the magnitude of the forces that stabilize the host/guest adducts of thiourea is necessary to understanding the types of interactions to expect in the structural analysis of the adducts. Heats of formation and decomposition can give an estimate of the order of magnitude of the forces, and also give an indication of the stability of these adducts.

The thiourea adducts will form without the presence of a solvent for the thiourea if the guest is liquid, indicating that the transformation is a reversible process. This is evident by the substantial volume increase and change in crystal morphology seen when pure crystalline thiourea is placed in contact with either cyclohexane or carbon tetrachloride. This leads to the chemical expression:

$$\text{COMPLEX} \longleftrightarrow \text{GUEST} + \text{Thiourea}$$

where the equilibrium is fast in solution and slower in the solid state. The enthalpy of dissociation is accessible through the vapor pressure of the guest, and is the enthalpy of dissociation of the guest and the reorganization of the thiourea to the orthorhombic form.

Experimental

Adduct Preparation

Several grams of both the carbon tetrachloride and cyclohexane adducts were formed by precipitation of a saturated thiourea solution with the appropriate guest. The white flocculent precipitate was filtered, and then washed with the appropriate guest to remove any excess mother liquor. These samples were then sealed in bottles until needed for the vapor pressure measurements.

Vapor Pressure Determination

Figure 35 diagrams the system used for the vapor pressure measurements. The sample was placed in a round bottomed flask and attached to the manometer and vacuum system. Then the system was evacuated to about 5 torr, and checked for leaks. The sample was immersed in a constant temperature bath, and the temperature recorded after a suitable period of time for equilibration. The sample was then exposed briefly to the vacuum, and the manometer monitored until a stable reading was achieved. This process was repeated until a series of evacuations gave consistent readings on the manometer. The vapor pressure and temperature were then recorded for later analysis.

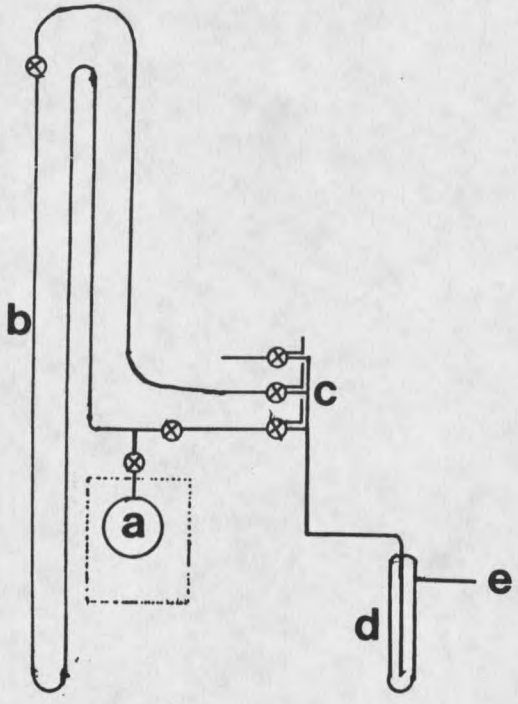


Figure 35. Schematic diagram of vapor pressure measurement apparatus. Details (a) round bottom flask, (b) manometer, (c) manifold, (d) trap, (e) to vacuum.

Data Analysis

The van't Hoff isochore is appropriate for the determination of the enthalpy of dissociation from the pressure and temperature data on these adducts. The data for each adduct was entered into a computer work sheet[16] for calculations, and the plot of the ln(P) v.s. 1/T results with a slope equal to the enthalpy divided by the gas constant. Figures 36 and 37 are the plots for the carbon tetrachloride and cyclohexane adducts.

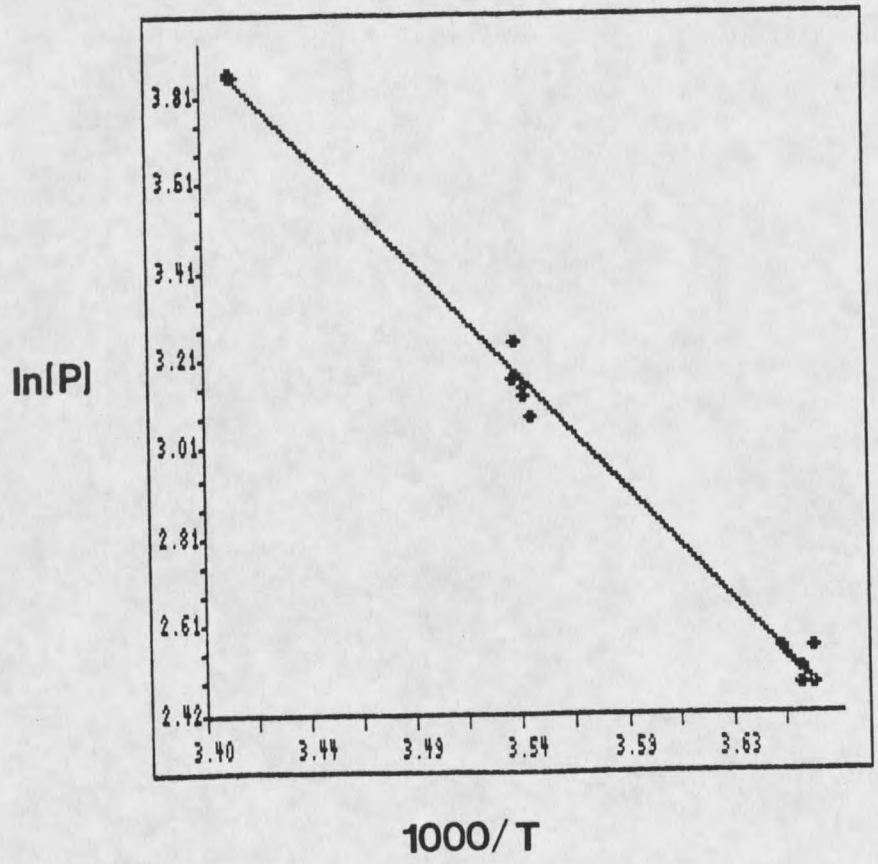


Figure 36. Plot of ln(P) v.s. 1/T for the cyclohexane adduct. The slope of the least squares line shown in the figure is -5.3158.

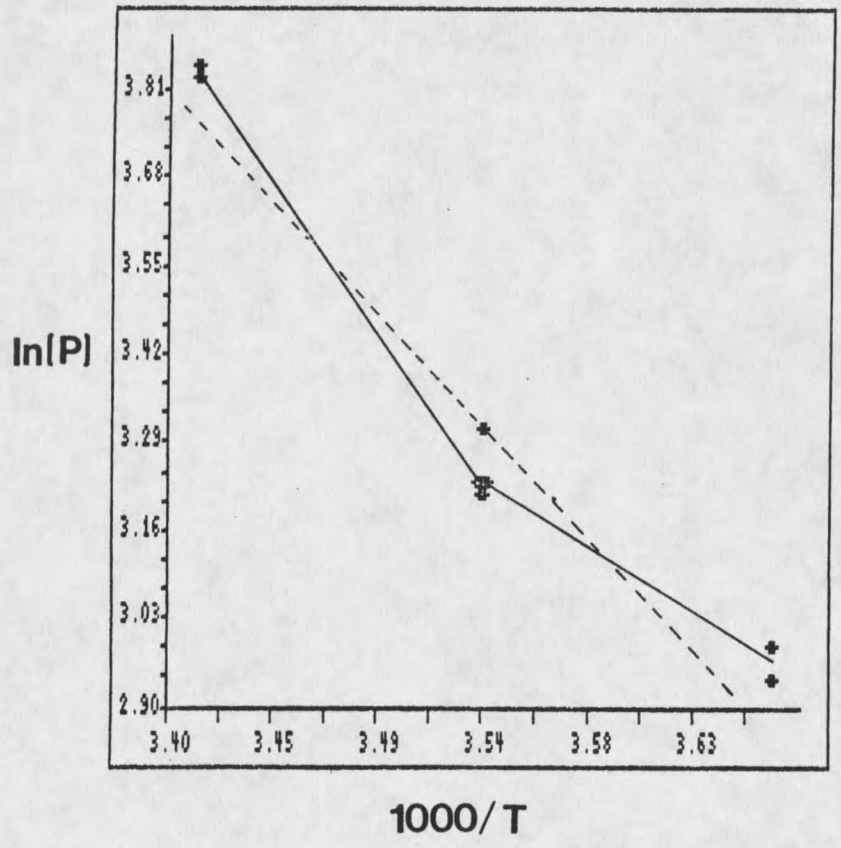


Figure 37. Plot of ln(P) v.s. 1/T for the carbon tetrachloride adduct. The dashed line is the least squares line for all of the data, and has a slope of -3.7326. The solid line on the left is the least squares line for the temperature range 9.5° to 19.8°, and has a slope of -4.8116. The solid line on the right is the least squares line for the temperature range 0.0° to 9.8°, and has a slope of -2.1901.

Results and Discussion

Enthalpies of dissociation were obtained for both the cyclohexane and carbon tetrachloride adducts which were comparable to those found in the literature.[19,45] These values are tabulated in Table 48, and compared to those previously reported. These enthalpies, as measured, include both the energy of binding the guest in the lattice, and the reorganization of the thiourea lattice to the orthorhombic form seen for pure thiourea at room temperature. Calculations assuming a 10-12 generalized hydrogen bond potential for the thiourea indicated that the hydrogen bonding energies were close to the same for both the rhombohedral host lattice and the orthorhombic thiourea, with the orthorhombic lattice slightly more stable.

As the method of vapor pressure measurement utilized was less accurate than that used by previous determinations, the differences between these values and the previously reported values is not significant. Some refinements to improve the quality and reproducibility of the data include isolation of the sample from the manometer and better temperature regulation of the apparatus. The method is not applicable to most of the adducts due to the small vapor pressures of the pure guest make determination of the vapor pressure of the adduct extremely difficult and

beyond the accuracy of the equipment used in this determination.

Table 48. Enthalpies of decomposition for selected thiourea adducts in Kj/mole.

Guest	Literature value[19,45]	This work
Cyclohexane	45.19	44.2
Carbon Tetrachloride	41.42	40.0[a]
		18.2[b]
		31.0[c]

[a] Value obtained for temperature range of 9.5° to 19.8°.
[b] Value obtained for temperature range of 0.0° to 9.8°.
[c] Value obtained for all data.

CHAPTER 11

CONCLUSION

Each of the adducts studied in this research have exhibited disorder in the guest model. This can be attributed to the very weak interactions that stabilize the guest molecule in the binding site and the high symmetry of the host lattice and binding site. The interactions involved are those typical of molecular crystals, being principally dispersion and dipole-induced dipole types of interactions with a r^{-6} distance dependence. The large dipole of thiourea makes these contributions sufficient to stabilize the adduct, but does not localize the guest completely. As the binding site appears to have two fold symmetry normal to the channel in all of the adducts, this symmetry is dominant in the guest disordering even when it is not present in the lattice symmetry.

Disorder Classification

The thiourea adducts display several types of disorder. As only three types of disorder have been previously defined,[20] these definitions of the various types of disorder are proposed for the classification of the thiourea adduct guest disorder. Types 1, 2, and 3

include the previous definitions of disorder by Westrum and McCullough.[20] Figure 38 illustrates each of these types of disorder.

1) Symmetry disorder: This is disorder introduced when the guest molecule does not conform to the site symmetry that it occupies. This disorder includes the internal rotational disorder seen in plastic crystals.

2) Positional disorder: This is the disorder of a molecule by translation of the center of mass of the molecule in the lattice.

3) Conformational disorder: This is disorder between two conformations of the same molecule.

4) Orientation disorder: This is disorder due to multiple possible orientations of the molecule in the same site. This is distinguished from type 1 disorder in that the disorder is not implicit in the crystallographic symmetry of the site. This type of disorder is a subset of positional disorder in mixed molecular crystals.

5) Site disorder: This is disorder due to a molecule occupying one site lapping over into a second site, blocking that site for other molecules. This results in lowered site occupancy and disorder. This type of disorder is usually accompanied by orientation disorder.

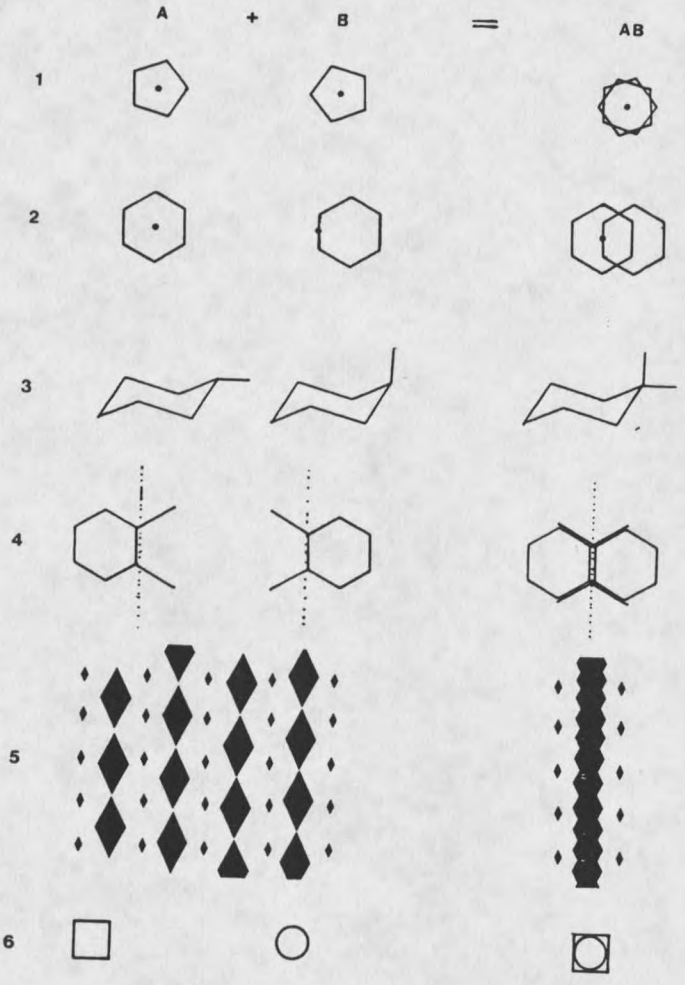


Figure 38. Illustration of the six types of disorder. Each of the components A and B are shown, as well as the resultant AB. The resultant model is the superposition of the two components. 1) Symmetry disorder. The dot represents a symmetry operator like a 2 fold axis or center. 3) Positional disorder. The dot represents a fixed point in the lattice. 2) Conformational disorder. The two conformers of monosubstituted cyclohexane add to give the image of a disubstituted cyclohexane. 4) Orientation disorder. The dotted line represents a site which can be approached from either direction. 5) Site disorder. The pattern on the left represents the actual crystal, with the small diamonds representing the relative positions of the sites. The larger diamonds are have a greater length than the distance between sites, giving a composite pattern like that seen on the right. 6) Substitutional disorder. The circle and square represent two distinct but similar atoms or molecules that can occupy the same crystallographic site.

6) Substitutional Disorder: This is disorder based on the substitution of one element or group for another element or group. This is illustrated by the partial replacement of sodium with potassium in a salt system, and by the mixed adduct, where the two trisubstituted aromatics occupy the same site.

The simplest disorder seen in the thiourea adducts is found in the carbon tetrachloride adduct. In this adduct, only symmetry disorder is seen as the carbon tetrachloride breaks the three fold symmetry of the site. This allows for a successful model of the disorder that is simple yet complete. The similar model used in the adamantane complex also includes a small translational component as well as a second major orientation of the molecule relative to the site.

The cyclohexane and bicyclo[2.2.2]octane adducts exhibit symmetry disorder as well as conformational disorder, although the conformational disorder is not immediately apparent in the bicyclo[2.2.2]octane. For steric reasons, the bicyclo[2.2.2]octane will exist in two slightly twisted conformations, which average to the fully eclipsed conformation used in the refinement model. The cyclohexane adduct was modeled equally well with either the boat or chair conformation, so either conformation could be present in the crystal.

The cis-p-menthane, 1,2,4-trimethylbenzene, 1,2,4-trichlorobenzene and the mixed TCB/TMB adducts all exhibit site disorder due to the size of each of these molecules. Although these adducts are reasonably stable, the interactions that stabilize these adducts is less than that seen in the stoichiometric adducts above. The superlattice phenomena seen and modeled in the cis-p-menthane adduct, and the diffuse scattering seen in the trichlorobenzene adduct are both direct results of the site disorder and orientation disorder seen in these structures.

Space Group Differences in the Thiourea Adducts

Two major groups of adducts are apparent in the structures that have been investigated. The aromatic adducts are monoclinic, with the channel along the a c diagonal of the primitive cell. The other adducts are rhombohedral, with the channel along the c axis. At first, these adducts appear to be quite different in packing and molecular interactions, but on further examination it is found that the thiourea host structure is almost the same for both types of adducts. The greatest difference in the adducts is the removal of the three fold symmetry along the channel in the monoclinic adducts, which allows for the distortion of the channel cross section from circular in the rhombohedral adducts to elliptical in the monoclinic

adducts. The majority of other symmetry elements are often present in both types of adducts, though they are not always required by the space group symmetry. The most prominent of these conserved symmetry operations is the apparent two fold axis coincident with the sulfur-carbon bond of the thiourea. This operation is only required in the adamatane adduct, but is seen in the disorder of all of the adducts studied. The glide planes seen in the adamatane adduct does not appear to be conserved when going to the lower symmetry adducts, but may be related to the glide plane in the monoclinic adducts.

Host/Guest Interactions

The major interactions between the thiourea host and the guest molecules are short range coulombic interactions and dispersion forces. The stabilization of the thiourea lattice by the guest is significant, yet small enough that the guest is not locked into a single position in each channel. The localization of the guest molecule at the binding site of three thioureas circling the channel indicates that there is a specific set of interactions that dominate for each guest molecule. The most prominent of these is the interaction of a slight positive charge on a localized center with the strong negative charge of the sulfur on thiourea. This characteristic can be postulated in each of adducts, and may be a significant contribution

to the stability of the adduct. The "supported hydrogen bond" proposed by Fetterly[19] does not encompass the variety of guest molecules and the interactions that can be discerned in these structures.

Predictions for Inclusion in Thiourea Adducts

Several high symmetry guests are immediately apparent for the formation of thiourea adducts. Hexamethylethane and hexachloroethane should both form adducts similar to the carbon tetrachloride and bicyclo[2.2.2]octane adducts. These molecules both show 32 symmetry, which is the site symmetry of the thiourea binding site as seen in the adamatane adduct. These molecules are also about 5Å in length, thereby avoiding the disordering seen in the bicyclo[2.2.2]octane adduct due to the excessive length of the molecule. Another bicyclic molecule that will probably adduct is bicyclo[1.1.1]pentane. These candidates for adduct formation are suggested for further structural studies. Other types of molecules that may adduct with thiourea include some of the silanes and boranes, especially those with high symmetry and cross sectional dimensions comparable with adamantane and bicyclo[2.2.2]octane.

Suggestions for Additional Research

Solid state NMR spectroscopy could help to resolve some of the disorder seen in the thiourea adducts, and either validate or disprove the disorder models advanced in this work. Additional structural studies on some of the simple, high symmetry molecules that are predicted to form adducts may add to the understanding of the structural features of these adducts. Lattice energy calculations with extended potential sets may give some insight into the interactions that dominate the selection between isomers and related guest molecules. Each of these major areas includes a wealth of potential insight into the dynamics of adduct formation and stability, and each is worthy of further research.

REFERENCES CITED

REFERENCES CITED

1 Allcock, H. R., Stein, M. T., and Bissell, E. C.; Journal of the American Chemical Society, 96:15, 4795-4800 (1974)

2 Allcock, H. R., and Siegel, L. A.; Journal of the American Chemical Society, 86, 5140-5144 (1964)

3 Angla, B.; Compt. rend., 224, 402-404 (1947)

4 Angla, B.; Compt. rend., 224, 1166-1167 (1947)

5 Angla, B.; Ann. de Chim., 12, 639-698 (1949)

6 Barlow, G. B., and Clamp, A. C.; Journal of the Chemical Society, 393-395 (1961)

7 Barrer, R. M.; Journal of the Chemical Society, 127-143 (1948)

8 Bear, R.; Journal of the American Chemical Society, 66, 2122 (1944)

9 Bengen, F., and Schlenk, W., Jr.; Experientia, 5, 200 (1949)

10 Bengen, M. F.; Angew. Chem., 63(9), 207-208 (1951)

11 Bondi, A.; Journal of Physical Chemistry, 68, 441-451 (1964)

12 Clausen, W. F.; Journal of Chemical Physics, 19, 259 (1951)

13 Dewar, M. J. S., and Theil, W.; Journal of the American Chemical Society, 99, 4899-4907 (1977)

14 Elcombe, M. M., and Taylor, J. C.; Acta Cryst., A24, 410-420 (1968)

15 Evans, D. F., and Richards, R. E.; Nature, 170, 246 (1952)

16 Fait, J. F.; WSHEET, A Worksheet for Chemists, Version 3.2, Department of Chemistry, Montana State University, Bozeman, MT (1987)

17 Fetterly, L. C.; United States Patent Office, 2520715 (1950)

18 Fetterly, L. C.; United States Patent Office, 2569984, 2569986 (1951)

19 Fetterly, L. C.; Non-stoichiometric Compounds, L. Mandelcorn, ed; Acedemic Press, New York NY, 491-567 (1964)

20 Fox, D., Labes, M. M., and Weissberger, A., ed.; Physics and Chemistry of the Organic Solid State, vol. 1, Interscience, New York

21 Fuller, E. J.; United States Patent Office, 3684701 (1972)

22 Hart, H., Lin, L-T. W., and Ward, D. W.; Journal of the Chemical Society, Chem. Commun., 1985, 293-4 (1985)

23 Hartley, H., and Thomas, N. G.; Journal of the Chemical Society, 1013- 1033 (1906)

24 International Tables for X-ray Crystallography, Vol 4., Kynoch Press, Birmingham, (1974)

25 Hermann, C., and Lenne, H. U.; Naturwissenschaften, 10, 234-235 (1952)

26 Kitaigorodsky, A. I.; Chem. Soc. Rev., 7(1), 133-163

27 Lawton, D., and Powell, H. M.; Journal of the Chemical Society, 2339-2358 (1958)

28 Lenne, H. U.; Acta Cryst., 7, 1-15 (1954)

29 McCandless, F. P.; Ind. Eng. Chem. Prod. Res. Develop., 10(4), 406-409 (1971)

30 McCandless, F. P.; Ind. Eng. Chem. Prod. Res. Dev., 19, 612-616 (1980)

31 McCandless, F. P.; Ind. Eng. Chem. Prod. Res. Dev., 21, 483-488 (1982)

32 McCandless, F. P., Cline, R. E., and Cloninger, M. O.; Ind. Eng. Chem. Prod. Res. Dev., 13, 214-216 (1974)

33 McLaughlin, R. L.; The Chemistry of Petroleum Hydrocarbons, Volume 1, B. T. Brooks et al. ed.; Reinhold Publishing Co., New York NY 241-274 (1954)

34 McLaughlin, R. L., and McClenahan, W. S.; Journal of the American Chemical Society., 74, 5804-5805 (1952)

35 Mikus, F. F., Hixon, R. M., and Rundle, R. E.; Journal of the American Chemical Society, 63, 1115-1123 (1946)

36 Mullen, D., Heger, G., and Treutmann, W.; Z. Kristallogr., 148, 95-100 (1978)

37 Newman, A. D. C., and Powell, H. M.; Journal of the Chemical Society, 3747-3451 (1952)

38 Palin, D. E., and Powell, H. E.; Nature, 156, 334-335 (1945)

39 Palin, D. E., and Powell, H. M.; Journal of the Chemical Society, 571-574 (1948)

40 Palin, D. E., and Powell, H. M.; Journal of the Chemical Society, 815-821 (1948)

41 Pauling, L., and Marsh, R. E.; Proc. Nat. Acad. Science, 38, 112 (1952)

42 Powell, H. M.; Journal of the Chemical Society, 298-300 (1950)

43 Powell, H. M.; Journal of the Chemical Society, 468-469 (1950)

44 Powell, H. M.; Nature, 170, 155 (1952)

45 Redlich, O., Gable, C. M., Beason, L. R., and Millar, R. W.; Journal of the American Chemical Society., 72, 4161-4162 (1950)

46 Redlich, O., Gable, C. M., Dunlop, A. K., and Millar, R. W.; Journal of the American Chemical Society., 72, 4153-4160 (1950)

47 Robertson, B. E., Rutherford, J. S., and Gopal, R.; personal communication

48 Rundle, R., and Edwards, F.; Journal of the American Chemical Society, 65, 2200 (1943)

49 Rundle, R., Foster, J., and Baldwin, R.; Journal of the American Chemical Society, 66, 2116 (1944)

50 Rundle, R., and French, D.; Journal of the American Chemical Society, 65, 1707 (1943)

51 Rundle, R., and French, D.; Journal of the American Chemical Society, 65, 558 (1943)

52 Schiessler, R. W., and Flitter, D.; Journal of the American Chemical Society., 74, 1720-1723 (1952)

53 Schlenk, H., and Holman, R. T.; Journal of the American Chemical Society., 72, 5001-5004 (1950)

54 Schlenk, H., and Sand, D. M.; Journal of the American Chemical Society., 83, 2312-2320 (1961?)

55 Schlenk, W., Jr.; Annal. d. Chem., 565, 204-240 (1949)

56 Schlenk, W., Jr.; Annal. d. Chem., 573, 142-162 (1951)

57 Sheldrick, G. M.; SHELXTL, An Integrated System for Solving, Refining, and Displaying Crystal Structures from Diffraction Data., Nicolet XRD Corporation, Madison, WI, Revisions 4.0 and 5.1 (1983, 1985)

58 Smith, A. E.; Acta Cryst., 5, 224-235 (1952)

59 Spinti, M. J.; Masters Thesis in Chemical Engineering, Montana State University, Bozeman, MT (1986)

60 Stackelberg, M., and Muller, H. R.; Z. Electrochem., 58, 25-40 (1954)

61 Stewart, J. M., and Hall, S. R., editors; The XTAL System of Crystallographic Programs, University of Maryland, Computer Science Center, College Park, MD (1983)

62 Stezowski, J. J.; Transactions of the American Crystallographic Association, 20, 73-82 (1984)

63 Swern, D.; Industrial and Engineering Chemistry, 47(2), 216-221 (1955)

64 Truter, E. V.; Journal of the Chemical Society, 2416-2419 (1951)

65 Welling, B. L.; Masters Thesis in Chemical Engineering, Montana State University, Bozeman, MT (1982)

66 Wick, T. A.; Masters Thesis in Chemical Engineering, Montana State University, Bozeman, MT (1986)

67 Williams, D. E., and Starr, T. L.; Computers and Chemistry, 1, 173-177 (1977)

68 Zimmerschied, W. J., Dinerstein, R. A., Weitkamp, A. W., and Marschner, R. F.; Journal of the American Chemical Society., 71, 2947 (1949)

69 Zimmerschied, W. J., Dinerstein, R. A., Weitkamp, A. W., and Marschner, R. F.; Industrial and Engineering Chemistry, 42(7), 1300-1306 (1950)

APPENDICES

APPENDIX A

TABLE 49

Table 49. Carbon Tetrachloride Thiourea Host/Guest Adduct F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
-1	2	0	234	204	6	-10	17	0	607	618	18
0	3	0	3292	3256	43	-7	17	0	718	615	-184
-2	4	0	806	806	8	-4	17	0	238	253	27
-4	5	0	1414	1418	10	-12	18	0	73	47	-79
-1	5	0	1436	1434	17	-9	18	0	198	149	34
-3	6	0	565	586	12	-6	18	0	131	53	-53
0	6	0	96	84	-34	-1	1	1	80	35	10
-5	7	0	130	161	-34	-3	2	1	429	441	7
-2	7	0	116	130	-29	0	2	1	64	14	-20
-7	8	0	102	58	-43	-5	3	1	2786	2767	9
-4	8	0	690	648	11	-2	3	1	428	444	7
-1	8	0	89	93	-42	1	3	1	777	800	12
-6	9	0	73	6	-58	-7	4	1	953	971	10
-3	9	0	42	16	-85	-4	4	1	67	35	-44
0	9	0	885	837	23	-1	4	1	780	774	8
-8	10	0	127	68	-41	2	4	1	791	786	28
-5	10	0	423	450	15	-9	5	1	171	135	23
-2	10	0	156	107	34	-6	5	1	1429	1410	10
-10	11	0	684	665	15	-3	5	1	2780	2736	31
-7	11	0	841	788	79	0	5	1	88	40	-31
-4	11	0	795	786	12	3	5	1	926	930	18
-1	11	0	696	660	24	-11	6	1	106	158	-59
-9	12	0	103	149	-49	-8	6	1	2009	1991	12
-6	12	0	578	600	22	-5	6	1	1430	1411	17
-3	12	0	154	152	-45	-2	6	1	790	787	10
0	12	0	95	142	-55	1	6	1	942	948	10
-11	13	0	142	62	-55	4	6	1	158	200	-40
-8	13	0	262	271	23	-13	7	1	338	322	25
-5	13	0	263	256	29	-10	7	1	180	140	-52
-2	13	0	82	74	-72	-7	7	1	47	6	-62
-13	14	0	148	135	-50	-4	7	1	957	981	11
-10	14	0	505	492	18	-1	7	1	951	950	9
-7	14	0	669	628	18	2	7	1	165	166	-45
-4	14	0	533	492	35	5	7	1	412	392	18
-1	14	0	159	126	-44	-15	8	1	319	345	38
-12	15	0	288	258	24	-12	8	1	726	718	15
-9	15	0	461	466	20	-9	8	1	1269	1242	12
-6	15	0	481	480	20	-6	8	1	2009	1992	18
-3	15	0	278	273	25	-3	8	1	925	911	12
0	15	0	168	144	34	0	8	1	70	7	-49
-14	16	0	217	182	31	3	8	1	46	59	-94
-11	16	0	248	249	29	6	8	1	87	16	-60
-8	16	0	234	241	28	-17	9	1	53	57	-107
-5	16	0	244	248	32	-11	9	1	848	865	24
-2	16	0	200	170	31	-8	9	1	1253	1243	18
-13	17	0	256	261	26	-5	9	1	135	122	-30

Table 49. (cont.)
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
-2	9	1	161	148	26	-8	15	1	337	328	25
1	9	1	135	118	-34	-5	15	1	147	172	-38
4	9	1	561	522	17	-2	15	1	477	469	20
7	9	1	116	128	-48	1	15	1	255	274	30
-16	10	1	209	206	-50	-13	16	1	156	146	-48
-13	10	1	176	154	36	-10	16	1	198	192	38
-10	10	1	92	10	-56	-7	16	1	116	118	-66
-7	10	1	189	160	24	-4	16	1	140	122	-38
-4	10	1	157	203	30	-1	16	1	299	279	38
-1	10	1	132	103	-41	-12	17	1	123	89	-47
2	10	1	187	210	38	-9	17	1	71	63	-89
5	10	1	154	151	-44	-6	17	1	116	98	-70
8	10	1	162	146	-46	-11	18	1	106	102	-80
-18	11	1	164	84	-53	-8	18	1	202	171	33
-15	11	1	231	220	30	0	1	2	1572	1594	16
-12	11	1	720	730	16	-2	2	2	1811	2033	-478
-9	11	1	842	872	17	1	2	2	458	454	7
-6	11	1	144	171	-46	-4	3	2	209	219	16
-3	11	1	95	63	-49	-1	3	2	459	486	9
0	11	1	134	18	-45	2	3	2	1054	1058	27
3	11	1	232	252	25	-6	4	2	494	451	11
6	11	1	76	94	-87	-3	4	2	196	232	13
-17	12	1	129	98	-59	0	4	2	1271	1222	31
-14	12	1	462	504	27	3	4	2	1168	1139	21
-11	12	1	720	730	17	-8	5	2	674	665	12
-8	12	1	707	723	15	-5	5	2	59	17	-45
-5	12	1	406	370	22	-2	5	2	1062	1063	10
-2	12	1	187	235	-54	1	5	2	898	887	10
1	12	1	495	522	18	4	5	2	432	418	20
4	12	1	175	127	29	-10	6	2	622	610	14
-16	13	1	107	138	-72	-7	6	2	201	210	19
-13	13	1	105	9	-44	-4	6	2	471	437	21
-10	13	1	165	161	33	-1	6	2	897	870	10
-7	13	1	354	333	32	2	6	2	1019	1026	8
-4	13	1	560	525	23	5	6	2	345	351	22
-1	13	1	521	528	18	-12	7	2	287	322	23
2	13	1	463	486	20	-9	7	2	263	255	26
-15	14	1	86	90	-71	-6	7	2	185	197	19
-12	14	1	462	499	20	-3	7	2	1171	1157	12
-9	14	1	246	260	25	0	7	2	2110	2102	6
-6	14	1	64	24	-81	3	7	2	1486	1486	13
-3	14	1	235	236	50	6	7	2	433	436	24
0	14	1	78	7	-61	-14	8	2	49	59	-99
3	14	1	56	19	-112	-11	8	2	313	303	20
-14	15	1	76	87	-86	-8	8	2	920	885	30
-11	15	1	196	214	39	-5	8	2	677	669	15

Table 49. (cont.)
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-2	8	2	1017	1004	27
1	8	2	94	53	-40
4	8	2	551	599	25
7	8	2	259	272	26
-16	9	2	142	107	-56
-13	9	2	87	102	-70
-10	9	2	218	196	19
-7	9	2	232	227	26
-4	9	2	421	411	20
-1	9	2	76	41	-52
2	9	2	90	14	-61
5	9	2	165	188	34
8	9	2	164	132	-50
-18	10	2	203	219	42
-15	10	2	50	10	-101
-12	10	2	271	259	23
-9	10	2	221	209	23
-6	10	2	608	635	18
-3	10	2	1492	1504	23
0	10	2	1240	1202	38
3	10	2	600	640	19
6	10	2	52	59	-104
-17	11	2	142	143	-52
-14	11	2	191	183	-47
-11	11	2	691	681	28
-8	11	2	317	296	22
-5	11	2	332	343	23
-2	11	2	61	6	-81
1	11	2	141	94	-52
4	11	2	178	156	37
7	11	2	281	248	40
-16	12	2	291	256	26
-13	12	2	278	284	33
-10	12	2	240	235	29
-7	12	2	311	345	32
-4	12	2	577	589	24
-1	12	2	115	108	-46
2	12	2	394	410	21
5	12	2	59	132	-120
-15	13	2	261	247	45
-12	13	2	283	265	43
-9	13	2	125	82	-49
-6	13	2	443	455	19
-3	13	2	615	654	18
0	13	2	357	420	21
3	13	2	150	152	-44
-17	14	2	453	424	28
-14	14	2	451	467	18
-11	14	2	203	172	34
-8	14	2	109	71	-60
-5	14	2	184	219	37
-2	14	2	403	413	21
1	14	2	185	140	-66
-16	15	2	360	370	31
-13	15	2	239	253	29
-10	15	2	87	11	-71
-7	15	2	224	264	38
-4	15	2	193	166	32
-1	15	2	158	151	-47
-15	16	2	352	377	27
-12	16	2	260	245	29
-9	16	2	113	101	-58
-6	16	2	69	64	-84
-3	16	2	172	146	-56
-14	17	2	424	428	42
-11	17	2	166	139	-48
-8	17	2	135	105	-49
-5	17	2	197	149	-44
-10	18	2	228	230	33
-7	18	2	275	246	39
0	0	3	109	52	-40
1	1	3	2045	2098	32
-1	2	3	2037	2086	62
2	2	3	1887	1881	72
-3	3	3	91	14	-32
0	3	3	36	9	-64
3	3	3	598	615	14
-5	4	3	1167	1165	13
-2	4	3	1901	1912	24
1	4	3	324	322	11
4	4	3	91	42	-41
-7	5	3	954	948	11
-4	5	3	1152	1164	17
-1	5	3	319	323	12
2	5	3	284	280	16
5	5	3	515	545	15
-9	6	3	308	303	21
-6	6	3	39	2	-68
-3	6	3	597	605	11
0	6	3	58	5	-54
3	6	3	521	498	31
6	6	3	466	81	-165

Table 49. (cont.)
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-11	7	3	206	161	24
-8	7	3	110	68	-37
-5	7	3	960	961	4
-2	7	3	298	290	18
1	7	3	76	101	-53
4	7	3	404	446	38
7	7	3	113	71	-58
-13	8	3	903	927	22
-10	8	3	404	395	12
-7	8	3	130	59	-34
-4	8	3	51	54	-71
-1	8	3	115	92	-36
2	8	3	364	403	17
5	8	3	582	609	17
8	8	3	564	595	20
-15	9	3	758	708	21
-12	9	3	87	43	-68
-9	9	3	57	3	-69
-6	9	3	307	306	17
-3	9	3	519	507	16
0	9	3	62	6	-67
3	9	3	372	337	24
6	9	3	498	487	20
9	9	3	554	576	33
-17	10	3	54	79	-110
-14	10	3	137	100	-47
-11	10	3	153	128	-34
-8	10	3	392	391	14
-5	10	3	515	549	20
-2	10	3	373	400	15
1	10	3	68	53	-76
4	10	3	50	18	-101
7	10	3	89	89	-69
-16	11	3	445	480	24
-13	11	3	186	180	32
-10	11	3	165	118	32
-7	11	3	192	155	30
-4	11	3	393	418	21
-1	11	3	124	60	-43
2	11	3	277	328	25
5	11	3	232	198	29
-15	12	3	536	482	39
-12	12	3	69	6	-65
-9	12	3	67	46	-81
-6	12	3	161	83	-42
-3	12	3	365	324	20
3	12	3	352	356	23
-17	13	3	140	102	-62
-14	13	3	111	125	-52
-11	13	3	172	181	32
-8	13	3	968	926	166
-5	13	3	565	608	20
-2	13	3	314	330	43
1	13	3	261	258	41
4	13	3	90	58	-75
-16	14	3	112	10	-64
-13	14	3	132	127	-46
-10	14	3	152	86	-45
-7	14	3	86	69	-68
-4	14	3	49	1	-100
-1	14	3	257	254	30
2	14	3	131	82	-54
-15	15	3	74	5	-80
-12	15	3	500	488	22
-9	15	3	757	707	18
-6	15	3	505	488	20
-3	15	3	353	334	22
0	15	3	128	17	-64
-14	16	3	79	15	-85
-11	16	3	463	468	22
-8	16	3	560	586	90
-5	16	3	213	196	35
-2	16	3	233	70	-82
-13	17	3	136	89	-50
-10	17	3	164	69	-64
-7	17	3	122	95	-70
-4	17	3	113	59	-67
-9	18	3	576	585	27
-1	1	4	644	624	14
-3	2	4	451	444	12
0	2	4	1282	1288	20
-5	3	4	289	302	14
-2	3	4	448	454	27
1	3	4	629	646	12
-7	4	4	772	787	13
-4	4	4	492	549	15
-1	4	4	631	677	11
2	4	4	537	527	24
-9	5	4	481	505	15
-6	5	4	570	567	12
-3	5	4	286	313	14
0	5	4	412	413	11

Table 49. (cont.)
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
3	5	4	313	297	17
-11	6	4	310	337	32
-8	6	4	108	13	-49
-5	6	4	559	573	11
-2	6	4	536	529	12
1	6	4	733	763	22
4	6	4	584	596	13
-13	7	4	174	117	30
-10	7	4	1261	1274	23
-7	7	4	1545	1560	17
-4	7	4	759	809	43
-1	7	4	747	753	16
2	7	4	89	79	-54
5	7	4	133	135	-43
-15	8	4	125	37	-49
-12	8	4	150	126	-58
-9	8	4	422	417	17
-6	8	4	96	5	-53
-3	8	4	335	306	23
0	8	4	336	332	20
3	8	4	163	167	34
6	8	4	168	161	-37
-17	9	4	78	10	-84
-14	9	4	313	339	45
-11	9	4	532	495	19
-8	9	4	403	419	16
-5	9	4	507	507	27
-2	9	4	76	48	-65
1	9	4	471	475	-113
4	9	4	50	55	-100
-16	10	4	92	45	-64
-13	10	4	574	603	22
-10	10	4	1835	1880	21
-7	10	4	1245	1269	13
-4	10	4	584	588	15
-1	10	4	428	464	24
2	10	4	224	210	27
5	10	4	200	162	-65
-15	11	4	184	201	-46
-12	11	4	470	445	48
-9	11	4	507	496	18
-6	11	4	331	328	25
-3	11	4	166	179	-38
0	11	4	372	388	17
3	11	4	324	316	24
6	11	4	275	269	44
-17	12	4	88	88	-83
-14	12	4	161	127	-39
-11	12	4	472	454	19
-8	12	4	141	147	-45
-5	12	4	164	128	-38
-2	12	4	254	203	25
1	12	4	246	232	33
4	12	4	293	306	46
-16	13	4	84	59	-82
-13	13	4	321	360	22
-10	13	4	570	597	18
-7	13	4	133	112	-45
-4	13	4	127	63	-41
-1	13	4	266	227	35
2	13	4	278	259	26
-15	14	4	170	211	-40
-12	14	4	123	132	-66
-9	14	4	326	329	21
-6	14	4	133	163	-40
-3	14	4	303	304	24
0	14	4	397	370	26
-14	15	4	164	177	-46
-11	15	4	202	197	30
-8	15	4	79	28	-77
-5	15	4	167	159	-40
-2	15	4	292	263	33
-13	16	4	105	89	-67
-10	16	4	98	21	-62
-7	16	4	126	83	-45
-4	16	4	285	317	33
-12	17	4	152	110	-44
-9	17	4	103	39	-70
-6	17	4	291	270	48
0	1	5	46	10	-44
-2	2	5	45	28	-54
1	2	5	762	788	10
-4	3	5	870	856	14
-1	3	5	770	780	10
2	3	5	500	513	32
-6	4	5	379	406	18
-3	4	5	872	846	10
0	4	5	89	2	-31
3	4	5	216	147	45
-8	5	5	825	839	20
-5	5	5	83	23	-46
-2	5	5	513	539	17

Table 49. (cont.)
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
1	5	5	442	462	14
4	5	5	943	975	22
-10	6	5	434	434	20
-7	6	5	489	470	16
-4	6	5	356	360	14
-1	6	5	440	468	19
2	6	5	955	925	21
5	6	5	533	518	18
-12	7	5	420	443	20
-9	7	5	183	138	-45
-6	7	5	494	469	13
-3	7	5	196	163	33
0	7	5	108	8	-42
3	7	5	48	74	-97
6	7	5	49	54	-98
-14	8	5	116	96	-51
-11	8	5	50	43	-100
-8	8	5	132	30	-33
-5	8	5	836	848	24
-2	8	5	928	931	16
1	8	5	1110	1130	27
4	8	5	783	848	28
7	8	5	123	70	-65
-16	9	5	54	75	-108
-13	9	5	61	24	-85
-10	9	5	149	185	-35
-7	9	5	159	141	24
-4	9	5	952	969	24
-1	9	5	1113	1143	18
2	9	5	810	778	18
5	9	5	217	194	28
8	9	5	71	40	-91
-15	10	5	328	314	24
-12	10	5	174	121	-44
-9	10	5	168	203	36
-6	10	5	418	430	32
-3	10	5	105	78	-46
0	10	5	63	1	-66
3	10	5	149	121	-51
6	10	5	54	25	-109
-17	11	5	163	82	-63
-14	11	5	193	197	-65
-11	11	5	69	37	-63
-8	11	5	49	20	-99
-5	11	5	518	511	17
-2	11	5	806	803	27
1	11	5	657	683	18
4	11	5	132	69	-38
-16	12	5	177	149	-43
-13	12	5	161	169	-40
-10	12	5	142	82	-46
-7	12	5	392	476	21
-4	12	5	790	861	27
-1	12	5	673	687	21
2	12	5	338	327	25
-15	13	5	526	542	26
-12	13	5	178	184	-67
-9	13	5	92	41	-55
-6	13	5	99	32	-63
-3	13	5	134	118	-42
0	13	5	70	4	-73
3	13	5	70	66	-90
-14	14	5	114	8	-53
-11	14	5	205	168	-76
-8	14	5	130	104	-57
-5	14	5	198	192	31
-2	14	5	363	324	25
1	14	5	112	82	-61
-13	15	5	540	544	21
-10	15	5	296	281	28
-7	15	5	143	53	-63
-4	15	5	83	56	-59
-1	15	5	80	82	-85
-12	16	5	183	149	-60
-9	16	5	116	47	-56
-6	16	5	69	38	-88
-3	16	5	98	65	-67
-11	17	5	55	83	-112
-8	17	5	55	39	-110
0	0	6	970	998	13
1	1	6	403	410	10
-1	2	6	410	420	13
2	2	6	1212	1205	19
-3	3	6	1546	1531	19
0	3	6	1620	1639	13
3	3	6	1018	1000	12
-5	4	6	192	188	18
-2	4	6	1228	1217	25
4	4	6	150	135	-41
-7	5	6	272	313	44
-4	5	6	194	190	26
-1	5	6	294	288	22

Table 49. (cont.)
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
2	5	6	321	325	17
5	5	6	145	108	-39
-9	6	6	47	46	-95
-6	6	6	391	377	53
-3	6	6	1024	993	22
0	6	6	498	500	19
3	6	6	131	95	-46
6	6	6	232	240	27
-11	7	6	211	208	29
-8	7	6	379	345	73
-5	7	6	297	346	19
-2	7	6	333	329	17
1	7	6	264	269	22
4	7	6	183	163	-52
7	7	6	615	597	56
-13	8	6	285	283	24
-10	8	6	234	250	45
-7	8	6	410	399	16
-4	8	6	133	120	-40
-1	8	6	253	271	42
2	8	6	300	293	21
5	8	6	238	275	26
8	8	6	323	339	29
-15	9	6	276	318	41
-12	9	6	171	151	-51
-9	9	6	257	214	22
-6	9	6	47	94	-95
-3	9	6	118	120	-46
0	9	6	276	285	20
3	9	6	233	224	44
6	9	6	312	334	26
-14	10	6	466	461	22
-11	10	6	254	248	31
-8	10	6	242	218	41
-5	10	6	165	146	-36
-2	10	6	307	318	25
1	10	6	176	231	34
4	10	6	449	482	22
-16	11	6	264	222	32
-13	11	6	188	163	34
-10	11	6	244	248	30
-7	11	6	241	212	23
-4	11	6	169	152	34
-1	11	6	202	207	41
2	11	6	215	181	-53
5	11	6	313	298	28
-12	12	6	117	40	-55
-6	12	6	286	272	23
-3	12	6	224	214	28
0	12	6	123	12	-43
3	12	6	137	127	-45
-14	13	6	92	68	-73
-11	13	6	171	158	36
-8	13	6	284	276	24
-5	13	6	278	244	24
-2	13	6	164	153	35
1	13	6	93	66	-68
-13	14	6	107	37	-69
-10	14	6	440	421	50
-7	14	6	624	599	28
-4	14	6	490	462	20
-1	14	6	102	39	-69
-12	15	6	138	149	-53
-9	15	6	285	286	40
-6	15	6	286	322	35
-3	15	6	132	117	-62
-11	16	6	243	237	31
-8	16	6	490	367	-168
-5	16	6	314	303	30
-1	1	7	67	8	-38
-3	2	7	443	467	17
0	2	7	82	3	-47
-5	3	7	489	467	-117
-2	3	7	433	455	15
1	3	7	488	493	17
-7	4	7	130	53	-34
-4	4	7	74	34	-47
-1	4	7	501	494	15
2	4	7	210	263	30
-9	5	7	772	763	15
-6	5	7	496	547	20
-3	5	7	422	421	19
0	5	7	87	28	-43
3	5	7	783	817	17
-11	6	7	701	635	62
-8	6	7	903	914	22
-5	6	7	502	536	21
-2	6	7	230	235	22
1	6	7	356	325	23
4	6	7	212	139	25
-13	7	7	132	60	-54
-10	7	7	149	74	-59

Table 49. (cont.)
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-7	7	7	100	16	-54
-4	7	7	101	68	-36
-1	7	7	371	348	17
2	7	7	87	29	-59
5	7	7	245	230	41
-15	8	7	128	56	-51
-12	8	7	623	599	28
-9	8	7	913	949	28
-6	8	7	912	925	25
-3	8	7	782	779	14
0	8	7	105	3	-40
3	8	7	109	75	-47
6	8	7	87	21	-66
-14	9	7	249	234	20
-11	9	7	692	658	19
-8	9	7	918	926	24
-5	9	7	765	752	15
-2	9	7	123	42	-50
1	9	7	157	129	-40
4	9	7	82	47	-75
7	9	7	150	117	-51
-16	10	7	71	33	-89
-13	10	7	107	46	-60
-10	10	7	49	15	-86
-7	10	7	89	52	-61
-4	10	7	202	147	27
-1	10	7	158	126	-42
2	10	7	169	140	33
5	10	7	231	211	39
-15	11	7	115	104	-61
-12	11	7	495	504	36
-9	11	7	690	717	23
-6	11	7	643	664	25
-3	11	7	71	96	-74
0	11	7	49	22	-86
3	11	7	174	200	38
-11	12	7	519	500	19
-8	12	7	612	619	19
-5	12	7	258	251	32
-2	12	7	144	133	-62
1	12	7	124	133	-52
-13	13	7	115	23	-62
-10	13	7	107	41	-58
-7	13	7	88	58	-63
-4	13	7	71	75	-83
-1	13	7	140	118	-46
2	13	7	404	391	24
-12	14	7	260	247	29
-9	14	7	252	228	26
-6	14	7	51	25	-103
-3	14	7	212	192	31
0	14	7	91	12	-62
-11	15	7	718	81	-248
-8	15	7	108	69	-69
-5	15	7	216	208	37
-2	15	7	422	404	24
-10	16	7	104	40	-69
-7	16	7	135	123	-54
0	1	8	715	714	11
-2	2	8	86	29	-44
1	2	8	65	3	-58
-4	3	8	448	462	14
-1	3	8	89	5	-46
2	3	8	121	77	-54
-6	4	8	334	366	19
-3	4	8	468	467	17
0	4	8	661	677	14
3	4	8	487	512	17
-8	5	8	126	118	-45
-5	5	8	247	248	18
-2	5	8	107	126	-44
1	5	8	587	580	20
4	5	8	430	401	18
-10	6	8	264	281	32
-7	6	8	296	276	27
-4	6	8	338	372	41
-1	6	8	584	567	21
2	6	8	306	325	27
5	6	8	274	264	23
-12	7	8	63	22	-84
-9	7	8	145	146	-47
-6	7	8	293	235	24
-3	7	8	490	485	16
0	7	8	961	957	30
3	7	8	750	737	17
6	7	8	188	154	41
-14	8	8	52	6	-105
-11	8	8	90	67	-64
-8	8	8	168	166	36
-5	8	8	71	112	-75
-2	8	8	306	322	23
1	8	8	561	559	17

Table 49. (cont.)
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
4	8	8	63	72	-91	-2	4	9	858	836	14
-13	9	8	104	4	-54	1	4	9	502	517	23
-10	9	8	189	122	-43	4	4	9	48	51	-97
-7	9	8	175	169	35	-7	5	9	199	186	33
-4	9	8	417	438	24	-4	5	9	252	262	38
-1	9	8	594	596	17	-1	5	9	512	523	16
2	9	8	444	476	21	2	5	9	452	426	18
5	9	8	165	187	-43	5	5	9	171	133	-40
-15	10	8	54	89	-109	-9	6	9	333	327	27
-12	10	8	191	174	42	-6	6	9	81	1	-62
-9	10	8	160	173	-40	-3	6	9	48	24	-97
-6	10	8	272	300	25	0	6	9	48	4	-84
-3	10	8	765	766	22	3	6	9	151	15	-58
0	10	8	1213	1194	19	6	6	9	318	335	27
3	10	8	505	500	20	-11	7	9	156	102	-59
-14	11	8	344	365	26	-8	7	9	49	102	-99
-11	11	8	293	300	31	-5	7	9	196	167	36
-8	11	8	105	43	-63	-2	7	9	451	396	38
-5	11	8	275	276	41	1	7	9	59	31	-82
-2	11	8	459	453	36	4	7	9	201	205	42
1	11	8	313	325	21	7	7	9	106	66	-72
4	11	8	88	119	-78	-13	8	9	360	352	32
-13	12	8	121	155	-54	-10	8	9	152	109	-56
-10	12	8	240	211	34	-7	8	9	103	98	-52
-7	12	8	117	24	-57	-4	8	9	47	61	-95
-4	12	8	86	69	-81	-1	8	9	46	56	-94
-1	12	8	321	323	25	2	8	9	164	113	34
2	12	8	53	18	-107	5	8	9	522	526	27
-12	13	8	194	131	-66	-12	9	9	294	307	53
-9	13	8	101	57	-52	-9	9	9	79	0	-65
-6	13	8	202	203	-46	-6	9	9	359	347	28
-3	13	8	519	498	32	-3	9	9	100	12	-60
-11	14	8	343	362	25	0	9	9	103	5	-53
-8	14	8	78	31	-77	3	9	9	146	179	-44
-5	14	8	192	202	40	-14	10	9	100	34	-76
-2	14	8	54	17	-109	-11	10	9	160	32	-43
-10	15	8	81	83	-79	-8	10	9	141	102	-39
-4	15	8	133	76	-60	-5	10	9	177	164	30
0	0	9	46	32	-81	-2	10	9	105	122	-67
1	1	9	1090	1128	16	1	10	9	52	37	-105
-1	2	9	1095	1109	15	4	10	9	70	35	-90
2	2	9	856	829	16	-13	11	9	248	267	31
-3	3	9	49	1	-86	-10	11	9	127	55	-46
0	3	9	85	2	-52	-7	11	9	86	88	-65
3	3	9	139	32	-41	-4	11	9	179	238	32
-5	4	9	254	259	34	-1	11	9	64	94	-90

Table 49. (cont.)
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
2	11	9	181	167	-54
-12	12	9	120	11	-53
-9	12	9	316	281	36
-6	12	9	302	341	25
-3	12	9	93	168	-71
0	12	9	90	33	-69
-11	13	9	286	242	28
-8	13	9	365	319	26
-5	13	9	552	513	32
-2	13	9	147	149	-47
-10	14	9	74	29	-88
-7	14	9	102	32	-64
-4	14	9	93	32	-77
-1	1	10	180	139	31
-3	2	10	94	88	-62
0	2	10	401	363	18
-5	3	10	322	273	26
-2	3	10	86	70	-67
1	3	10	47	64	-96
-7	4	10	630	649	17
-4	4	10	699	670	17
-1	4	10	93	41	-62
2	4	10	146	145	-40
-9	5	10	244	225	35
-6	5	10	457	452	25
-3	5	10	283	296	25
0	5	10	126	53	-57
3	5	10	298	259	42
-11	6	10	151	108	-34
-8	6	10	520	532	18
-5	6	10	445	477	22
-2	6	10	105	121	-49
1	6	10	118	24	-50
4	6	10	265	247	26
-13	7	10	328	297	29
-10	7	10	684	654	22
-7	7	10	997	968	17
-4	7	10	632	657	25
-1	7	10	118	5	-46
2	7	10	103	13	-58
5	7	10	170	141	-42
-12	8	10	343	348	33
-9	8	10	335	330	34
-6	8	10	505	507	19
-3	8	10	295	289	24
0	8	10	156	93	-44
3	8	10	77	93	-77
-11	9	10	163	130	-51
-8	9	10	334	355	29
-5	9	10	248	258	31
-2	9	10	115	34	-63
1	9	10	89	56	-49
4	9	10	99	28	-73
-13	10	10	395	403	25
-10	10	10	534	505	24
-7	10	10	661	658	20
-4	10	10	273	296	32
-1	10	10	75	45	-54
2	10	10	53	4	-108
-12	11	10	170	184	-51
-9	11	10	145	122	-48
-6	11	10	145	97	29
-3	11	10	67	51	-92
0	11	10	308	245	28
-11	12	10	205	143	-65
-8	12	10	384	329	29
-5	12	10	177	158	-43
-2	12	10	53	15	-106
-10	13	10	401	365	24
-7	13	10	293	289	28
-4	13	10	128	19	-55
0	1	11	48	13	-83
-2	2	11	47	24	-82
1	2	11	75	96	-67
-4	3	11	205	231	29
-1	3	11	81	58	-57
2	3	11	530	522	25
-6	4	11	186	170	-43
-3	4	11	219	208	33
0	4	11	105	18	-47
3	4	11	113	81	-58
-8	5	11	119	108	-49
-2	5	11	532	491	29
1	5	11	752	763	22
4	5	11	358	349	23
-10	6	11	77	46	-78
-7	6	11	175	184	35
-4	6	11	161	168	32
-1	6	11	612	710	10
2	6	11	639	641	27
5	6	11	241	217	51
-12	7	11	131	78	-50

Table 49. (cont.)
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-9	7	11	119	67	-38
-6	7	11	199	179	31
-3	7	11	109	85	-50
0	7	11	107	27	-50
3	7	11	103	35	-63
-11	8	11	175	32	-68
-8	8	11	72	37	-72
-5	8	11	141	132	-44
-2	8	11	664	644	30
1	8	11	617	630	21
4	8	11	321	296	31
-10	9	11	74	100	-86
-7	9	11	154	143	-34
-4	9	11	357	374	42
-1	9	11	629	584	20
2	9	11	463	456	22
-9	10	11	103	111	-58
-6	10	11	52	85	-104
-3	10	11	53	16	-108
0	10	11	96	15	-62
-8	11	11	107	85	-70
-5	11	11	252	227	37
-2	11	11	440	434	26
-7	12	11	147	131	-50
-4	12	11	304	303	35
0	0	12	1318	1262	56
1	1	12	573	540	19
-1	2	12	576	588	18
2	2	12	168	117	-57
-3	3	12	685	649	18
0	3	12	618	607	16
3	3	12	245	239	3
-5	4	12	279	323	24
-2	4	12	146	106	-40
1	4	12	229	240	27
4	4	12	51	50	-103
-7	5	12	70	35	-75
-4	5	12	294	243	44
-1	5	12	249	206	40
2	5	12	123	20	-51
5	5	12	138	107	-44
-9	6	12	83	37	-80
-6	6	12	273	258	3
-3	6	12	224	155	44
0	6	12	227	177	25
3	6	12	96	59	-73
-8	7	12	53	50	-107
-5	7	12	51	22	-103
-2	7	12	108	49	-65
1	7	12	68	28	-87
-10	8	12	74	65	-87
-7	8	12	112	67	-68
-4	8	12	62	11	-88
-1	8	12	95	5	-64
2	8	12	156	157	-45
-9	9	12	117	82	-64
-6	9	12	63	37	-91
-3	9	12	86	19	-80
0	9	12	138	92	-41
-8	10	12	141	28	-55
-5	10	12	54	119	-109
-2	10	12	139	110	-55
-1	1	13	101	20	-48
-3	2	13	178	145	-42
0	2	13	74	51	-63
-5	3	13	400	395	21
-2	3	13	134	130	-43
1	3	13	130	156	-34
-7	4	13	143	75	-65
-4	4	13	71	10	-73
-1	4	13	138	97	-33
2	4	13	188	173	35
-6	5	13	493	521	24
-3	5	13	407	375	21
0	5	13	105	30	-50
3	5	13	120	107	-62
-8	6	13	474	453	46
-5	6	13	509	489	21
-2	6	13	153	169	-47
1	6	13	134	102	-45
-7	7	13	83	34	-68
-4	7	13	127	91	-59
-1	7	13	55	127	-111
-6	8	13	510	490	25
-3	8	13	167	142	-50
0	1	14	52	2	-91
-2	2	14	54	37	-94
1	2	14	93	70	-60
-4	3	14	116	109	-59
-1	3	14	69	26	-91
2	3	14	196	190	-43
-6	4	14	55	34	-111

Table 49. (cont.)
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-3	4	14	107	46	-65
0	4	14	307	308	23
-5	5	14	69	7	-90
-2	5	14	218	175	41
-4	6	14	146	16	-63

APPENDIX B

TABLE 50

Table 50. Cyclohexane (boat) Thiourea Host/Guest Adduct
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
-1	2	0	860	836	10	-13	17	0	133	128	-32
0	3	0	2852	3009	16	-10	17	0	236	235	15
-2	4	0	929	952	11	-7	17	0	244	231	17
-4	5	0	1174	1083	12	-4	17	0	122	124	24
-1	5	0	1175	1036	11	-1	17	0	59	34	-58
-3	6	0	116	138	13	-15	18	0	94	44	-44
0	6	0	481	577	5	-12	18	0	99	77	-37
-5	7	0	105	220	-31	-9	18	0	112	97	-30
-2	7	0	70	168	-22	-6	18	0	132	76	-41
-7	8	0	515	474	8	-3	18	0	112	36	-33
-4	8	0	571	496	5	0	18	0	93	30	-37
-1	8	0	518	453	7	-17	19	0	41	2	-81
-6	9	0	114	153	15	-14	19	0	109	56	-32
-3	9	0	124	150	15	-11	19	0	115	120	-35
0	9	0	381	415	7	-8	19	0	134	120	-32
-8	10	0	272	246	9	-5	19	0	73	58	-50
-5	10	0	284	252	9	-2	19	0	71	3	-47
-2	10	0	276	295	14	-16	20	0	74	58	-53
-10	11	0	44	22	-55	-13	20	0	148	138	-44
-7	11	0	326	354	9	-10	20	0	182	188	28
-4	11	0	326	313	9	-7	20	0	142	137	26
-1	11	0	65	3	-44	-4	20	0	101	54	-44
-9	12	0	112	121	22	-15	21	0	96	57	-43
-6	12	0	230	263	14	-12	21	0	90	75	-45
-3	12	0	75	118	-48	-9	21	0	109	72	-50
0	12	0	115	118	21	-6	21	0	70	51	-53
-11	13	0	93	40	-35	-14	22	0	64	10	-61
-8	13	0	80	76	-42	-11	22	0	144	33	-50
-5	13	0	91	94	-40	-8	22	0	106	12	-50
-2	13	0	91	19	-33	-1	1	1	59	52	9
-13	14	0	58	67	-47	-3	2	1	208	262	5
-10	14	0	217	208	18	0	2	1	37	41	-19
-7	14	0	346	339	13	-5	3	1	1479	1406	23
-4	14	0	217	180	13	-2	3	1	210	214	4
-1	14	0	96	74	-28	1	3	1	1306	1295	19
-12	15	0	96	109	-28	-7	4	1	88	44	16
-9	15	0	144	165	20	-4	4	1	25	80	-44
-6	15	0	142	168	21	-1	4	1	1314	1398	22
-3	15	0	136	112	26	2	4	1	213	223	9
0	15	0	96	55	-31	-9	5	1	525	523	6
-14	16	0	66	12	-50	-6	5	1	1730	1719	10
-11	16	0	89	72	-35	-3	5	1	1482	1315	22
-8	16	0	116	124	23	0	5	1	51	12	-27
-5	16	0	56	72	-51	3	5	1	37	47	-46
-2	16	0	37	21	-74	-11	6	1	285	289	18
-16	17	0	38	36	-77	-8	6	1	1180	1213	11

Table 50. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-5	6	1	1735	1780	22
-2	6	1	216	256	7
1	6	1	636	614	7
4	6	1	236	240	13
-13	7	1	82	44	-32
-10	7	1	162	166	13
-7	7	1	84	52	-31
-4	7	1	90	28	-23
-1	7	1	643	606	6
2	7	1	372	386	10
5	7	1	242	252	13
-15	8	1	214	207	19
-12	8	1	372	362	9
-9	8	1	947	939	7
-6	8	1	1190	1106	10
-3	8	1	35	67	-47
0	8	1	45	26	-40
3	8	1	118	103	20
6	8	1	200	197	14
-17	9	1	68	37	-49
-14	9	1	277	285	12
-11	9	1	663	709	7
-8	9	1	951	972	8
-5	9	1	521	529	7
-2	9	1	366	389	8
1	9	1	113	69	-26
4	9	1	140	115	21
7	9	1	45	19	-60
-19	10	1	59	40	-58
-16	10	1	62	6	-50
-13	10	1	140	130	-32
-10	10	1	62	33	-40
-7	10	1	147	183	22
-4	10	1	243	244	10
-1	10	1	81	73	-38
2	10	1	98	15	-36
5	10	1	35	58	-70
8	10	1	83	28	-37
-21	11	1	59	12	-59
-18	11	1	78	2	-47
-15	11	1	192	190	20
-12	11	1	471	482	9
-9	11	1	664	675	15
-6	11	1	286	267	10
-3	11	1	126	140	23
0	11	1	75	21	-36
3	11	1	121	107	25
6	11	1	50	18	-58
9	11	1	40	18	-81
-20	12	1	72	13	-51
-17	12	1	37	70	-75
-14	12	1	309	326	19
-11	12	1	469	488	9
-8	12	1	384	363	13
-5	12	1	243	253	11
-2	12	1	99	19	-40
1	12	1	177	184	24
4	12	1	99	67	-29
7	12	1	39	58	-79
10	12	1	41	20	-82
-22	13	1	77	7	-45
-19	13	1	49	47	-66
-16	13	1	94	53	-40
-13	13	1	53	7	-41
-10	13	1	140	137	28
-7	13	1	64	21	-41
-4	13	1	136	119	19
-1	13	1	187	181	22
2	13	1	102	92	-29
5	13	1	119	111	23
8	13	1	76	26	-49
-21	14	1	80	25	-54
-18	14	1	81	15	-49
-15	14	1	140	139	23
-12	14	1	304	309	18
-9	14	1	293	287	11
-6	14	1	202	211	26
-3	14	1	97	122	-26
0	14	1	82	5	-40
3	14	1	37	41	-74
6	14	1	66	0	-59
-20	15	1	59	8	-63
-17	15	1	62	47	-40
-14	15	1	153	139	31
-11	15	1	198	182	15
-8	15	1	217	212	13
-5	15	1	67	54	-47
-2	15	1	78	98	-43
1	15	1	121	90	-28
4	15	1	87	92	-52
-19	16	1	105	16	-32
-16	16	1	71	2	-33

Table 50. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
-13	16	1	54	45	-52	-1	3	2	232	197	10
-10	16	1	97	6	-33	2	3	2	729	663	14
-7	16	1	80	15	-37	-6	4	2	123	92	18
-4	16	1	83	78	-38	-3	4	2	101	105	15
-1	16	1	100	92	-35	0	4	2	1220	1155	1
2	16	1	150	119	-34	3	4	2	993	1046	1
5	16	1	42	53	-83	-8	5	2	644	576	7
-18	17	1	40	7	-80	-5	5	2	77	172	-18
-15	17	1	38	46	-54	-2	5	2	732	684	16
-12	17	1	112	62	-31	1	5	2	801	690	1
-9	17	1	80	47	-43	4	5	2	320	302	8
-6	17	1	69	13	-49	-10	6	2	436	450	10
-3	17	1	52	33	-59	-7	6	2	145	113	11
0	17	1	62	5	-48	-4	6	2	118	100	13
3	17	1	59	6	-64	-1	6	2	802	696	9
-20	18	1	42	1	-83	2	6	2	976	923	13
-17	18	1	62	3	-59	5	6	2	285	270	11
-14	18	1	51	16	-63	-12	7	2	143	137	25
-11	18	1	38	2	-75	-9	7	2	77	88	-28
-8	18	1	90	27	-38	-6	7	2	136	109	13
-5	18	1	130	108	22	-3	7	2	1019	1040	14
-2	18	1	116	114	-31	0	7	2	1292	1316	12
1	18	1	121	103	-33	3	7	2	872	890	7
-19	19	1	41	4	-71	6	7	2	427	429	15
-16	19	1	63	20	-59	-14	8	2	78	58	-47
-13	19	1	39	40	-79	-11	8	2	120	134	19
-10	19	1	85	42	-40	-8	8	2	63	60	-34
-7	19	1	59	60	-59	-5	8	2	641	622	7
-4	19	1	98	93	-38	-2	8	2	974	951	10
-1	19	1	120	104	-36	1	8	2	498	482	12
-18	20	1	60	5	-64	4	8	2	402	420	21
-15	20	1	108	3	-47	7	8	2	150	140	18
-12	20	1	67	16	-52	-16	9	2	70	45	-42
-9	20	1	64	20	-59	-13	9	2	88	79	-33
-6	20	1	49	1	-69	-10	9	2	62	55	-43
-3	20	1	88	8	-47	-7	9	2	67	118	-28
-14	21	1	76	17	-49	-4	9	2	325	323	8
-11	21	1	53	10	-68	-1	9	2	499	497	9
-8	21	1	97	24	-37	2	9	2	232	251	14
-5	21	1	74	53	-51	5	9	2	87	67	-42
-13	22	1	73	3	-58	8	9	2	37	30	-73
-10	22	1	41	18	-82	-18	10	2	56	24	-54
0	1	2	813	663	14	-15	10	2	62	4	-49
-2	2	2	1575	1475	20	-12	10	2	108	83	-28
1	2	2	227	194	9	-9	10	2	57	57	-45
-4	3	2	96	87	14	-6	10	2	439	445	7

Table 50. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-3	10	2	871	853	6
0	10	2	564	535	7
3	10	2	437	451	9
6	10	2	127	118	23
9	10	2	39	24	-78
-20	11	2	80	27	-51
-17	11	2	109	24	-33
-14	11	2	61	4	-48
-11	11	2	79	64	-27
-8	11	2	118	134	20
-5	11	2	286	302	10
-2	11	2	237	262	11
1	11	2	213	235	17
4	11	2	111	127	24
7	11	2	78	23	-40
10	11	2	41	8	-81
-22	12	2	42	7	-84
-19	12	2	39	1	-78
-16	12	2	55	34	-56
-13	12	2	35	70	-70
-10	12	2	122	107	20
-7	12	2	140	149	18
-4	12	2	396	460	13
-1	12	2	218	245	14
2	12	2	160	182	19
5	12	2	78	26	-47
8	12	2	108	34	-46
-21	13	2	60	31	-59
-18	13	2	87	59	-34
-15	13	2	56	51	-50
-12	13	2	48	75	-56
-9	13	2	108	102	-24
-6	13	2	426	418	10
-3	13	2	443	429	9
0	13	2	333	342	12
3	13	2	177	160	36
6	13	2	81	9	-41
9	13	2	57	4	-66
-20	14	2	79	56	-50
-17	14	2	104	136	-31
-14	14	2	172	171	18
-11	14	2	62	4	-48
-8	14	2	76	66	-42
-5	14	2	73	78	-34
-2	14	2	183	185	15
1	14	2	117	83	24
4	14	2	38	24	-77
7	14	2	41	11	-82
-19	15	2	68	39	-47
-16	15	2	113	96	-29
-13	15	2	86	30	-44
-10	15	2	69	7	-46
-7	15	2	157	150	-46
-4	15	2	124	132	-29
-1	15	2	88	87	-40
2	15	2	82	35	-32
5	15	2	124	31	-48
-21	16	2	122	30	-36
-18	16	2	89	85	-43
-15	16	2	109	111	-28
-12	16	2	66	37	-46
-9	16	2	62	43	-51
-6	16	2	106	104	-28
-3	16	2	152	155	20
0	16	2	70	71	-33
3	16	2	40	6	-81
-20	17	2	86	90	-54
-17	17	2	177	180	20
-14	17	2	146	139	27
-11	17	2	79	36	-35
-8	17	2	114	37	-44
-5	17	2	48	24	-62
-2	17	2	87	29	-31
1	17	2	79	0	-44
-19	18	2	84	60	-43
-16	18	2	90	78	-42
-13	18	2	106	60	22
-10	18	2	38	33	-75
-7	18	2	52	26	-60
-4	18	2	75	29	-44
-1	18	2	74	4	-54
2	18	2	41	19	-83
-18	19	2	101	56	-40
-15	19	2	114	38	-32
-12	19	2	82	4	-50
-9	19	2	95	28	-40
-6	19	2	39	9	-79
-3	19	2	65	7	-58
0	19	2	59	21	-55
-17	20	2	98	83	-39
-14	20	2	66	57	-60
-11	20	2	66	34	-52

Table 50. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-8	20	2	105	36	-36
-5	20	2	87	33	-42
-2	20	2	55	19	-68
-16	21	2	90	29	-52
-13	21	2	104	32	-38
-10	21	2	74	10	-55
-7	21	2	81	12	-48
-12	22	2	95	3	-51
-9	22	2	80	6	-47
0	0	3	92	12	-28
1	1	3	2068	2102	39
-1	2	3	2094	2088	71
2	2	3	1566	1556	30
-3	3	3	43	18	-33
0	3	3	26	38	-44
3	3	3	59	92	-26
-5	4	3	1361	1320	12
-2	4	3	1583	1512	31
1	4	3	757	717	16
4	4	3	240	209	10
-7	5	3	713	701	12
-4	5	3	1372	1327	21
-1	5	3	761	765	17
2	5	3	301	316	7
5	5	3	70	17	-40
-9	6	3	271	241	8
-6	6	3	54	5	-32
-3	6	3	43	45	-34
0	6	3	52	71	-29
3	6	3	229	264	10
6	6	3	144	139	31
-11	7	3	175	195	19
-8	7	3	90	63	-23
-5	7	3	723	709	17
-2	7	3	305	264	9
1	7	3	219	199	9
4	7	3	150	133	20
7	7	3	55	17	-50
-13	8	3	312	297	10
-10	8	3	43	18	-53
-7	8	3	101	72	-29
-4	8	3	236	238	10
-1	8	3	225	238	10
2	8	3	74	20	-39
5	8	3	143	125	20
8	8	3	287	279	19
-15	9	3	284	295	15
-12	9	3	34	32	-69
-9	9	3	52	9	-42
-6	9	3	279	246	13
-3	9	3	230	239	10
0	9	3	77	18	-31
3	9	3	184	188	30
6	9	3	190	196	19
9	9	3	208	203	20
-17	10	3	37	6	-74
-14	10	3	35	18	-69
-11	10	3	34	31	-69
-8	10	3	54	26	-47
-5	10	3	56	14	-44
-2	10	3	70	29	-33
1	10	3	34	7	-68
4	10	3	35	10	-69
7	10	3	72	22	-48
10	10	3	73	0	-53
-19	11	3	160	156	32
-16	11	3	254	257	15
-13	11	3	101	67	-25
-10	11	3	43	30	-58
-7	11	3	176	214	15
-4	11	3	136	118	19
-1	11	3	71	5	-37
2	11	3	129	120	25
5	11	3	154	147	-45
8	11	3	157	160	30
-21	12	3	113	82	-37
-18	12	3	161	158	25
-15	12	3	155	153	34
-12	12	3	77	18	-35
-9	12	3	94	19	-30
-6	12	3	109	146	22
-3	12	3	179	188	17
0	12	3	65	10	-37
3	12	3	109	98	-35
6	12	3	128	127	19
9	12	3	114	83	-36
-20	13	3	40	2	-81
-17	13	3	38	26	-76
-14	13	3	73	61	-36
-11	13	3	85	58	-37
-8	13	3	314	279	11
-5	13	3	147	120	18

Table 50. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-2	13	3	119	119	24
1	13	3	116	80	-39
4	13	3	76	10	-38
7	13	3	108	23	-40
-19	14	3	41	83	-82
-16	14	3	114	65	-28
-13	14	3	95	57	-43
-10	14	3	35	24	-70
-7	14	3	47	27	-55
-4	14	3	85	16	-42
-1	14	3	72	81	-47
2	14	3	122	84	26
5	14	3	121	99	-36
-21	15	3	41	23	-83
-18	15	3	39	8	-78
-15	15	3	72	3	-39
-12	15	3	137	151	21
-9	15	3	281	304	12
-6	15	3	210	206	21
-3	15	3	107	95	-31
0	15	3	63	2	-47
3	15	3	95	70	-40
6	15	3	95	42	-52
-20	16	3	66	43	-55
-17	16	3	103	66	-36
-14	16	3	92	78	-36
-11	16	3	261	258	13
-8	16	3	276	271	13
-5	16	3	149	140	23
-2	16	3	114	85	-26
1	16	3	39	4	-78
4	16	3	41	12	-82
-19	17	3	95	45	-50
-16	17	3	83	68	-51
-13	17	3	106	38	-40
-10	17	3	49	11	-60
-7	17	3	37	15	-74
-4	17	3	47	7	-64
-1	17	3	69	2	-48
2	17	3	62	32	-61
-18	18	3	81	1	-44
-15	18	3	65	14	-49
-12	18	3	162	161	17
-9	18	3	205	206	17
-6	18	3	143	129	18
-3	18	3	105	75	-36
0	18	3	51	2	-60
-17	19	3	94	47	-42
-14	19	3	85	95	-46
-11	19	3	161	160	27
-8	19	3	179	157	24
-5	19	3	117	100	-41
-2	19	3	71	32	-51
-16	20	3	89	46	-51
-13	20	3	40	9	-80
-10	20	3	40	3	-80
-7	20	3	90	21	-50
-4	20	3	54	9	-68
-15	21	3	41	24	-82
-12	21	3	118	80	-44
-9	21	3	123	79	-48
-6	21	3	77	43	-51
-1	1	4	424	245	5
-3	2	4	348	336	7
0	2	4	1231	1334	16
-5	3	4	256	203	8
-2	3	4	355	320	7
1	3	4	529	565	14
-7	4	4	506	561	6
-4	4	4	240	277	7
-1	4	4	533	580	20
2	4	4	519	470	10
-9	5	4	430	408	7
-6	5	4	516	439	9
-3	5	4	257	227	8
0	5	4	483	419	10
3	5	4	30	4	-60
-11	6	4	281	307	10
-8	6	4	274	260	8
-5	6	4	523	449	8
-2	6	4	513	487	13
1	6	4	346	372	7
4	6	4	421	439	8
-13	7	4	247	242	12
-10	7	4	823	830	13
-7	7	4	872	881	12
-4	7	4	508	564	10
-1	7	4	343	362	9
2	7	4	240	254	17
5	7	4	34	20	-68
-15	8	4	36	49	-71
-12	8	4	122	109	25

Table 50. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-9	8	4	526	509	8
-6	8	4	280	279	10
-3	8	4	30	11	-59
0	8	4	200	213	15
3	8	4	86	111	-30
6	8	4	35	58	-70
-17	9	4	64	11	-47
-14	9	4	135	132	-34
-11	9	4	439	465	10
-8	9	4	526	525	7
-5	9	4	441	467	9
-2	9	4	248	265	10
1	9	4	177	167	20
4	9	4	86	60	-38
7	9	4	44	39	-63
-19	10	4	59	52	-59
-16	10	4	148	113	20
-13	10	4	440	433	14
-10	10	4	1043	1044	12
-7	10	4	837	834	14
-4	10	4	431	413	7
-1	10	4	189	168	14
2	10	4	91	57	-31
5	10	4	82	44	-31
8	10	4	84	68	-32
-21	11	4	41	4	-82
-18	11	4	99	91	-27
-15	11	4	157	171	20
-12	11	4	290	306	12
-9	11	4	449	466	8
-6	11	4	282	309	10
-3	11	4	104	116	-28
0	11	4	89	53	-28
3	11	4	104	90	-33
6	11	4	74	76	-42
9	11	4	71	9	-57
-20	12	4	40	1	-81
-17	12	4	92	59	-37
-14	12	4	84	29	-34
-11	12	4	288	290	11
-8	12	4	110	130	-28
-5	12	4	59	49	-43
-2	12	4	61	77	-48
1	12	4	52	38	-53
4	12	4	69	62	-45
7	12	4	40	2	-79
-19	13	4	40	18	-80
-16	13	4	87	59	-37
-13	13	4	263	268	11
-10	13	4	441	431	13
-7	13	4	255	232	16
-4	13	4	104	72	-31
-1	13	4	51	11	-54
2	13	4	83	60	-41
5	13	4	60	48	-59
8	13	4	100	12	-40
-21	14	4	67	26	-55
-18	14	4	50	58	-67
-15	14	4	89	88	-36
-12	14	4	57	32	-53
-9	14	4	124	123	23
-6	14	4	94	64	-33
-3	14	4	108	81	-32
0	14	4	103	125	-33
3	14	4	146	125	18
6	14	4	91	44	-51
-20	15	4	68	7	-53
-17	15	4	88	23	-40
-14	15	4	107	88	-39
-11	15	4	157	161	25
-8	15	4	84	46	-36
-5	15	4	95	51	-37
-2	15	4	84	71	-45
1	15	4	90	72	-27
4	15	4	72	40	-55
-19	16	4	41	14	-82
-16	16	4	90	40	-44
-13	16	4	94	62	-38
-10	16	4	106	102	-28
-7	16	4	76	36	-39
-4	16	4	102	54	-44
-1	16	4	102	70	-23
2	16	4	68	59	-59
-18	17	4	41	20	-81
-15	17	4	58	31	-59
-12	17	4	61	64	-54
-9	17	4	65	15	-51
-6	17	4	38	82	-76
-3	17	4	142	133	18
0	17	4	128	129	25
3	17	4	105	77	-42
-17	18	4	41	27	-82

Table 50. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-14	18	4	57	64	-61
-11	18	4	104	88	-27
-8	18	4	87	72	-28
-5	18	4	59	58	-60
-2	18	4	41	62	-81
1	18	4	42	48	-84
-16	19	4	70	18	-58
-13	19	4	60	23	-59
-10	19	4	90	53	-49
-7	19	4	72	3	-54
-4	19	4	78	40	-53
-1	19	4	100	47	-42
-15	20	4	41	6	-81
-12	20	4	57	6	-63
-9	20	4	63	9	-59
-6	20	4	79	50	-53
-3	20	4	72	78	-55
-14	21	4	87	25	-44
-11	21	4	41	4	-82
-8	21	4	41	15	-83
0	1	5	51	55	-27
-2	2	5	37	20	-35
1	2	5	677	715	5
-4	3	5	699	656	5
-1	3	5	683	653	10
2	3	5	274	297	9
-6	4	5	394	410	8
-3	4	5	708	724	12
0	4	5	39	4	-33
3	4	5	150	152	13
-8	5	5	692	717	12
-5	5	5	60	29	-27
-2	5	5	274	300	7
1	5	5	320	277	7
4	5	5	641	632	18
-10	6	5	55	64	-48
-7	6	5	280	270	11
-4	6	5	396	365	10
-1	6	5	322	307	10
2	6	5	716	739	19
5	6	5	460	468	11
-12	7	5	242	223	16
-9	7	5	208	199	14
-6	7	5	290	240	10
-3	7	5	158	129	15
0	7	5	31	14	-54
3	7	5	97	138	-26
6	7	5	59	67	-44
-14	8	5	75	11	-44
-11	8	5	90	80	-30
-8	8	5	32	18	-56
-5	8	5	700	742	6
-2	8	5	724	701	17
1	8	5	776	791	2
4	8	5	488	484	13
7	8	5	59	13	-51
-16	9	5	69	63	-51
-13	9	5	111	119	-28
-10	9	5	113	131	22
-7	9	5	200	182	16
-4	9	5	649	620	14
-1	9	5	794	832	17
2	9	5	578	593	13
5	9	5	177	181	18
8	9	5	56	72	-60
-18	10	5	109	12	-44
-15	10	5	90	48	-31
-12	10	5	114	93	22
-9	10	5	105	119	-23
-6	10	5	77	43	-36
-3	10	5	128	131	18
0	10	5	35	27	-60
3	10	5	81	59	-39
6	10	5	131	81	-29
9	10	5	87	12	-38
-20	11	5	40	16	-81
-17	11	5	68	53	-52
-14	11	5	61	68	-46
-11	11	5	63	0	-35
-8	11	5	64	95	-46
-5	11	5	467	483	9
-2	11	5	576	594	9
1	11	5	422	429	23
4	11	5	92	96	-35
7	11	5	47	18	-67
10	11	5	83	6	-53
-19	12	5	84	37	-45
-16	12	5	113	96	-38
-13	12	5	44	14	-60
-10	12	5	82	88	-34
-7	12	5	246	221	13
-4	12	5	489	502	8

Table 50. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-1	12	5	424	443	10
2	12	5	201	208	17
5	12	5	91	97	-30
8	12	5	69	5	-57
-21	13	5	67	9	-56
-18	13	5	80	36	-51
-15	13	5	126	127	24
-12	13	5	96	11	-26
-9	13	5	109	123	-26
-6	13	5	97	84	-30
-3	13	5	35	38	-71
0	13	5	50	6	-50
3	13	5	67	61	-53
6	13	5	40	17	-80
-20	14	5	49	13	-70
-17	14	5	91	32	-47
-14	14	5	37	5	-64
-11	14	5	85	82	-35
-8	14	5	54	7	-47
-5	14	5	193	195	15
-2	14	5	205	203	15
1	14	5	84	74	-40
4	14	5	78	15	-51
7	14	5	42	1	-145
-19	15	5	62	73	-58
-16	15	5	179	175	19
-13	15	5	160	137	24
-10	15	5	88	62	-36
-7	15	5	36	15	-72
-4	15	5	117	90	-36
-1	15	5	105	75	-28
2	15	5	49	55	-68
5	15	5	42	1	-83
-18	16	5	165	108	-52
-15	16	5	179	175	24
-12	16	5	125	97	-31
-9	16	5	89	67	-41
-6	16	5	82	92	-40
-3	16	5	72	65	-51
0	16	5	81	1	-45
3	16	5	41	10	-82
-17	17	5	41	3	-71
-14	17	5	75	29	-45
-11	17	5	80	48	-43
-8	17	5	83	80	-48
-5	17	5	112	92	-30
-2	17	5	69	51	-56
1	17	5	41	14	-82
-19	18	5	92	69	-48
-16	18	5	99	105	-42
-13	18	5	105	37	-46
-10	18	5	67	5	-54
-7	18	5	106	6	-45
-4	18	5	53	8	-65
-1	18	5	81	12	-52
-18	19	5	42	69	-104
-15	19	5	106	70	-38
-12	19	5	50	36	-69
-9	19	5	68	26	-50
-6	19	5	60	25	-61
-3	19	5	41	13	-82
-14	20	5	81	11	-45
-11	20	5	70	15	-55
-8	20	5	77	5	-54
-5	20	5	63	2	-62
-13	21	5	74	9	-57
-10	21	5	102	2	-50
-7	21	5	42	5	-145
0	0	6	556	471	12
1	1	6	689	773	6
-1	2	6	696	798	13
2	2	6	1213	1159	20
-3	3	6	1277	1230	17
0	3	6	1399	1388	20
3	3	6	910	928	16
-5	4	6	340	280	13
-2	4	6	1223	1140	22
1	4	6	340	334	15
4	4	6	125	101	26
-7	5	6	320	311	9
-4	5	6	347	286	7
-1	5	6	338	330	12
2	5	6	263	248	9
5	5	6	144	129	20
-9	6	6	51	60	-49
-6	6	6	280	314	9
-3	6	6	923	916	20
0	6	6	466	483	9
3	6	6	100	48	-29
6	6	6	91	13	-38
-11	7	6	88	16	-28
-8	7	6	78	85	-33

Table 50. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
-5	7	6	314	304	8	-6	12	6	70	21	-44
-2	7	6	280	244	9	-3	12	6	34	23	-69
1	7	6	78	11	-40	0	12	6	99	71	-40
4	7	6	35	60	-69	3	12	6	125	42	-31
7	7	6	243	256	19	6	12	6	137	104	-35
-13	8	6	120	121	-38	-20	13	6	120	65	-36
-10	8	6	78	67	-36	-17	13	6	138	114	-32
-7	8	6	101	63	-32	-14	13	6	93	52	-30
-4	8	6	128	116	17	-11	13	6	124	105	-28
-1	8	6	55	14	-46	-8	13	6	112	112	23
2	8	6	139	126	28	-5	13	6	116	103	-34
5	8	6	90	109	-31	-2	13	6	152	116	32
8	8	6	109	129	-28	1	13	6	80	33	-45
-15	9	6	140	131	21	4	13	6	105	124	-31
-12	9	6	35	7	-69	7	13	6	102	66	-35
-9	9	6	158	164	15	-19	14	6	60	1	-63
-6	9	6	48	36	-51	-16	14	6	93	2	-47
-3	9	6	94	32	-39	-13	14	6	80	62	-39
0	9	6	125	144	22	-10	14	6	200	204	19
3	9	6	67	30	-39	-7	14	6	250	255	25
6	9	6	116	145	-27	-4	14	6	207	211	20
9	9	6	129	131	26	-1	14	6	110	25	-32
-17	10	6	231	228	13	2	14	6	58	27	-59
-14	10	6	207	210	15	5	14	6	41	3	-82
-11	10	6	85	74	-41	-18	15	6	126	69	-43
-8	10	6	109	76	-27	-15	15	6	90	63	-31
-5	10	6	162	138	16	-12	15	6	99	71	-29
-2	10	6	145	134	17	-9	15	6	158	145	20
1	10	6	83	18	-39	-6	15	6	148	136	30
4	10	6	191	208	23	-3	15	6	95	28	-37
7	10	6	215	244	13	0	15	6	39	18	-67
10	10	6	84	92	-48	3	15	6	76	59	-49
-19	11	6	86	38	-43	-17	16	6	40	38	-81
-16	11	6	105	95	-35	-14	16	6	39	3	-78
-13	11	6	110	106	-30	-11	16	6	104	85	-30
-10	11	6	82	52	-33	-8	16	6	133	125	22
-7	11	6	60	52	-44	-5	16	6	130	118	26
-4	11	6	71	62	-45	-2	16	6	39	26	-78
-1	11	6	35	20	-69	1	16	6	64	27	-55
2	11	6	115	123	-29	-19	17	6	41	17	-83
5	11	6	141	114	23	-16	17	6	64	36	-59
8	11	6	41	45	-81	-13	17	6	160	119	30
-18	12	6	121	102	-33	-10	17	6	220	234	12
-15	12	6	134	61	-48	-7	17	6	243	244	12
-12	12	6	57	20	-43	-4	17	6	62	123	-62
-9	12	6	35	13	-69	-1	17	6	85	33	-51

Table 50. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
2	17	6	42	26	-84
-18	18	6	86	37	-42
-15	18	6	110	68	-41
-12	18	6	115	112	-31
-9	18	6	126	133	27
-6	18	6	93	95	-38
-3	18	6	87	58	-41
0	18	6	90	39	-48
-17	19	6	62	18	-58
-14	19	6	55	3	-66
-11	19	6	71	38	-56
-8	19	6	65	46	-59
-5	19	6	52	5	-68
-2	19	6	41	20	-82
-13	20	6	83	70	-54
-10	20	6	138	94	-34
-7	20	6	42	63	-84
-1	1	7	41	14	-39
-3	2	7	338	361	8
0	2	7	45	6	-35
-5	3	7	219	220	12
-2	3	7	336	330	10
1	3	7	305	296	21
-7	4	7	82	57	-30
-4	4	7	30	2	-52
-1	4	7	310	306	12
2	4	7	247	276	12
-9	5	7	563	589	14
-6	5	7	379	426	13
-3	5	7	209	221	12
0	5	7	57	2	-38
3	5	7	493	489	11
-11	6	7	401	404	14
-8	6	7	595	583	8
-5	6	7	379	396	9
-2	6	7	239	252	14
1	6	7	214	214	11
4	6	7	76	42	-36
-13	7	7	71	15	-46
-10	7	7	81	66	-34
-7	7	7	40	8	-51
-4	7	7	72	49	-33
-1	7	7	211	225	16
2	7	7	74	96	-37
5	7	7	159	175	18
-15	8	7	72	19	-49
-12	8	7	378	398	10
-9	8	7	648	665	8
-6	8	7	593	605	9
-3	8	7	503	510	7
0	8	7	58	12	-36
3	8	7	79	49	-35
6	8	7	57	29	-54
-17	9	7	97	71	-47
-14	9	7	194	199	23
-11	9	7	437	460	15
-8	9	7	645	657	13
-5	9	7	574	577	7
-2	9	7	110	109	22
1	9	7	81	77	-35
4	9	7	70	83	-47
7	9	7	89	69	-33
-19	10	7	51	19	-69
-16	10	7	73	87	-44
-13	10	7	36	9	-72
-10	10	7	66	5	-38
-7	10	7	48	72	-56
-4	10	7	75	31	-36
-1	10	7	79	56	-31
2	10	7	36	34	-71
5	10	7	72	40	-49
8	10	7	72	9	-50
-18	11	7	40	6	-80
-15	11	7	110	88	-35
-12	11	7	310	313	16
-9	11	7	448	445	9
-6	11	7	404	411	9
-3	11	7	58	64	-50
0	11	7	81	7	-35
3	11	7	82	64	-38
6	11	7	55	49	-63
9	11	7	42	14	-83
-20	12	7	96	1	-51
-17	12	7	58	78	-61
-14	12	7	172	169	18
-11	12	7	317	314	13
-8	12	7	384	380	12
-5	12	7	169	170	19
-2	12	7	52	48	-54
1	12	7	67	13	-44
4	12	7	105	75	-39
7	12	7	41	30	-82

Table 50. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
-19	13	7	77	13	-53	-16	19	7	42	10	-83
-16	13	7	65	32	-50	-13	19	7	41	15	-82
-13	13	7	37	5	-64	-10	19	7	58	16	-63
-10	13	7	36	11	-72	-7	19	7	41	35	-82
-7	13	7	70	19	-41	-4	19	7	103	70	-36
-4	13	7	90	74	-42	-12	20	7	76	2	-50
-1	13	7	37	4	-73	-9	20	7	68	15	-53
2	13	7	119	109	18	0	1	8	110	58	-34
5	13	7	67	17	-58	-2	2	8	272	251	12
-18	14	7	41	19	-81	1	2	8	189	212	11
-15	14	7	97	84	-35	-4	3	8	229	232	17
-12	14	7	175	174	20	-1	3	8	168	199	13
-9	14	7	204	191	18	2	3	8	71	76	-30
-6	14	7	62	37	-46	-6	4	8	181	166	13
-3	14	7	49	48	-60	-3	4	8	231	228	11
0	14	7	78	7	-35	0	4	8	433	471	7
3	14	7	110	36	-41	3	4	8	432	434	14
-17	15	7	55	46	-65	-8	5	8	119	114	23
-14	15	7	100	81	-41	-5	5	8	193	193	19
-11	15	7	93	88	-36	-2	5	8	78	90	-27
-8	15	7	37	12	-74	1	5	8	282	298	10
-5	15	7	74	36	-41	4	5	8	172	193	17
-2	15	7	111	101	23	-10	6	8	240	237	13
1	15	7	163	150	22	-7	6	8	230	230	18
4	15	7	68	64	-61	-4	6	8	184	162	15
-19	16	7	63	7	-62	-1	6	8	291	301	10
-16	16	7	53	3	-58	2	6	8	221	211	12
-13	16	7	57	43	-59	5	6	8	212	228	14
-10	16	7	109	90	-28	-12	7	8	86	2	-35
-7	16	7	103	73	-35	-9	7	8	34	41	-68
-4	16	7	88	85	-38	-6	7	8	221	235	15
-1	16	7	162	155	-44	-3	7	8	445	450	11
2	16	7	111	85	-36	0	7	8	732	717	8
-18	17	7	41	9	-83	3	7	8	512	507	9
-15	17	7	104	50	-44	6	7	8	132	142	21
-12	17	7	92	81	-42	-14	8	8	88	58	-37
-9	17	7	97	69	-37	-11	8	8	100	102	-29
-6	17	7	49	57	-67	-8	8	8	226	222	13
-3	17	7	63	42	-55	-5	8	8	121	137	25
0	17	7	41	1	-71	-2	8	8	216	212	15
-17	18	7	101	8	-44	1	8	8	337	350	13
-14	18	7	75	17	-55	4	8	8	87	89	-32
-11	18	7	51	9	-67	7	8	8	64	27	-53
-8	18	7	40	10	-80	-16	9	8	52	35	-62
-5	18	7	41	19	-81	-13	9	8	56	49	-54
-2	18	7	104	89	-42	-10	9	8	133	117	25

Table 50. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-7	9	8	34	49	-68
-4	9	8	172	199	16
-1	9	8	325	349	10
2	9	8	289	307	28
5	9	8	106	104	-30
8	9	8	114	18	-35
-18	10	8	57	24	-63
-15	10	8	66	34	-52
-12	10	8	95	47	-31
-9	10	8	109	111	-25
-6	10	8	243	248	13
-3	10	8	516	517	8
0	10	8	627	659	12
3	10	8	276	274	17
6	10	8	97	84	-33
9	10	8	82	27	-45
-17	11	8	114	39	-34
-14	11	8	66	68	-52
-11	11	8	96	19	-33
-8	11	8	100	117	-45
-5	11	8	218	231	27
-2	11	8	274	300	12
1	11	8	207	206	16
4	11	8	111	113	22
7	11	8	86	45	-46
-19	12	8	42	18	-83
-16	12	8	78	39	-44
-13	12	8	64	16	-52
-10	12	8	82	48	-36
-7	12	8	98	14	-33
-4	12	8	88	85	-32
-1	12	8	214	207	15
2	12	8	62	30	-55
5	12	8	40	24	-80
-18	13	8	98	16	-50
-15	13	8	69	49	-48
-12	13	8	66	24	-51
-9	13	8	76	40	-39
-6	13	8	156	145	27
-3	13	8	284	277	12
0	13	8	168	177	19
3	13	8	79	48	-51
6	13	8	92	12	-52
-17	14	8	96	82	-50
-14	14	8	132	92	27
-11	14	8	38	67	-75
-8	14	8	48	50	-61
-5	14	8	141	90	-37
-2	14	8	47	18	-64
1	14	8	82	56	-46
4	14	8	74	34	-51
-16	15	8	40	48	-81
-13	15	8	112	50	-36
-10	15	8	94	44	-45
-7	15	8	87	40	-35
-4	15	8	140	118	18
-1	15	8	94	61	-34
2	15	8	65	11	-60
-18	16	8	102	30	-51
-15	16	8	51	46	-68
-12	16	8	49	39	-66
-9	16	8	86	35	-37
-6	16	8	99	88	-47
-3	16	8	81	49	-43
0	16	8	89	30	-45
-17	17	8	125	80	-44
-14	17	8	98	80	-37
-11	17	8	89	39	-50
-8	17	8	39	10	-79
-5	17	8	85	32	-50
-2	17	8	60	15	-62
-16	18	8	98	29	-41
-13	18	8	57	15	-65
-10	18	8	50	27	-70
-7	18	8	41	50	-82
-4	18	8	79	34	-48
-12	19	8	81	20	-47
-9	19	8	54	22	-68
-6	19	8	61	7	-59
0	0	9	34	2	-83
1	1	9	918	931	15
-1	2	9	933	946	11
2	2	9	659	645	10
-3	3	9	58	17	-38
0	3	9	87	8	-25
3	3	9	112	124	-25
-5	4	9	328	320	14
-2	4	9	660	647	13
1	4	9	458	471	11
4	4	9	133	125	-33
-7	5	9	185	178	14
-4	5	9	329	323	9

Table 50. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-1	5	9	471	467	24
2	5	9	317	297	12
5	5	9	66	25	-40
-9	6	9	95	82	-26
-6	6	9	92	14	-38
-3	6	9	119	140	21
0	6	9	72	2	-40
3	6	9	93	82	-37
6	6	9	120	117	24
-11	7	9	89	80	-35
-8	7	9	166	163	16
-5	7	9	184	172	14
-2	7	9	317	303	11
1	7	9	130	108	-43
4	7	9	47	39	-58
7	7	9	38	23	-75
-13	8	9	132	114	-29
-10	8	9	36	2	-71
-7	8	9	140	151	21
-4	8	9	121	106	-28
-1	8	9	113	92	-27
2	8	9	35	10	-70
5	8	9	168	175	27
8	8	9	171	151	23
-15	9	9	96	100	-34
-12	9	9	86	104	-33
-9	9	9	45	14	-51
-6	9	9	89	63	-33
-3	9	9	81	91	-34
0	9	9	45	7	-52
3	9	9	69	65	-43
6	9	9	164	161	25
9	9	9	143	116	-36
-17	10	9	41	14	-81
-14	10	9	87	22	-34
-11	10	9	36	8	-72
-8	10	9	48	8	-57
-5	10	9	35	17	-70
-2	10	9	76	28	-40
1	10	9	36	34	-73
4	10	9	38	2	-76
7	10	9	58	6	-64
-19	11	9	101	93	-48
-16	11	9	97	88	-36
-13	11	9	109	91	-29
-10	11	9	53	3	-55
-7	11	9	95	72	-39
-4	11	9	92	42	-32
-1	11	9	65	28	-50
2	11	9	80	30	-37
5	11	9	126	124	-27
8	11	9	99	85	-42
-18	12	9	117	71	-31
-15	12	9	65	41	-56
-12	12	9	62	3	-43
-9	12	9	87	96	-32
-6	12	9	138	116	-34
-3	12	9	108	61	-33
0	12	9	67	1	-38
3	12	9	125	80	-47
6	12	9	122	90	-36
-17	13	9	41	15	-82
-14	13	9	127	71	-36
-11	13	9	117	97	-27
-8	13	9	112	119	-31
-5	13	9	155	171	20
-2	13	9	88	34	-37
1	13	9	75	27	-50
4	13	9	49	5	-70
-16	14	9	115	58	-41
-13	14	9	99	76	-35
-10	14	9	59	31	-52
-7	14	9	49	29	-61
-4	14	9	93	8	-34
-1	14	9	39	28	-78
2	14	9	41	32	-82
-15	15	9	41	2	-70
-12	15	9	90	39	-45
-9	15	9	115	98	-33
-6	15	9	155	157	29
-3	15	9	68	82	-57
0	15	9	62	0	-54
-17	16	9	77	8	-56
-14	16	9	62	59	-62
-11	16	9	111	94	-49
-8	16	9	161	152	22
-5	16	9	147	124	23
-2	16	9	41	31	-81
1	16	9	73	29	-57
-16	17	9	52	9	-70
-13	17	9	108	17	-45
-10	17	9	68	16	-53

Table 50. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-7	17	9	51	4	-69
-4	17	9	55	2	-65
-1	17	9	42	27	-84
-12	18	9	75	72	-51
-9	18	9	96	115	-39
-6	18	9	100	90	-45
-11	19	9	101	94	-41
-8	19	9	62	83	-61
-1	1	10	96	62	-28
-3	2	10	136	126	21
0	2	10	205	190	11
-5	3	10	137	151	19
-2	3	10	122	127	19
1	3	10	45	14	-66
-7	4	10	415	422	9
-4	4	10	453	453	11
-1	4	10	75	17	-43
2	4	10	63	32	-42
-9	5	10	137	125	28
-6	5	10	270	272	15
-3	5	10	159	152	28
0	5	10	51	35	-41
3	5	10	172	187	17
-11	6	10	90	96	-36
-8	6	10	271	292	14
-5	6	10	280	273	14
-2	6	10	82	34	-41
1	6	10	34	52	-69
4	6	10	146	162	21
-13	7	10	198	178	17
-10	7	10	359	366	13
-7	7	10	583	607	11
-4	7	10	422	425	15
-1	7	10	84	65	-28
2	7	10	55	46	-48
5	7	10	113	88	-37
-15	8	10	87	75	-42
-12	8	10	200	207	17
-9	8	10	243	230	20
-6	8	10	275	290	14
-3	8	10	182	186	15
0	8	10	94	41	-29
3	8	10	71	49	-38
6	8	10	57	26	-58
-17	9	10	89	3	-42
-14	9	10	39	31	-78
-11	9	10	108	96	-27
-8	9	10	240	233	15
-5	9	10	118	125	24
-2	9	10	36	36	-71
1	9	10	36	8	-73
4	9	10	63	47	-46
7	9	10	41	35	-81
-16	10	10	124	61	-37
-13	10	10	219	212	15
-10	10	10	279	294	15
-7	10	10	364	361	18
-4	10	10	169	175	17
-1	10	10	37	6	-73
2	10	10	101	4	-43
5	10	10	64	26	-53
8	10	10	41	11	-83
-18	11	10	42	10	-83
-15	11	10	40	71	-81
-12	11	10	146	128	-32
-9	11	10	111	93	-26
-6	11	10	97	96	-29
-3	11	10	65	42	-50
0	11	10	63	38	-48
3	11	10	60	20	-59
6	11	10	63	10	-63
-17	12	10	73	13	-57
-14	12	10	64	82	-59
-11	12	10	115	136	-33
-8	12	10	205	210	20
-5	12	10	111	96	-33
-2	12	10	80	14	-36
1	12	10	39	34	-78
4	12	10	63	4	-60
-16	13	10	41	80	-83
-13	13	10	179	179	20
-10	13	10	214	207	14
-7	13	10	189	180	25
-4	13	10	38	53	-77
-1	13	10	98	25	-46
2	13	10	84	35	-44
-15	14	10	62	46	-61
-12	14	10	102	77	-35
-9	14	10	39	32	-78
-6	14	10	65	19	-54
-3	14	10	55	28	-61
0	14	10	108	87	-34

Table 50. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
3	14	10	138	63	-52
-14	15	10	83	48	-48
-11	15	10	71	74	-57
-8	15	10	79	83	-46
-5	15	10	98	35	-48
-2	15	10	55	45	-66
1	15	10	81	46	-47
-13	16	10	60	73	-65
-10	16	10	98	60	-35
-7	16	10	66	37	-58
-4	16	10	74	1	-50
-1	16	10	42	37	-83
-12	17	10	91	10	-51
-9	17	10	98	7	-41
-6	17	10	95	12	-44
-3	17	10	77	63	-50
-11	18	10	62	12	-64
-8	18	10	74	13	-59
0	1	11	34	2	-59
-2	2	11	55	4	-40
1	2	11	34	46	-69
-4	3	11	140	134	20
-1	3	11	50	53	-53
2	3	11	289	292	14
-6	4	11	159	150	20
-3	4	11	135	138	-39
0	4	11	58	3	-41
3	4	11	76	70	-37
-8	5	11	93	41	-43
-5	5	11	43	4	-52
-2	5	11	287	285	13
1	5	11	463	480	18
4	5	11	250	246	14
-10	6	11	100	95	-38
-7	6	11	156	162	26
-4	6	11	160	161	19
-1	6	11	471	483	13
2	6	11	346	362	16
5	6	11	156	141	27
-12	7	11	101	106	-35
-9	7	11	131	121	21
-6	7	11	168	156	16
-3	7	11	66	72	-44
0	7	11	47	2	-54
3	7	11	37	17	-74
6	7	11	92	4	-43
-14	8	11	115	74	-34
-11	8	11	70	36	-51
-8	8	11	70	1	-44
-5	8	11	36	41	-72
-2	8	11	357	366	12
1	8	11	332	333	12
4	8	11	166	154	18
7	8	11	81	82	-46
-16	9	11	71	15	-57
-13	9	11	39	14	-78
-10	9	11	92	26	-45
-7	9	11	121	126	25
-4	9	11	229	254	18
-1	9	11	328	331	16
2	9	11	239	245	15
5	9	11	145	123	27
8	9	11	61	11	-64
-15	10	11	40	19	-81
-12	10	11	49	10	-65
-9	10	11	54	25	-57
-6	10	11	77	88	-41
-3	10	11	98	19	-37
0	10	11	53	1	-53
3	10	11	112	37	-46
6	10	11	72	7	-58
-17	11	11	107	16	-46
-14	11	11	87	18	-50
-11	11	11	53	4	-54
-8	11	11	61	42	-54
-5	11	11	161	150	19
-2	11	11	257	248	22
1	11	11	193	169	33
4	11	11	120	80	-35
-16	12	11	41	14	-82
-13	12	11	79	52	-53
-10	12	11	39	4	-77
-7	12	11	127	109	26
-4	12	11	157	153	19
-1	12	11	175	167	25
2	12	11	111	117	-36
-15	13	11	42	41	-83
-12	13	11	40	51	-81
-9	13	11	39	15	-77
-6	13	11	39	12	-78
-3	13	11	100	40	-38
0	13	11	50	3	-61

Table 50. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
3	13	11	63	0	-62	7	7	12	118	106	-40
-14	14	11	69	0	-47	-13	8	12	108	22	-47
-11	14	11	100	23	-42	-10	8	12	84	41	-30
-8	14	11	71	77	-50	-7	8	12	117	86	-34
-5	14	11	116	126	-29	-4	8	12	101	86	-35
-2	14	11	141	122	29	-1	8	12	66	67	-51
1	14	11	102	67	-39	2	8	12	111	89	23
-13	15	11	41	41	-83	5	8	12	71	43	-56
-10	15	11	41	21	-81	8	8	12	90	47	-44
-7	15	11	98	76	-41	-15	9	12	105	63	-51
-4	15	11	82	77	-54	-12	9	12	79	54	-44
-1	15	11	42	63	-84	-9	9	12	72	74	-38
-12	16	11	54	17	-68	-6	9	12	54	51	-59
-9	16	11	77	10	-54	-3	9	12	96	73	-35
-6	16	11	55	1	-67	0	9	12	97	108	-32
-3	16	11	67	7	-54	3	9	12	39	19	-79
-11	17	11	77	14	-49	6	9	12	64	43	-56
-8	17	11	73	10	-57	-14	10	12	100	71	-39
0	0	12	869	881	20	-11	10	12	68	17	-54
1	1	12	361	375	10	-8	10	12	68	27	-40
-1	2	12	373	383	10	-5	10	12	65	52	-47
2	2	12	111	96	-25	-2	10	12	110	81	-24
-3	3	12	482	485	8	1	10	12	102	15	-45
0	3	12	455	453	13	4	10	12	119	58	-49
3	3	12	192	182	15	-13	11	12	108	9	-40
-5	4	12	196	205	22	-10	11	12	56	10	-61
-2	4	12	103	86	-27	-7	11	12	125	82	-31
1	4	12	187	182	16	-4	11	12	117	89	-38
4	4	12	90	82	-40	-1	11	12	39	9	-78
-7	5	12	36	7	-73	2	11	12	71	2	-56
-4	5	12	202	216	23	-15	12	12	42	41	-84
-1	5	12	190	188	28	-12	12	12	64	40	-50
2	5	12	36	20	-73	-9	12	12	99	61	-45
5	5	12	125	66	-45	-6	12	12	102	77	-37
-9	6	12	89	57	-45	-3	12	12	58	18	-61
-6	6	12	200	204	14	0	12	12	99	31	-32
-3	6	12	198	181	20	3	12	12	42	26	-84
0	6	12	175	173	16	-14	13	12	41	26	-83
3	6	12	71	74	-41	-11	13	12	79	18	-53
6	6	12	39	73	-79	-8	13	12	82	14	-43
-11	7	12	76	83	-44	-5	13	12	86	35	-47
-8	7	12	79	77	-36	-2	13	12	90	1	-49
-5	7	12	36	9	-73	1	13	12	112	21	-47
-2	7	12	49	11	-59	-13	14	12	50	20	-72
1	7	12	102	64	-35	-10	14	12	82	69	-54
4	7	12	95	95	-37	-7	14	12	104	102	-36

Table 50. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
-4	14	12	79	53	-47	-2	9	13	83	79	-41
-1	14	12	41	21	-83	1	9	13	57	6	-61
-12	15	12	61	42	-65	4	9	13	79	29	-47
-9	15	12	120	63	-30	-13	10	13	42	23	-84
-6	15	12	95	43	-42	-10	10	13	73	4	-46
-3	15	12	42	25	-83	-7	10	13	53	35	-65
-8	16	12	91	47	-52	-4	10	13	39	13	-78
-1	1	13	59	2	-42	-1	10	13	91	1	-48
-3	2	13	79	66	-46	2	10	13	41	6	-81
0	2	13	36	0	-62	-12	11	13	157	145	-44
-5	3	13	194	202	17	-9	11	13	219	200	23
-2	3	13	66	63	-49	-6	11	13	93	108	-40
1	3	13	100	71	-32	-3	11	13	78	60	-52
-7	4	13	46	19	-64	0	11	13	52	8	-60
-4	4	13	62	1	-47	3	11	13	75	28	-52
-1	4	13	66	69	-50	-11	12	13	151	141	25
2	4	13	77	87	-42	-8	12	13	145	110	28
-9	5	13	146	128	15	-5	12	13	82	67	-48
-6	5	13	243	267	14	-2	12	13	96	1	-42
-3	5	13	199	203	20	1	12	13	89	44	-44
0	5	13	71	1	-36	-10	13	13	42	25	-83
3	5	13	106	67	-30	-7	13	13	61	3	-58
-11	6	13	141	105	-31	-4	13	13	41	33	-82
-8	6	13	251	255	13	-1	13	13	96	50	-51
-5	6	13	256	267	13	-9	14	13	124	78	-36
-2	6	13	105	88	-31	-6	14	13	119	56	-47
1	6	13	66	77	-52	-3	14	13	56	35	-68
4	6	13	39	20	-77	0	1	14	69	17	-39
-13	7	13	69	2	-58	-2	2	14	92	24	-38
-10	7	13	73	31	-49	1	2	14	100	26	-45
-7	7	13	50	0	-56	-4	3	14	84	49	-42
-4	7	13	37	21	-75	-1	3	14	67	24	-51
-1	7	13	123	74	23	2	3	14	98	102	-23
2	7	13	86	76	-45	-6	4	14	77	15	-39
5	7	13	116	62	-30	-3	4	14	48	50	-63
-12	8	13	134	109	26	0	4	14	171	160	25
-9	8	13	232	239	24	3	4	14	197	189	32
-6	8	13	257	251	10	-8	5	14	96	91	-39
-3	8	13	88	68	-38	-5	5	14	62	39	-33
0	8	13	69	5	-43	-2	5	14	112	107	20
3	8	13	104	49	-38	1	5	14	125	97	-32
6	8	13	103	52	-42	4	5	14	113	63	-48
-14	9	13	106	78	-40	-10	6	14	99	104	-42
-11	9	13	204	196	18	-7	6	14	72	34	-46
-8	9	13	260	236	14	-4	6	14	83	14	-39
-5	9	13	116	126	22	-1	6	14	79	92	-41

Table 50. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
2	6	14	165	144	25
5	6	14	108	80	-38
-12	7	14	41	18	-82
-9	7	14	95	1	-49
-6	7	14	66	36	-50
-3	7	14	188	191	25
0	7	14	240	247	13
3	7	14	189	191	24
6	7	14	88	85	-46
-11	8	14	60	42	-63
-8	8	14	71	12	-45
-5	8	14	128	91	-34
-2	8	14	143	146	-33
1	8	14	116	96	-39
4	8	14	108	72	-35
-13	9	14	64	9	-62
-10	9	14	41	3	-82
-7	9	14	63	3	-59
-4	9	14	98	65	-39
-1	9	14	134	100	-34
2	9	14	71	74	-60
-12	10	14	42	26	-84
-9	10	14	79	8	-50
-6	10	14	100	110	-43
-3	10	14	211	197	20
0	10	14	170	151	25
-11	11	14	42	9	-73
-8	11	14	41	42	-82
-5	11	14	108	80	-50
-2	11	14	93	71	-43
1	11	14	115	53	-37
-10	12	14	104	23	-50
-7	12	14	68	22	-54
-4	12	14	107	78	-35
-1	12	14	76	57	-53
-9	13	14	74	14	-52
-6	13	14	97	89	-43
0	0	15	77	1	-59
1	1	15	241	256	17
-1	2	15	258	253	15
2	2	15	197	202	34
-3	3	15	40	2	-69
0	3	15	65	3	-51
3	3	15	67	21	-57

APPENDIX C

TABLE 51

Table 51. Cyclohexane (chair) Thiourea Host/Guest Adduct
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
-1	2	0	852	843	10	-13	17	0	132	121	-32
0	3	0	2827	2984	16	-10	17	0	234	225	15
-2	4	0	920	922	11	-7	17	0	242	230	17
-4	5	0	1164	1108	12	-4	17	0	121	120	24
-1	5	0	1164	1036	11	-1	17	0	58	27	-58
-3	6	0	115	128	13	-15	18	0	93	41	-44
0	6	0	477	564	5	-12	18	0	98	77	-37
-5	7	0	104	160	-31	-9	18	0	111	92	-30
-2	7	0	70	143	-22	-6	18	0	131	70	-41
-7	8	0	510	491	8	-3	18	0	111	29	-33
-4	8	0	566	463	5	0	18	0	92	26	-37
-1	8	0	513	470	7	-17	19	0	40	4	-81
-6	9	0	113	147	15	-14	19	0	108	54	-32
-3	9	0	123	161	15	-11	19	0	114	116	-35
0	9	0	378	386	7	-8	19	0	133	121	-32
-8	10	0	270	270	9	-5	19	0	73	59	-50
-5	10	0	282	260	9	-2	19	0	70	3	-47
-2	10	0	273	262	14	-16	20	0	73	57	-53
-10	11	0	43	7	-55	-13	20	0	147	137	-44
-7	11	0	323	328	9	-10	20	0	180	186	28
-4	11	0	323	333	9	-7	20	0	141	134	26
-1	11	0	64	3	-44	-4	20	0	100	49	-44
-9	12	0	111	123	22	-15	21	0	95	57	-43
-6	12	0	228	233	14	-12	21	0	89	75	-45
-3	12	0	75	121	-48	-9	21	0	108	70	-50
0	12	0	113	126	21	-6	21	0	70	48	-53
-11	13	0	92	33	-35	-14	22	0	64	9	-61
-8	13	0	79	81	-42	-11	22	0	142	33	-50
-5	13	0	90	75	-40	-8	22	0	105	13	-50
-2	13	0	90	27	-33	-1	1	1	58	56	9
-13	14	0	58	58	-47	-3	2	1	206	224	5
-10	14	0	215	181	18	0	2	1	36	39	-19
-7	14	0	343	337	13	-5	3	1	1466	1438	23
-4	14	0	215	199	13	-2	3	1	208	197	4
-1	14	0	95	71	-28	1	3	1	1295	1311	19
-12	15	0	95	111	-28	-7	4	1	87	58	16
-9	15	0	142	157	20	-4	4	1	25	72	-44
-6	15	0	141	161	21	-1	4	1	1302	1346	22
-3	15	0	135	110	26	2	4	1	211	201	9
0	15	0	95	50	-31	-9	5	1	520	471	6
-14	16	0	65	16	-50	-6	5	1	1715	1704	10
-11	16	0	88	65	-35	-3	5	1	1469	1371	22
-8	16	0	115	115	23	0	5	1	51	30	-27
-5	16	0	55	67	-51	3	5	1	37	20	-46
-2	16	0	36	20	-74	-11	6	1	282	299	18
-16	17	0	38	35	-77	-8	6	1	1169	1196	11

Table 51. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-5	6	1	1719	1701	22
-2	6	1	214	212	7
1	6	1	631	611	7
4	6	1	234	263	13
-13	7	1	81	16	-32
-10	7	1	161	140	13
-7	7	1	83	26	-31
-4	7	1	89	25	-23
-1	7	1	637	628	6
2	7	1	368	354	10
5	7	1	240	221	13
-15	8	1	212	205	19
-12	8	1	369	335	9
-9	8	1	939	934	7
-6	8	1	1179	1171	10
-3	8	1	35	15	-47
0	8	1	44	6	-40
3	8	1	117	122	20
6	8	1	198	208	14
-17	9	1	67	46	-49
-14	9	1	275	295	12
-11	9	1	657	690	7
-8	9	1	943	904	8
-5	9	1	516	482	7
-2	9	1	363	391	8
1	9	1	112	78	-26
4	9	1	138	113	21
7	9	1	44	22	-60
-19	10	1	59	37	-58
-16	10	1	62	6	-50
-13	10	1	138	124	-32
-10	10	1	62	6	-40
-7	10	1	145	162	22
-4	10	1	241	267	10
-1	10	1	80	71	-38
2	10	1	97	33	-36
5	10	1	35	51	-70
8	10	1	82	23	-37
-21	11	1	58	12	-59
-18	11	1	77	3	-47
-15	11	1	190	185	20
-12	11	1	466	485	9
-9	11	1	658	704	15
-6	11	1	284	307	10
-3	11	1	125	144	23
0	11	1	74	10	-36
3	11	1	120	111	25
6	11	1	50	18	-58
9	11	1	40	18	-81
-20	12	1	71	14	-51
-17	12	1	37	72	-75
-14	12	1	306	328	19
-11	12	1	464	472	9
-8	12	1	380	332	13
-5	12	1	241	249	11
-2	12	1	98	17	-40
1	12	1	176	180	24
4	12	1	98	67	-29
7	12	1	39	55	-79
10	12	1	41	20	-82
-22	13	1	76	8	-45
-19	13	1	49	42	-66
-16	13	1	93	53	-40
-13	13	1	53	12	-41
-10	13	1	139	114	28
-7	13	1	63	15	-41
-4	13	1	135	112	19
-1	13	1	186	187	22
2	13	1	102	95	-29
5	13	1	118	110	23
8	13	1	75	24	-49
-21	14	1	79	26	-54
-18	14	1	80	16	-49
-15	14	1	139	140	23
-12	14	1	301	316	18
-9	14	1	291	291	11
-6	14	1	200	217	26
-3	14	1	96	119	-26
0	14	1	82	7	-40
3	14	1	37	45	-74
6	14	1	65	3	-59
-20	15	1	59	11	-63
-17	15	1	61	49	-40
-14	15	1	151	141	31
-11	15	1	196	177	15
-8	15	1	215	206	13
-5	15	1	67	57	-47
-2	15	1	77	90	-43
1	15	1	120	80	-28
4	15	1	86	88	-52
-19	16	1	104	14	-32
-16	16	1	71	1	-33

Table 51. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-13	16	1	53	40	-52
-10	16	1	96	11	-33
-7	16	1	79	23	-37
-4	16	1	82	67	-38
-1	16	1	99	87	-35
2	16	1	149	114	-34
5	16	1	41	49	-83
-18	17	1	40	8	-80
-15	17	1	38	46	-54
-12	17	1	111	59	-31
-9	17	1	79	39	-43
-6	17	1	69	18	-49
-3	17	1	52	36	-59
0	17	1	62	5	-48
3	17	1	59	7	-64
-20	18	1	41	2	-83
-17	18	1	61	3	-59
-14	18	1	50	19	-63
-11	18	1	37	5	-75
-8	18	1	90	26	-38
-5	18	1	128	106	22
-2	18	1	115	111	-31
1	18	1	120	101	-33
-19	19	1	41	7	-71
-16	19	1	62	23	-59
-13	19	1	39	44	-79
-10	19	1	84	40	-40
-7	19	1	59	54	-59
-4	19	1	97	89	-38
-1	19	1	118	103	-36
-18	20	1	59	8	-64
-15	20	1	107	2	-47
-12	20	1	66	16	-52
-9	20	1	63	19	-59
-6	20	1	49	0	-69
-3	20	1	87	8	-47
-14	21	1	75	17	-49
-11	21	1	52	7	-68
-8	21	1	97	20	-37
-5	21	1	74	51	-51
-13	22	1	72	2	-58
-10	22	1	41	15	-82
0	1	2	806	656	14
-2	2	2	1561	1547	20
1	2	2	225	199	9
-4	3	2	95	80	14
-1	3	2	230	229	10
2	3	2	723	720	14
-6	4	2	122	90	18
-3	4	2	100	79	15
0	4	2	1209	1126	1
3	4	2	984	971	1
-8	5	2	638	605	7
-5	5	2	76	234	-18
-2	5	2	725	638	16
1	5	2	794	770	1
4	5	2	317	343	8
-10	6	2	432	419	10
-7	6	2	144	86	11
-4	6	2	117	79	13
-1	6	2	795	687	9
2	6	2	967	1014	13
5	6	2	282	293	11
-12	7	2	142	146	25
-9	7	2	76	94	-28
-6	7	2	135	91	13
-3	7	2	1010	1095	14
0	7	2	1280	1279	12
3	7	2	864	829	7
6	7	2	423	405	15
-14	8	2	77	59	-47
-11	8	2	119	126	19
-8	8	2	63	103	-34
-5	8	2	636	549	7
-2	8	2	965	903	10
1	8	2	493	514	12
4	8	2	399	443	21
7	8	2	149	143	18
-16	9	2	70	48	-42
-13	9	2	87	78	-33
-10	9	2	62	80	-43
-7	9	2	66	165	-28
-4	9	2	322	256	8
-1	9	2	494	517	9
2	9	2	230	286	14
5	9	2	86	74	-42
8	9	2	36	24	-73
-18	10	2	55	20	-54
-15	10	2	61	5	-49
-12	10	2	107	87	-28
-9	10	2	57	57	-45
-6	10	2	435	495	7

Table 51. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-3	10	2	863	898	6
0	10	2	559	517	7
3	10	2	433	423	9
6	10	2	125	111	23
9	10	2	39	25	-78
-20	11	2	80	23	-51
-17	11	2	108	18	-33
-14	11	2	60	2	-48
-11	11	2	78	74	-27
-8	11	2	117	139	20
-5	11	2	283	259	10
-2	11	2	235	247	11
1	11	2	211	249	17
4	11	2	110	136	24
7	11	2	77	18	-40
10	11	2	40	3	-81
-22	12	2	41	6	-84
-19	12	2	39	4	-78
-16	12	2	54	27	-56
-13	12	2	34	76	-70
-10	12	2	121	104	20
-7	12	2	139	126	18
-4	12	2	392	433	13
-1	12	2	217	241	14
2	12	2	159	187	19
5	12	2	78	31	-47
8	12	2	107	29	-46
-21	13	2	59	29	-59
-18	13	2	86	55	-34
-15	13	2	56	44	-50
-12	13	2	47	82	-56
-9	13	2	107	111	-24
-6	13	2	422	437	10
-3	13	2	439	441	9
0	13	2	330	330	12
3	13	2	175	159	36
6	13	2	81	8	-41
9	13	2	57	5	-66
-20	14	2	78	52	-50
-17	14	2	103	128	-31
-14	14	2	170	171	18
-11	14	2	61	5	-48
-8	14	2	76	61	-42
-5	14	2	73	57	-34
-2	14	2	181	186	15
1	14	2	116	88	24
4	14	2	38	26	-77
7	14	2	41	10	-82
-19	15	2	68	35	-47
-16	15	2	112	95	-29
-13	15	2	85	26	-44
-10	15	2	68	12	-46
-7	15	2	155	136	-46
-4	15	2	123	129	-29
-1	15	2	87	82	-40
2	15	2	82	36	-32
5	15	2	123	30	-48
-21	16	2	121	28	-36
-18	16	2	88	80	-43
-15	16	2	109	113	-28
-12	16	2	65	38	-46
-9	16	2	62	45	-51
-6	16	2	105	106	-28
-3	16	2	150	159	20
0	16	2	70	71	-33
3	16	2	40	5	-81
-20	17	2	85	86	-54
-17	17	2	176	179	20
-14	17	2	145	136	27
-11	17	2	78	31	-35
-8	17	2	113	38	-44
-5	17	2	47	21	-62
-2	17	2	87	36	-31
1	17	2	79	3	-44
-19	18	2	83	60	-43
-16	18	2	89	77	-42
-13	18	2	105	57	22
-10	18	2	37	28	-75
-7	18	2	52	24	-60
-4	18	2	74	29	-44
-1	18	2	73	0	-54
2	18	2	41	21	-83
-18	19	2	101	55	-40
-15	19	2	113	37	-32
-12	19	2	82	1	-50
-9	19	2	95	29	-40
-6	19	2	39	11	-79
-3	19	2	65	6	-58
0	19	2	58	22	-55
-17	20	2	97	81	-39
-14	20	2	65	54	-60
-11	20	2	65	31	-52

Table 51. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-8	20	2	104	38	-36
-5	20	2	86	35	-42
-2	20	2	55	18	-68
-16	21	2	90	28	-52
-13	21	2	103	33	-38
-10	21	2	74	11	-55
-7	21	2	81	14	-48
-12	22	2	94	7	-51
-9	22	2	79	6	-47
0	0	3	91	22	-28
1	1	3	2050	2096	39
-1	2	3	2075	2112	71
2	2	3	1552	1538	30
-3	3	3	43	18	-33
0	3	3	25	33	-44
3	3	3	58	19	-26
-5	4	3	1349	1319	12
-2	4	3	1568	1491	31
1	4	3	750	742	16
4	4	3	238	222	10
-7	5	3	707	740	12
-4	5	3	1359	1349	21
-1	5	3	754	749	17
2	5	3	298	278	7
5	5	3	69	8	-40
-9	6	3	269	245	8
-6	6	3	53	8	-32
-3	6	3	43	30	-34
0	6	3	52	13	-29
3	6	3	227	225	10
6	6	3	143	140	31
-11	7	3	174	207	19
-8	7	3	89	95	-23
-5	7	3	716	683	17
-2	7	3	303	252	9
1	7	3	217	230	9
4	7	3	149	143	20
7	7	3	54	24	-50
-13	8	3	309	288	10
-10	8	3	43	3	-53
-7	8	3	100	84	-29
-4	8	3	234	235	10
-1	8	3	223	243	10
2	8	3	74	13	-39
5	8	3	142	136	20
8	8	3	284	276	19
-15	9	3	282	299	15
-12	9	3	34	35	-69
-9	9	3	52	18	-42
-6	9	3	277	265	13
-3	9	3	228	225	10
0	9	3	76	19	-31
3	9	3	182	175	30
6	9	3	188	191	19
9	9	3	206	198	20
-17	10	3	36	8	-74
-14	10	3	34	23	-69
-11	10	3	34	11	-69
-8	10	3	53	11	-47
-5	10	3	56	34	-44
-2	10	3	70	19	-33
1	10	3	34	15	-68
4	10	3	34	22	-69
7	10	3	71	23	-48
10	10	3	72	3	-53
-19	11	3	158	149	32
-16	11	3	252	250	15
-13	11	3	100	54	-25
-10	11	3	42	43	-58
-7	11	3	174	225	15
-4	11	3	135	141	19
-1	11	3	70	18	-37
2	11	3	128	131	25
5	11	3	153	146	-45
8	11	3	156	154	30
-21	12	3	112	81	-37
-18	12	3	160	153	25
-15	12	3	154	149	34
-12	12	3	76	14	-35
-9	12	3	93	13	-30
-6	12	3	108	134	22
-3	12	3	177	179	17
0	12	3	64	2	-37
3	12	3	108	91	-35
6	12	3	127	118	19
9	12	3	113	82	-36
-20	13	3	40	0	-81
-17	13	3	37	29	-76
-14	13	3	73	71	-36
-11	13	3	84	46	-37
-8	13	3	312	296	11
-5	13	3	145	128	18

Table 51. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-2	13	3	118	109	24
1	13	3	115	79	-39
4	13	3	75	10	-38
7	13	3	107	22	-40
-19	14	3	40	78	-82
-16	14	3	113	60	-28
-13	14	3	94	58	-43
-10	14	3	34	37	-70
-7	14	3	46	21	-55
-4	14	3	84	29	-42
-1	14	3	71	79	-47
2	14	3	121	86	26
5	14	3	120	95	-36
-21	15	3	41	21	-83
-18	15	3	39	2	-78
-15	15	3	72	0	-39
-12	15	3	136	146	21
-9	15	3	278	299	12
-6	15	3	208	189	21
-3	15	3	106	88	-31
0	15	3	62	2	-47
3	15	3	94	68	-40
6	15	3	94	42	-52
-20	16	3	66	44	-55
-17	16	3	102	65	-36
-14	16	3	91	67	-36
-11	16	3	259	258	13
-8	16	3	274	272	13
-5	16	3	148	130	23
-2	16	3	113	79	-26
1	16	3	39	2	-78
4	16	3	41	8	-82
-19	17	3	94	41	-50
-16	17	3	82	67	-51
-13	17	3	105	37	-40
-10	17	3	49	6	-60
-7	17	3	36	13	-74
-4	17	3	47	2	-64
-1	17	3	69	2	-48
2	17	3	62	27	-61
-18	18	3	80	1	-44
-15	18	3	64	6	-49
-12	18	3	160	161	17
-9	18	3	203	204	17
-6	18	3	142	122	18
-3	18	3	104	74	-36
0	18	3	51	3	-60
-17	19	3	93	43	-42
-14	19	3	84	91	-46
-11	19	3	160	160	27
-8	19	3	177	156	24
-5	19	3	116	95	-41
-2	19	3	70	31	-51
-16	20	3	88	49	-51
-13	20	3	40	8	-80
-10	20	3	40	3	-80
-7	20	3	89	24	-50
-4	20	3	54	8	-68
-15	21	3	41	21	-82
-12	21	3	117	79	-44
-9	21	3	122	76	-48
-6	21	3	76	39	-51
-1	1	4	420	246	5
-3	2	4	345	340	7
0	2	4	1220	1300	16
-5	3	4	254	196	8
-2	3	4	352	317	7
1	3	4	524	542	14
-7	4	4	501	542	6
-4	4	4	238	305	7
-1	4	4	528	580	20
2	4	4	514	475	10
-9	5	4	426	414	7
-6	5	4	511	439	9
-3	5	4	254	197	8
0	5	4	479	426	10
3	5	4	29	26	-60
-11	6	4	278	308	10
-8	6	4	272	262	8
-5	6	4	518	418	8
-2	6	4	508	457	13
1	6	4	342	349	7
4	6	4	418	405	8
-13	7	4	244	231	12
-10	7	4	816	820	13
-7	7	4	864	925	12
-4	7	4	503	582	10
-1	7	4	340	370	9
2	7	4	238	260	17
5	7	4	34	31	-68
-15	8	4	35	51	-71
-12	8	4	121	133	25

Table 51. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-9	8	4	521	523	8
-6	8	4	278	250	10
-3	8	4	29	46	-59
0	8	4	198	219	15
3	8	4	85	116	-30
6	8	4	35	65	-70
-17	9	4	63	9	-47
-14	9	4	134	130	-34
-11	9	4	435	454	10
-8	9	4	521	522	7
-5	9	4	437	409	9
-2	9	4	246	252	10
1	9	4	175	157	20
4	9	4	85	50	-38
7	9	4	44	37	-63
-19	10	4	59	53	-59
-16	10	4	147	107	20
-13	10	4	436	425	14
-10	10	4	1034	1044	12
-7	10	4	830	830	14
-4	10	4	427	409	7
-1	10	4	187	185	14
2	10	4	91	64	-31
5	10	4	82	43	-31
8	10	4	83	65	-32
-21	11	4	41	4	-82
-18	11	4	98	90	-27
-15	11	4	156	173	20
-12	11	4	287	310	12
-9	11	4	445	447	8
-6	11	4	280	291	10
-3	11	4	103	92	-28
0	11	4	88	60	-28
3	11	4	103	86	-33
6	11	4	73	72	-42
9	11	4	70	6	-57
-20	12	4	40	1	-81
-17	12	4	91	62	-37
-14	12	4	84	28	-34
-11	12	4	285	302	11
-8	12	4	109	117	-28
-5	12	4	58	21	-43
-2	12	4	60	84	-48
1	12	4	52	37	-53
4	12	4	69	62	-45
7	12	4	39	3	-79
-19	13	4	40	17	-80
-16	13	4	87	58	-37
-13	13	4	260	272	11
-10	13	4	437	424	13
-7	13	4	252	232	16
-4	13	4	103	74	-31
-1	13	4	50	4	-54
2	13	4	82	63	-41
5	13	4	59	46	-59
8	13	4	99	11	-40
-21	14	4	67	27	-55
-18	14	4	50	58	-67
-15	14	4	88	87	-36
-12	14	4	56	21	-53
-9	14	4	123	127	23
-6	14	4	93	70	-33
-3	14	4	107	85	-32
0	14	4	102	120	-33
3	14	4	145	123	18
6	14	4	91	41	-51
-20	15	4	68	7	-53
-17	15	4	87	24	-40
-14	15	4	106	94	-39
-11	15	4	155	160	25
-8	15	4	83	34	-36
-5	15	4	94	46	-37
-2	15	4	83	76	-45
1	15	4	89	69	-27
4	15	4	72	40	-55
-19	16	4	41	16	-82
-16	16	4	89	45	-44
-13	16	4	93	57	-38
-10	16	4	105	101	-28
-7	16	4	75	39	-39
-4	16	4	101	53	-44
-1	16	4	101	67	-23
2	16	4	67	57	-59
-18	17	4	40	22	-81
-15	17	4	58	36	-59
-12	17	4	60	65	-54
-9	17	4	65	6	-51
-6	17	4	38	76	-76
-3	17	4	140	130	18
0	17	4	127	124	25
3	17	4	104	73	-42
-17	18	4	40	31	-82

Table 51. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-14	18	4	57	64	-61
-11	18	4	103	86	-27
-8	18	4	86	68	-28
-5	18	4	58	57	-60
-2	18	4	40	60	-81
1	18	4	41	45	-84
-16	19	4	69	18	-58
-13	19	4	59	22	-59
-10	19	4	89	57	-49
-7	19	4	71	5	-54
-4	19	4	77	40	-53
-1	19	4	99	46	-42
-15	20	4	40	7	-81
-12	20	4	57	9	-63
-9	20	4	62	4	-59
-6	20	4	79	46	-53
-3	20	4	72	75	-55
-14	21	4	87	28	-44
-11	21	4	41	3	-82
-8	21	4	41	14	-83
0	1	5	51	40	-27
-2	2	5	36	39	-35
1	2	5	671	708	5
-4	3	5	693	657	5
-1	3	5	677	691	10
2	3	5	271	288	9
-6	4	5	390	423	8
-3	4	5	702	673	12
0	4	5	39	29	-33
3	4	5	149	170	13
-8	5	5	686	708	12
-5	5	5	60	10	-27
-2	5	5	271	278	7
1	5	5	317	297	7
4	5	5	635	641	18
-10	6	5	54	66	-48
-7	6	5	277	251	11
-4	6	5	393	401	10
-1	6	5	319	332	10
2	6	5	710	687	19
5	6	5	456	462	11
-12	7	5	240	223	16
-9	7	5	207	187	14
-6	7	5	287	268	10
-3	7	5	157	172	15
0	7	5	31	23	-54
3	7	5	96	106	-26
6	7	5	59	63	-44
-14	8	5	74	16	-44
-11	8	5	90	82	-30
-8	8	5	32	8	-56
-5	8	5	694	698	6
-2	8	5	718	675	17
1	8	5	769	797	2
4	8	5	483	505	13
7	8	5	58	18	-51
-16	9	5	68	56	-51
-13	9	5	110	127	-28
-10	9	5	112	127	22
-7	9	5	199	183	16
-4	9	5	643	653	14
-1	9	5	787	814	17
2	9	5	573	563	13
5	9	5	176	175	18
8	9	5	55	69	-60
-18	10	5	108	16	-44
-15	10	5	90	47	-31
-12	10	5	113	89	22
-9	10	5	104	118	-23
-6	10	5	76	71	-36
-3	10	5	127	117	18
0	10	5	34	1	-60
3	10	5	80	48	-39
6	10	5	130	84	-29
9	10	5	86	10	-38
-20	11	5	40	15	-81
-17	11	5	68	49	-52
-14	11	5	60	74	-46
-11	11	5	62	5	-35
-8	11	5	64	72	-46
-5	11	5	463	458	9
-2	11	5	570	581	9
1	11	5	418	440	23
4	11	5	91	101	-35
7	11	5	47	17	-67
10	11	5	83	6	-53
-19	12	5	84	31	-45
-16	12	5	112	89	-38
-13	12	5	44	12	-60
-10	12	5	81	79	-34
-7	12	5	244	228	13
-4	12	5	485	517	8

Table 51. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
-1	12	5	421	431	10	-2	17	5	68	48	-56
2	12	5	199	196	17	1	17	5	41	15	-82
5	12	5	90	94	-30	-19	18	5	91	65	-48
8	12	5	69	3	-57	-16	18	5	99	101	-42
-21	13	5	66	7	-56	-13	18	5	104	29	-46
-18	13	5	79	32	-51	-10	18	5	66	11	-54
-15	13	5	125	129	24	-7	18	5	105	9	-45
-12	13	5	95	13	-26	-4	18	5	53	8	-65
-9	13	5	108	123	-26	-1	18	5	81	13	-52
-6	13	5	96	63	-30	-18	19	5	42	65	-104
-3	13	5	35	39	-71	-15	19	5	105	63	-38
0	13	5	49	5	-50	-12	19	5	50	34	-69
3	13	5	67	62	-53	-9	19	5	68	24	-50
6	13	5	40	17	-80	-6	19	5	59	23	-61
-20	14	5	48	12	-70	-3	19	5	41	11	-82
-17	14	5	91	29	-47	-14	20	5	80	11	-45
-14	14	5	37	5	-64	-11	20	5	70	17	-55
-11	14	5	84	87	-35	-8	20	5	76	4	-54
-8	14	5	54	14	-47	-5	20	5	63	1	-62
-5	14	5	191	190	15	-13	21	5	73	8	-57
-2	14	5	203	201	15	-10	21	5	101	1	-50
1	14	5	84	75	-40	-7	21	5	41	5	-145
4	14	5	77	16	-51	0	0	6	551	465	12
7	14	5	41	2	-145	1	1	6	683	764	6
-19	15	5	62	69	-58	-1	2	6	690	772	13
-16	15	5	177	176	19	2	2	6	1202	1179	20
-13	15	5	159	137	24	-3	3	6	1266	1217	17
-10	15	5	87	55	-36	0	3	6	1386	1389	20
-7	15	5	35	21	-72	3	3	6	902	928	16
-4	15	5	116	95	-36	-5	4	6	337	286	13
-1	15	5	104	70	-28	-2	4	6	1212	1198	22
2	15	5	49	56	-68	1	4	6	337	307	15
5	15	5	41	2	-83	4	4	6	124	100	26
-18	16	5	164	108	-52	-7	5	6	317	315	9
-15	16	5	177	175	24	-4	5	6	344	313	7
-12	16	5	124	92	-31	-1	5	6	335	320	12
-9	16	5	88	69	-41	2	5	6	261	239	9
-6	16	5	82	95	-40	5	5	6	142	128	20
-3	16	5	71	63	-51	-9	6	6	51	57	-49
0	16	5	80	1	-45	-6	6	6	278	267	9
3	16	5	41	11	-82	-3	6	6	915	908	20
-17	17	5	40	3	-71	0	6	6	462	481	9
-14	17	5	74	28	-45	3	6	6	99	80	-29
-11	17	5	79	52	-43	6	6	6	90	9	-38
-8	17	5	82	80	-48	-11	7	6	88	20	-28
-5	17	5	111	93	-30	-8	7	6	77	77	-33

Table 51. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-5	7	6	311	329	8
-2	7	6	277	260	9
1	7	6	77	39	-40
4	7	6	34	52	-69
7	7	6	241	249	19
-13	8	6	119	118	-38
-10	8	6	77	57	-36
-7	8	6	100	53	-32
-4	8	6	127	150	17
-1	8	6	55	35	-46
2	8	6	138	130	28
5	8	6	90	98	-31
8	8	6	108	126	-28
-15	9	6	139	132	21
-12	9	6	34	10	-69
-9	9	6	156	169	15
-6	9	6	47	40	-51
-3	9	6	93	42	-39
0	9	6	124	135	22
3	9	6	67	14	-39
6	9	6	115	136	-27
9	9	6	128	128	26
-17	10	6	228	224	13
-14	10	6	205	204	15
-11	10	6	84	71	-41
-8	10	6	108	64	-27
-5	10	6	161	129	16
-2	10	6	144	128	17
1	10	6	82	30	-39
4	10	6	189	201	23
7	10	6	213	239	13
10	10	6	83	91	-48
-19	11	6	85	39	-43
-16	11	6	104	93	-35
-13	11	6	109	108	-30
-10	11	6	81	53	-33
-7	11	6	60	58	-44
-4	11	6	70	59	-45
-1	11	6	34	33	-69
2	11	6	114	116	-29
5	11	6	139	111	23
8	11	6	40	45	-81
-18	12	6	120	100	-33
-15	12	6	133	58	-48
-12	12	6	56	24	-43
-9	12	6	34	9	-69
-6	12	6	69	27	-44
-3	12	6	34	30	-69
0	12	6	98	70	-40
3	12	6	124	32	-31
6	12	6	136	99	-35
-20	13	6	119	63	-36
-17	13	6	137	107	-32
-14	13	6	92	52	-30
-11	13	6	123	100	-28
-8	13	6	111	105	23
-5	13	6	115	104	-34
-2	13	6	150	116	32
1	13	6	79	31	-45
4	13	6	105	120	-31
7	13	6	101	64	-35
-19	14	6	59	4	-63
-16	14	6	92	0	-47
-13	14	6	79	58	-39
-10	14	6	198	196	19
-7	14	6	248	248	25
-4	14	6	205	209	20
-1	14	6	109	24	-32
2	14	6	57	29	-59
5	14	6	40	3	-82
-18	15	6	125	66	-43
-15	15	6	89	60	-31
-12	15	6	98	68	-29
-9	15	6	157	147	20
-6	15	6	147	139	30
-3	15	6	94	30	-37
0	15	6	38	13	-67
3	15	6	76	56	-49
-17	16	6	40	34	-81
-14	16	6	39	3	-78
-11	16	6	103	78	-30
-8	16	6	132	124	22
-5	16	6	129	121	26
-2	16	6	39	26	-78
1	16	6	63	27	-55
-19	17	6	41	16	-83
-16	17	6	64	33	-59
-13	17	6	159	112	30
-10	17	6	218	228	12
-7	17	6	241	240	12
-4	17	6	61	119	-62
-1	17	6	85	27	-51

Table 51. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
2	17	6	41	25	-84
-18	18	6	85	32	-42
-15	18	6	109	68	-41
-12	18	6	114	113	-31
-9	18	6	125	131	27
-6	18	6	92	93	-38
-3	18	6	86	56	-41
0	18	6	89	37	-48
-17	19	6	62	19	-58
-14	19	6	55	8	-66
-11	19	6	71	35	-56
-8	19	6	64	46	-59
-5	19	6	51	4	-68
-2	19	6	41	23	-82
-13	20	6	82	66	-54
-10	20	6	137	89	-34
-7	20	6	42	58	-84
-1	1	7	40	22	-39
-3	2	7	335	361	8
0	2	7	45	26	-35
-5	3	7	217	226	12
-2	3	7	333	327	10
1	3	7	302	296	21
-7	4	7	82	56	-30
-4	4	7	30	17	-52
-1	4	7	307	306	12
2	4	7	245	276	12
-9	5	7	558	575	14
-6	5	7	375	404	13
-3	5	7	207	229	12
0	5	7	57	14	-38
3	5	7	488	502	11
-11	6	7	397	398	14
-8	6	7	590	578	8
-5	6	7	376	390	9
-2	6	7	236	260	14
1	6	7	212	216	11
4	6	7	75	45	-36
-13	7	7	71	19	-46
-10	7	7	80	77	-34
-7	7	7	39	3	-51
-4	7	7	71	59	-33
-1	7	7	209	220	16
2	7	7	73	95	-37
5	7	7	158	164	18
-15	8	7	71	20	-49
-12	8	7	375	388	10
-9	8	7	642	652	8
-6	8	7	588	595	9
-3	8	7	498	505	7
0	8	7	57	4	-36
3	8	7	78	47	-35
6	8	7	56	30	-54
-17	9	7	96	68	-47
-14	9	7	192	199	23
-11	9	7	433	447	15
-8	9	7	639	654	13
-5	9	7	569	577	7
-2	9	7	109	117	22
1	9	7	81	64	-35
4	9	7	69	76	-47
7	9	7	88	66	-33
-19	10	7	51	17	-69
-16	10	7	72	87	-44
-13	10	7	36	12	-72
-10	10	7	65	4	-38
-7	10	7	48	71	-56
-4	10	7	75	46	-36
-1	10	7	78	61	-31
2	10	7	35	31	-71
5	10	7	72	38	-49
8	10	7	72	9	-50
-18	11	7	39	7	-80
-15	11	7	109	90	-35
-12	11	7	307	303	16
-9	11	7	444	445	9
-6	11	7	401	407	9
-3	11	7	58	64	-50
0	11	7	80	8	-35
3	11	7	81	67	-38
6	11	7	55	48	-63
9	11	7	41	14	-83
-20	12	7	95	3	-51
-17	12	7	57	77	-61
-14	12	7	170	170	18
-11	12	7	314	310	13
-8	12	7	381	382	12
-5	12	7	167	171	19
-2	12	7	52	50	-54
1	12	7	66	9	-44
4	12	7	104	70	-39
7	12	7	40	29	-82

Table 51. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-19	13	7	76	11	-53
-16	13	7	65	32	-50
-13	13	7	36	1	-64
-10	13	7	36	13	-72
-7	13	7	69	24	-41
-4	13	7	90	74	-42
-1	13	7	36	4	-73
2	13	7	118	107	18
5	13	7	66	16	-58
-18	14	7	40	21	-81
-15	14	7	96	85	-35
-12	14	7	173	168	20
-9	14	7	202	191	18
-6	14	7	62	33	-46
-3	14	7	49	50	-60
0	14	7	77	7	-35
3	14	7	109	33	-41
-17	15	7	54	47	-65
-14	15	7	99	84	-41
-11	15	7	92	83	-36
-8	15	7	37	8	-74
-5	15	7	73	33	-41
-2	15	7	110	97	23
1	15	7	161	147	22
4	15	7	68	61	-61
-19	16	7	63	6	-62
-16	16	7	52	4	-58
-13	16	7	57	41	-59
-10	16	7	108	92	-28
-7	16	7	102	71	-35
-4	16	7	87	79	-38
-1	16	7	161	153	-44
2	16	7	110	86	-36
-18	17	7	41	13	-83
-15	17	7	103	54	-44
-12	17	7	91	79	-42
-9	17	7	96	68	-37
-6	17	7	49	59	-67
-3	17	7	62	45	-55
0	17	7	41	2	-71
-17	18	7	101	11	-44
-14	18	7	75	20	-55
-11	18	7	50	8	-67
-8	18	7	39	14	-80
-5	18	7	40	11	-81
-2	18	7	103	85	-42
-16	19	7	41	10	-83
-13	19	7	41	10	-82
-10	19	7	57	10	-63
-7	19	7	41	29	-82
-4	19	7	102	66	-36
-12	20	7	76	8	-50
-9	20	7	67	13	-53
0	1	8	109	77	-34
-2	2	8	270	257	12
1	2	8	188	198	11
-4	3	8	227	228	17
-1	3	8	166	181	13
2	3	8	71	63	-30
-6	4	8	180	195	13
-3	4	8	229	203	11
0	4	8	429	454	7
3	4	8	428	445	14
-8	5	8	118	121	23
-5	5	8	191	220	19
-2	5	8	77	99	-27
1	5	8	279	284	10
4	5	8	171	177	17
-10	6	8	238	230	13
-7	6	8	228	221	18
-4	6	8	182	184	15
-1	6	8	288	288	10
2	6	8	219	206	12
5	6	8	210	220	14
-12	7	8	85	2	-35
-9	7	8	34	55	-68
-6	7	8	219	204	15
-3	7	8	441	418	11
0	7	8	725	731	8
3	7	8	507	511	9
6	7	8	130	141	21
-14	8	8	87	56	-37
-11	8	8	99	98	-29
-8	8	8	224	234	13
-5	8	8	120	154	25
-2	8	8	214	221	15
1	8	8	334	330	13
4	8	8	86	77	-32
7	8	8	64	26	-53
-16	9	8	52	38	-62
-13	9	8	55	41	-54
-10	9	8	132	111	25

Table 51. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
-7	9	8	34	60	-68	-8	14	8	48	55	-61
-4	9	8	170	195	16	-5	14	8	140	94	-37
-1	9	8	323	348	10	-2	14	8	46	17	-64
2	9	8	286	291	28	1	14	8	81	58	-46
5	9	8	105	99	-30	4	14	8	73	32	-51
8	9	8	113	23	-35	-16	15	8	40	46	-81
-18	10	8	57	21	-63	-13	15	8	111	53	-36
-15	10	8	65	36	-52	-10	15	8	94	42	-45
-12	10	8	94	47	-31	-7	15	8	86	39	-35
-9	10	8	108	115	-25	-4	15	8	138	117	18
-6	10	8	241	233	13	-1	15	8	93	62	-34
-3	10	8	511	507	8	2	15	8	64	13	-60
0	10	8	621	658	12	-18	16	8	101	26	-51
3	10	8	274	274	17	-15	16	8	50	44	-68
6	10	8	96	88	-33	-12	16	8	49	38	-66
9	10	8	81	28	-45	-9	16	8	85	40	-37
-17	11	8	113	33	-34	-6	16	8	99	89	-47
-14	11	8	65	71	-52	-3	16	8	80	46	-43
-11	11	8	96	17	-33	0	16	8	88	31	-45
-8	11	8	99	113	-45	-17	17	8	124	74	-44
-5	11	8	216	242	27	-14	17	8	97	78	-37
-2	11	8	271	291	12	-11	17	8	88	35	-50
1	11	8	205	203	16	-8	17	8	39	16	-79
4	11	8	110	109	22	-5	17	8	85	31	-50
7	11	8	85	42	-46	-2	17	8	60	16	-62
-19	12	8	41	19	-83	-16	18	8	97	25	-41
-16	12	8	77	38	-44	-13	18	8	56	11	-65
-13	12	8	64	17	-52	-10	18	8	49	26	-70
-10	12	8	82	50	-36	-7	18	8	40	50	-82
-7	12	8	97	7	-33	-4	18	8	78	34	-48
-4	12	8	87	85	-32	-12	19	8	80	18	-47
-1	12	8	212	206	15	-9	19	8	54	26	-68
2	12	8	61	23	-55	-6	19	8	61	7	-59
5	12	8	40	22	-80	0	0	9	34	4	-83
-18	13	8	97	11	-50	1	1	9	910	937	15
-15	13	8	68	51	-48	-1	2	9	924	927	11
-12	13	8	65	19	-51	2	2	9	653	650	10
-9	13	8	75	40	-39	-3	3	9	57	1	-38
-6	13	8	155	143	27	0	3	9	87	6	-25
-3	13	8	282	269	12	3	3	9	111	119	-25
0	13	8	166	178	19	-5	4	9	325	332	14
3	13	8	79	48	-51	-2	4	9	655	653	13
6	13	8	91	11	-52	1	4	9	454	462	11
-17	14	8	95	78	-50	4	4	9	132	110	-33
-14	14	8	131	94	27	-7	5	9	184	182	14
-11	14	8	37	74	-75	-4	5	9	326	316	9

Table 51. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-1	5	9	467	456	24
2	5	9	314	310	12
5	5	9	65	10	-40
-9	6	9	94	78	-26
-6	6	9	92	8	-38
-3	6	9	118	126	21
0	6	9	71	4	-40
3	6	9	92	85	-37
6	6	9	119	125	24
-11	7	9	88	88	-35
-8	7	9	165	167	16
-5	7	9	183	187	14
-2	7	9	314	294	11
1	7	9	129	94	-43
4	7	9	46	41	-58
7	7	9	37	23	-75
-13	8	9	131	110	-29
-10	8	9	35	13	-71
-7	8	9	139	146	21
-4	8	9	120	94	-28
-1	8	9	112	94	-27
2	8	9	35	28	-70
5	8	9	166	175	27
8	8	9	169	146	23
-15	9	9	95	95	-34
-12	9	9	85	106	-33
-9	9	9	44	10	-51
-6	9	9	88	67	-33
-3	9	9	81	82	-34
0	9	9	45	3	-52
3	9	9	68	69	-43
6	9	9	162	162	25
9	9	9	142	112	-36
-17	10	9	40	16	-81
-14	10	9	86	21	-34
-11	10	9	36	15	-72
-8	10	9	48	11	-57
-5	10	9	35	20	-70
-2	10	9	75	23	-40
1	10	9	36	38	-73
4	10	9	38	7	-76
7	10	9	57	7	-64
-19	11	9	100	89	-48
-16	11	9	96	84	-36
-13	11	9	108	90	-29
-10	11	9	52	1	-55
-7	11	9	94	64	-39
-4	11	9	91	48	-32
-1	11	9	64	35	-50
2	11	9	79	29	-37
5	11	9	125	123	-27
8	11	9	98	80	-42
-18	12	9	116	64	-31
-15	12	9	65	38	-56
-12	12	9	62	7	-43
-9	12	9	87	93	-32
-6	12	9	137	118	-34
-3	12	9	107	64	-33
0	12	9	66	3	-38
3	12	9	124	79	-47
6	12	9	121	90	-36
-17	13	9	41	17	-82
-14	13	9	125	72	-36
-11	13	9	116	91	-27
-8	13	9	111	118	-31
-5	13	9	153	173	20
-2	13	9	87	26	-37
1	13	9	74	28	-50
4	13	9	49	4	-70
-16	14	9	114	57	-41
-13	14	9	98	79	-35
-10	14	9	59	34	-52
-7	14	9	49	32	-61
-4	14	9	93	6	-34
-1	14	9	39	29	-78
2	14	9	40	28	-82
-15	15	9	40	4	-70
-12	15	9	90	31	-45
-9	15	9	114	94	-33
-6	15	9	153	159	29
-3	15	9	67	78	-57
0	15	9	62	1	-54
-17	16	9	76	6	-56
-14	16	9	62	56	-62
-11	16	9	110	89	-49
-8	16	9	160	150	22
-5	16	9	146	121	23
-2	16	9	40	29	-81
1	16	9	73	28	-57
-16	17	9	52	7	-70
-13	17	9	107	20	-45
-10	17	9	67	20	-53

Table 51. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-7	17	9	50	4	-69
-4	17	9	55	3	-65
-1	17	9	42	26	-84
-12	18	9	74	66	-51
-9	18	9	95	112	-39
-6	18	9	99	87	-45
-11	19	9	100	91	-41
-8	19	9	62	78	-61
-1	1	10	95	45	-28
-3	2	10	135	120	21
0	2	10	203	200	11
-5	3	10	136	153	19
-2	3	10	121	121	19
1	3	10	45	17	-66
-7	4	10	411	417	9
-4	4	10	449	453	11
-1	4	10	75	22	-43
2	4	10	62	29	-42
-9	5	10	135	136	28
-6	5	10	268	286	15
-3	5	10	158	161	28
0	5	10	51	43	-41
3	5	10	171	184	17
-11	6	10	90	92	-36
-8	6	10	269	287	14
-5	6	10	277	278	14
-2	6	10	81	30	-41
1	6	10	34	54	-69
4	6	10	144	166	21
-13	7	10	197	171	17
-10	7	10	356	361	13
-7	7	10	577	592	11
-4	7	10	418	411	15
-1	7	10	84	52	-28
2	7	10	54	50	-48
5	7	10	112	86	-37
-15	8	10	87	78	-42
-12	8	10	198	208	17
-9	8	10	240	236	20
-6	8	10	272	287	14
-3	8	10	181	184	15
0	8	10	93	35	-29
3	8	10	70	50	-38
6	8	10	56	19	-58
-17	9	10	89	5	-42
-14	9	10	39	24	-78
-11	9	10	107	94	-27
-8	9	10	238	233	15
-5	9	10	117	132	24
-2	9	10	35	40	-71
1	9	10	36	12	-73
4	9	10	63	43	-46
7	9	10	40	34	-81
-16	10	10	123	58	-37
-13	10	10	217	206	15
-10	10	10	277	293	15
-7	10	10	361	354	18
-4	10	10	167	166	17
-1	10	10	36	5	-73
2	10	10	100	5	-43
5	10	10	63	27	-53
8	10	10	41	10	-83
-18	11	10	41	8	-83
-15	11	10	40	72	-81
-12	11	10	145	124	-32
-9	11	10	110	89	-26
-6	11	10	96	91	-29
-3	11	10	64	49	-50
0	11	10	62	38	-48
3	11	10	59	21	-59
6	11	10	62	8	-63
-17	12	10	72	14	-57
-14	12	10	63	82	-59
-11	12	10	113	134	-33
-8	12	10	203	205	20
-5	12	10	110	91	-33
-2	12	10	80	14	-36
1	12	10	39	38	-78
4	12	10	63	1	-60
-16	13	10	41	81	-83
-13	13	10	177	178	20
-10	13	10	212	205	14
-7	13	10	188	173	25
-4	13	10	38	54	-77
-1	13	10	97	23	-46
2	13	10	83	34	-44
-15	14	10	61	46	-61
-12	14	10	101	74	-35
-9	14	10	39	26	-78
-6	14	10	64	21	-54
-3	14	10	55	24	-61
0	14	10	107	88	-34

Table 51. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
3	14	10	136	60	-52	-14	8	11	114	71	-34
-14	15	10	82	50	-48	-11	8	11	69	36	-51
-11	15	10	70	74	-57	-8	8	11	70	3	-44
-8	15	10	79	78	-46	-5	8	11	35	39	-72
-5	15	10	97	35	-48	-2	8	11	354	356	12
-2	15	10	54	46	-66	1	8	11	329	327	12
1	15	10	81	44	-47	4	8	11	164	151	18
-13	16	10	59	76	-65	7	8	11	81	81	-46
-10	16	10	97	59	-35	-16	9	11	71	15	-57
-7	16	10	66	40	-58	-13	9	11	38	12	-78
-4	16	10	73	6	-50	-10	9	11	91	20	-45
-1	16	10	41	36	-83	-7	9	11	119	119	25
-12	17	10	90	12	-51	-4	9	11	227	247	18
-9	17	10	97	2	-41	-1	9	11	325	332	16
-6	17	10	94	8	-44	2	9	11	237	241	15
-3	17	10	76	60	-50	5	9	11	144	119	27
-11	18	10	62	6	-64	8	9	11	60	13	-64
-8	18	10	73	9	-59	-15	10	11	40	18	-81
0	1	11	34	0	-59	-12	10	11	49	11	-65
-2	2	11	54	3	-40	-9	10	11	54	22	-57
1	2	11	34	52	-69	-6	10	11	76	93	-41
-4	3	11	138	126	20	-3	10	11	97	12	-37
-1	3	11	49	56	-53	0	10	11	53	2	-53
2	3	11	287	288	14	3	10	11	111	33	-46
-6	4	11	158	146	20	6	10	11	71	7	-58
-3	4	11	133	125	-39	-17	11	11	106	17	-46
0	4	11	58	4	-41	-14	11	11	86	14	-50
3	4	11	76	65	-37	-11	11	11	52	0	-54
-8	5	11	92	42	-43	-8	11	11	61	38	-54
-5	5	11	42	2	-52	-5	11	11	160	146	19
-2	5	11	284	281	13	-2	11	11	254	247	22
1	5	11	459	463	18	1	11	11	191	165	33
4	5	11	248	243	14	4	11	11	119	78	-35
-10	6	11	99	95	-38	-16	12	11	41	13	-82
-7	6	11	155	156	26	-13	12	11	78	52	-53
-4	6	11	158	156	19	-10	12	11	38	10	-77
-1	6	11	466	476	13	-7	12	11	126	108	26
2	6	11	343	367	16	-4	12	11	155	153	19
5	6	11	154	139	27	-1	12	11	173	162	25
-12	7	11	101	109	-35	2	12	11	110	115	-36
-9	7	11	130	122	21	-15	13	11	41	44	-83
-6	7	11	166	159	16	-12	13	11	40	53	-81
-3	7	11	66	80	-44	-9	13	11	38	16	-77
0	7	11	46	9	-54	-6	13	11	39	9	-78
3	7	11	37	15	-74	-3	13	11	99	42	-38
6	7	11	91	0	-43	0	13	11	49	3	-61

Table 51. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
3	13	11	62	1	-62
-14	14	11	69	2	-47
-11	14	11	99	21	-42
-8	14	11	71	81	-50
-5	14	11	115	128	-29
-2	14	11	139	119	29
1	14	11	102	64	-39
-13	15	11	41	38	-83
-10	15	11	40	23	-81
-7	15	11	97	81	-41
-4	15	11	82	76	-54
-1	15	11	41	62	-84
-12	16	11	54	12	-68
-9	16	11	77	11	-54
-6	16	11	54	1	-67
-3	16	11	67	5	-54
-11	17	11	77	15	-49
-8	17	11	73	14	-57
0	0	12	861	873	20
1	1	12	358	368	10
-1	2	12	369	367	10
2	2	12	110	89	-25
-3	3	12	478	481	8
0	3	12	451	453	13
3	3	12	190	184	15
-5	4	12	195	207	22
-2	4	12	102	85	-27
1	4	12	185	181	16
4	4	12	89	75	-40
-7	5	12	36	12	-73
-4	5	12	200	209	23
-1	5	12	189	186	28
2	5	12	36	28	-73
5	5	12	124	65	-45
-9	6	12	88	53	-45
-6	6	12	198	209	14
-3	6	12	196	184	20
0	6	12	174	178	16
3	6	12	70	72	-41
6	6	12	39	67	-79
-11	7	12	75	80	-44
-8	7	12	78	75	-36
-5	7	12	36	2	-73
-2	7	12	49	15	-59
1	7	12	102	62	-35
4	7	12	95	87	-37
7	7	12	117	102	-40
-13	8	12	107	23	-47
-10	8	12	83	38	-30
-7	8	12	116	89	-34
-4	8	12	100	81	-35
-1	8	12	66	66	-51
2	8	12	110	83	23
5	8	12	70	44	-56
8	8	12	89	47	-44
-15	9	12	104	59	-51
-12	9	12	78	52	-44
-9	9	12	72	75	-38
-6	9	12	53	55	-59
-3	9	12	95	68	-35
0	9	12	96	101	-32
3	9	12	39	14	-79
6	9	12	64	40	-56
-14	10	12	99	67	-39
-11	10	12	68	14	-54
-8	10	12	68	24	-40
-5	10	12	65	54	-47
-2	10	12	109	79	-24
1	10	12	101	10	-45
4	10	12	118	56	-49
-13	11	12	107	12	-40
-10	11	12	55	9	-61
-7	11	12	123	78	-31
-4	11	12	116	91	-38
-1	11	12	39	13	-78
2	11	12	70	6	-56
-15	12	12	42	39	-84
-12	12	12	64	39	-50
-9	12	12	99	61	-45
-6	12	12	101	77	-37
-3	12	12	58	23	-61
0	12	12	98	28	-32
3	12	12	42	23	-84
-14	13	12	41	24	-83
-11	13	12	78	23	-53
-8	13	12	82	9	-43
-5	13	12	85	36	-47
-2	13	12	90	2	-49
1	13	12	111	22	-47
-13	14	12	50	18	-72
-10	14	12	81	65	-54
-7	14	12	103	101	-36

Table 51. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-4	14	12	78	56	-47
-1	14	12	41	20	-83
-12	15	12	61	44	-65
-9	15	12	119	65	-30
-6	15	12	95	43	-42
-3	15	12	41	23	-83
-8	16	12	90	44	-52
-1	1	13	59	4	-42
-3	2	13	78	67	-46
0	2	13	35	8	-62
-5	3	13	192	199	17
-2	3	13	65	67	-49
1	3	13	99	67	-32
-7	4	13	46	21	-64
-4	4	13	61	0	-47
-1	4	13	65	59	-50
2	4	13	76	85	-42
-9	5	13	145	122	15
-6	5	13	240	262	14
-3	5	13	197	197	20
0	5	13	70	2	-36
3	5	13	105	67	-30
-11	6	13	140	104	-31
-8	6	13	249	247	13
-5	6	13	254	264	13
-2	6	13	104	92	-31
1	6	13	66	70	-52
4	6	13	38	12	-77
-13	7	13	68	1	-58
-10	7	13	72	37	-49
-7	7	13	49	1	-56
-4	7	13	37	19	-75
-1	7	13	122	73	23
2	7	13	86	73	-45
5	7	13	115	62	-30
-12	8	13	133	108	26
-9	8	13	230	229	24
-6	8	13	254	249	10
-3	8	13	87	72	-38
0	8	13	68	1	-43
3	8	13	103	52	-38
6	8	13	102	48	-42
-14	9	13	105	75	-40
-11	9	13	203	196	18
-8	9	13	258	230	14
-5	9	13	115	127	22
-2	9	13	82	77	-41
1	9	13	57	3	-61
4	9	13	78	28	-47
-13	10	13	41	23	-84
-10	10	13	72	1	-46
-7	10	13	53	37	-65
-4	10	13	39	11	-78
-1	10	13	90	1	-48
2	10	13	40	4	-81
-12	11	13	155	143	-44
-9	11	13	217	193	23
-6	11	13	92	108	-40
-3	11	13	78	58	-52
0	11	13	51	5	-60
3	11	13	74	25	-52
-11	12	13	150	142	25
-8	12	13	143	104	28
-5	12	13	81	63	-48
-2	12	13	95	2	-42
1	12	13	89	41	-44
-10	13	13	41	25	-83
-7	13	13	60	7	-58
-4	13	13	41	32	-82
-1	13	13	96	47	-51
-9	14	13	123	75	-36
-6	14	13	118	55	-47
-3	14	13	56	37	-68
0	1	14	69	17	-39
-2	2	14	91	25	-38
1	2	14	99	32	-45
-4	3	14	83	60	-42
-1	3	14	66	18	-51
2	3	14	97	104	-23
-6	4	14	76	17	-39
-3	4	14	47	42	-63
0	4	14	169	158	25
3	4	14	195	186	32
-8	5	14	95	85	-39
-5	5	14	61	41	-33
-2	5	14	111	104	20
1	5	14	124	91	-32
4	5	14	112	65	-48
-10	6	14	98	101	-42
-7	6	14	71	34	-46
-4	6	14	82	7	-39
-1	6	14	78	92	-41

Table 51. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
2	6	14	163	142	25
5	6	14	107	77	-38
-12	7	14	40	19	-82
-9	7	14	94	0	-49
-6	7	14	65	38	-50
-3	7	14	187	187	25
0	7	14	238	239	13
3	7	14	187	191	24
6	7	14	87	85	-46
-11	8	14	60	38	-63
-8	8	14	71	12	-45
-5	8	14	127	95	-34
-2	8	14	142	143	-33
1	8	14	115	96	-39
4	8	14	107	73	-35
-13	9	14	63	10	-62
-10	9	14	41	1	-82
-7	9	14	62	1	-59
-4	9	14	97	60	-39
-1	9	14	133	94	-34
2	9	14	70	75	-60
-12	10	14	41	24	-84
-9	10	14	78	7	-50
-6	10	14	99	108	-43
-3	10	14	209	189	20
0	10	14	169	149	25
-11	11	14	42	4	-73
-8	11	14	41	41	-82
-5	11	14	107	81	-50
-2	11	14	92	73	-43
1	11	14	114	50	-37
-10	12	14	103	20	-50
-7	12	14	67	22	-54
-4	12	14	106	73	-35
-1	12	14	76	56	-53
-9	13	14	73	15	-52
-6	13	14	96	88	-43
0	0	15	76	10	-59
1	1	15	238	256	17
-1	2	15	255	248	15
2	2	15	195	205	34
-3	3	15	40	3	-69
0	3	15	64	1	-51
3	3	15	67	14	-57

APPENDIX D

TABLE 52

Table 52. Bicyclo[2.2.2]octane Thiourea Host/Guest Adduct F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
-1	2	0	380	425	2	-13	17	0	216	233	8
0	3	0	2436	3054	21	-10	17	0	400	424	13
-2	4	0	956	886	17	-7	17	0	402	418	13
-4	5	0	1382	1420	7	-4	17	0	209	238	7
-1	5	0	1398	1422	25	-1	17	0	75	86	16
-3	6	0	73	65	4	-15	18	0	128	105	9
0	6	0	562	538	10	-12	18	0	183	166	7
-5	7	0	25	18	-12	-9	18	0	225	201	6
-2	7	0	28	6	-13	-6	18	0	191	160	7
-7	8	0	710	703	6	-3	18	0	120	112	9
-4	8	0	722	582	14	0	18	0	106	95	11
-1	8	0	716	684	11	-17	19	0	36	2	-31
-6	9	0	256	288	3	-14	19	0	95	99	11
-3	9	0	259	258	7	-11	19	0	229	220	11
0	9	0	600	553	8	-8	19	0	234	219	14
-8	10	0	358	360	7	-5	19	0	113	101	14
-5	10	0	336	317	8	-2	19	0	42	2	-29
-2	10	0	356	379	5	-19	20	0	63	52	-22
-10	11	0	21	12	-23	-16	20	0	137	136	13
-7	11	0	438	408	7	-13	20	0	274	298	12
-4	11	0	438	419	12	-10	20	0	370	403	9
-1	11	0	50	22	10	-7	20	0	289	291	10
-9	12	0	42	83	-13	-4	20	0	145	141	11
-6	12	0	187	214	7	-1	20	0	75	52	-27
-3	12	0	39	86	-13	-18	21	0	100	87	12
0	12	0	105	134	6	-15	21	0	132	139	15
-11	13	0	56	30	12	-12	21	0	182	170	13
-8	13	0	62	92	10	-9	21	0	187	167	8
-5	13	0	65	117	-22	-6	21	0	135	137	12
-2	13	0	64	30	9	-3	21	0	74	86	18
-13	14	0	88	102	9	0	21	0	47	40	-27
-10	14	0	316	273	10	-20	22	0	54	17	-26
-7	14	0	541	476	9	-17	22	0	63	21	-20
-4	14	0	320	273	9	-14	22	0	25	43	-44
-1	14	0	89	98	11	-11	22	0	101	106	18
-12	15	0	169	156	9	-8	22	0	48	41	-26
-9	15	0	202	208	6	-5	22	0	37	16	-33
-6	15	0	196	195	6	-2	22	0	26	15	-47
-3	15	0	181	159	9	-22	23	0	56	3	-30
0	15	0	139	112	6	-19	23	0	26	22	-46
-14	16	0	70	36	12	-16	23	0	74	69	-19
-11	16	0	125	126	7	-13	23	0	123	132	11
-8	16	0	198	203	6	-10	23	0	119	130	11
-5	16	0	123	139	7	-7	23	0	88	71	14
-2	16	0	71	36	15	-4	23	0	41	24	-31
-16	17	0	69	81	17	-1	23	0	27	2	-47

Table 52. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-21	24	0	27	8	-47
-18	24	0	26	28	-46
-15	24	0	47	27	-32
-12	24	0	25	4	-45
-9	24	0	55	29	-29
-6	24	0	60	28	-22
-3	24	0	27	7	-47
-20	25	0	28	15	-48
-17	25	0	51	27	-28
-14	25	0	56	72	-26
-11	25	0	80	69	-21
-8	25	0	27	27	-48
-5	25	0	39	16	-38
-19	26	0	62	28	-26
-16	26	0	47	44	-32
-13	26	0	83	41	-28
-10	26	0	61	44	-28
-7	26	0	64	28	-29
-15	27	0	28	18	-49
-12	27	0	28	17	-50
-1	1	1	56	51	6
-3	2	1	293	274	5
0	2	1	40	42	4
-5	3	1	1578	1568	24
-2	3	1	290	313	2
1	3	1	1264	1250	16
-7	4	1	207	220	4
-4	4	1	26	2	-10
-1	4	1	1273	1231	20
2	4	1	107	65	4
-9	5	1	534	504	11
-6	5	1	1699	1748	20
-3	5	1	1569	1632	7
0	5	1	19	7	-13
3	5	1	113	102	19
-11	6	1	376	395	9
-8	6	1	1418	1380	28
-5	6	1	1687	1752	22
-2	6	1	102	67	4
1	6	1	858	806	11
4	6	1	412	384	7
-13	7	1	37	8	-15
-10	7	1	176	164	4
-7	7	1	29	12	-13
-4	7	1	208	193	5
-1	7	1	862	807	11
2	7	1	434	416	6
5	7	1	354	361	5
-15	8	1	389	383	8
-12	8	1	553	540	12
-9	8	1	1198	1141	19
-6	8	1	1406	1394	16
-3	8	1	99	105	5
0	8	1	46	2	-14
3	8	1	220	217	4
6	8	1	324	321	6
-17	9	1	148	143	8
-14	9	1	456	457	18
-11	9	1	927	926	20
-8	9	1	1184	1156	12
-5	9	1	531	488	8
-2	9	1	440	455	10
1	9	1	149	133	5
4	9	1	134	137	7
7	9	1	58	27	-16
-19	10	1	72	88	14
-16	10	1	20	17	-43
-13	10	1	218	189	6
-10	10	1	53	13	12
-7	10	1	175	168	6
-4	10	1	414	392	7
-1	10	1	154	133	7
2	10	1	31	10	-19
5	10	1	107	107	8
8	10	1	48	2	-20
-21	11	1	36	1	-30
-18	11	1	41	52	-21
-15	11	1	350	343	8
-12	11	1	729	714	13
-9	11	1	923	921	16
-6	11	1	377	379	4
-3	11	1	226	224	5
0	11	1	22	1	-19
3	11	1	211	196	6
6	11	1	45	9	-17
9	11	1	91	79	12
-23	12	1	34	1	-35
-20	12	1	72	68	14
-17	12	1	191	178	8
-14	12	1	549	527	15
-11	12	1	711	728	6
-8	12	1	554	520	14

Table 52. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
-5	12	1	361	366	12	-25	16	1	92	80	19
-2	12	1	16	23	-28	-22	16	1	54	43	-29
1	12	1	237	237	5	-19	16	1	48	17	-27
4	12	1	122	125	11	-16	16	1	33	1	-25
7	12	1	117	116	9	-13	16	1	81	92	10
10	12	1	25	44	-44	-10	16	1	28	7	-26
-25	13	1	45	42	-30	-7	16	1	57	29	-20
-22	13	1	49	5	-28	-4	16	1	129	130	11
-19	13	1	71	79	18	-1	16	1	165	158	10
-16	13	1	80	85	11	2	16	1	224	233	8
-13	13	1	18	1	-28	5	16	1	119	132	14
-10	13	1	217	195	5	8	16	1	48	25	-32
-7	13	1	31	8	-17	11	16	1	52	41	-29
-4	13	1	140	139	6	-27	17	1	57	12	-32
-1	13	1	245	231	5	-24	17	1	26	2	-46
2	13	1	138	130	7	-21	17	1	31	26	-36
5	13	1	190	193	9	-18	17	1	55	75	-18
8	13	1	48	37	-28	-15	17	1	151	152	14
11	13	1	26	4	-46	-12	17	1	180	178	10
-27	14	1	42	30	-37	-9	17	1	149	135	9
-24	14	1	34	8	-37	-6	17	1	44	19	-19
-21	14	1	39	17	-31	-3	17	1	21	38	-37
-18	14	1	44	36	-17	0	17	1	31	0	-27
-15	14	1	295	289	6	3	17	1	41	25	-30
-12	14	1	538	538	14	6	17	1	38	1	-35
-9	14	1	448	446	11	9	17	1	28	37	-49
-6	14	1	324	327	5	-26	18	1	80	74	18
-3	14	1	211	207	10	-23	18	1	54	39	-30
0	14	1	32	3	-21	-20	18	1	59	35	-26
3	14	1	45	40	-20	-17	18	1	60	78	-20
6	14	1	23	18	-41	-14	18	1	56	34	-16
9	14	1	51	29	-28	-11	18	1	61	55	-21
12	14	1	36	45	-40	-8	18	1	21	1	-38
-26	15	1	105	82	23	-5	18	1	185	193	14
-23	15	1	77	61	18	-2	18	1	233	230	7
-20	15	1	57	19	-23	1	18	1	241	243	10
-17	15	1	139	147	8	4	18	1	135	130	18
-14	15	1	290	298	7	7	18	1	62	10	-23
-11	15	1	339	347	9	-25	19	1	87	53	-29
-8	15	1	382	380	8	-22	19	1	26	29	-46
-5	15	1	106	115	9	-19	19	1	51	1	-20
-2	15	1	140	133	7	-16	19	1	51	23	-21
1	15	1	154	162	8	-13	19	1	68	79	16
4	15	1	210	207	14	-10	19	1	70	79	13
7	15	1	89	81	14	-7	19	1	106	122	10
10	15	1	48	4	-28	-4	19	1	206	205	7

Table 52. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-1	19	1	242	243	13
2	19	1	144	161	12
5	19	1	69	69	-21
-24	20	1	42	1	-32
-21	20	1	32	26	-39
-18	20	1	49	38	-22
-15	20	1	52	21	-21
-12	20	1	66	68	-20
-9	20	1	80	81	13
-6	20	1	35	18	-32
-3	20	1	57	25	-26
0	20	1	30	1	-34
3	20	1	37	13	-37
6	20	1	77	44	-29
-23	21	1	45	16	-30
-20	21	1	26	26	-45
-17	21	1	45	24	-29
-14	21	1	24	16	-43
-11	21	1	41	7	-30
-8	21	1	54	39	-19
-5	21	1	123	131	10
-2	21	1	166	160	12
1	21	1	92	99	16
4	21	1	41	18	-36
-25	22	1	29	15	-50
-22	22	1	49	0	-25
-19	22	1	57	27	-25
-16	22	1	66	41	-25
-13	22	1	38	1	-33
-10	22	1	57	43	-19
-7	22	1	91	80	13
-4	22	1	123	128	12
-1	22	1	91	100	15
2	22	1	60	54	-25
-24	23	1	73	18	-28
-21	23	1	39	15	-35
-18	23	1	50	39	-31
-15	23	1	75	61	-19
-12	23	1	26	4	-45
-9	23	1	59	26	-27
-6	23	1	35	2	-37
-3	23	1	45	14	-29
0	23	1	27	1	-41
-23	24	1	55	18	-25
-20	24	1	27	2	-48
-17	24	1	32	1	-39
-14	24	1	48	3	-25
-11	24	1	31	4	-39
-8	24	1	26	26	-46
-5	24	1	69	69	-20
-2	24	1	63	56	-30
-22	25	1	28	14	-50
-19	25	1	45	53	-35
-16	25	1	71	82	-24
-13	25	1	40	42	-35
-10	25	1	27	5	-47
-7	25	1	27	10	-48
-4	25	1	42	20	-36
-18	26	1	45	75	-33
-15	26	1	82	81	17
-12	26	1	61	45	-27
-9	26	1	62	38	-28
-6	26	1	29	43	-51
-17	27	1	29	12	-51
-14	27	1	59	30	-28
-11	27	1	28	41	-49
0	1	2	1123	1113	20
-2	2	2	1693	1802	70
1	2	2	356	313	4
-4	3	2	178	170	6
-1	3	2	355	296	9
2	3	2	866	843	11
-6	4	2	148	90	5
-3	4	2	175	179	3
0	4	2	1162	1045	10
3	4	2	1088	1087	14
-8	5	2	794	689	11
-5	5	2	72	88	4
-2	5	2	862	856	8
1	5	2	939	905	9
4	5	2	379	336	7
-10	6	2	593	623	13
-7	6	2	232	203	4
-4	6	2	145	107	5
-1	6	2	941	941	10
2	6	2	1183	1130	15
5	6	2	351	337	6
-12	7	2	141	151	5
-9	7	2	154	137	5
-6	7	2	230	187	5
-3	7	2	1082	1066	5
0	7	2	1423	1330	19

Table 52. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
3	7	2	1123	1122	16
6	7	2	688	661	21
-14	8	2	66	90	10
-11	8	2	184	212	4
-8	8	2	48	43	8
-5	8	2	786	722	6
-2	8	2	1180	1155	19
1	8	2	629	624	10
4	8	2	584	588	14
7	8	2	231	245	7
-16	9	2	131	132	7
-13	9	2	209	181	7
-10	9	2	51	73	9
-7	9	2	150	144	6
-4	9	2	383	338	7
-1	9	2	635	624	11
2	9	2	320	341	5
5	9	2	93	120	8
8	9	2	31	41	-25
-18	10	2	89	76	11
-15	10	2	41	3	-17
-12	10	2	232	173	4
-9	10	2	48	78	9
-6	10	2	594	617	10
-3	10	2	1126	1084	15
0	10	2	734	685	12
3	10	2	715	683	16
6	10	2	228	228	6
9	10	2	28	5	-33
-20	11	2	58	37	-25
-17	11	2	35	22	-26
-14	11	2	18	33	-32
-11	11	2	93	32	6
-8	11	2	182	202	4
-5	11	2	354	353	4
-2	11	2	324	344	8
1	11	2	324	348	5
4	11	2	232	235	9
7	11	2	93	82	11
10	11	2	45	16	-24
-22	12	2	44	20	-30
-19	12	2	47	47	-26
-16	12	2	20	8	-35
-13	12	2	71	93	10
-10	12	2	220	179	5
-7	12	2	133	152	5
-4	12	2	580	590	9
-1	12	2	340	350	4
2	12	2	343	344	9
5	12	2	92	83	17
8	12	2	41	36	-28
11	12	2	39	30	-33
-24	13	2	26	13	-45
-21	13	2	93	86	14
-18	13	2	156	145	12
-15	13	2	122	95	11
-12	13	2	105	98	-34
-9	13	2	201	183	5
-6	13	2	687	662	13
-3	13	2	717	669	20
0	13	2	588	584	12
3	13	2	319	341	7
6	13	2	52	50	-19
9	13	2	58	1	-19
12	13	2	55	31	-28
-26	14	2	41	11	-36
-23	14	2	46	42	-25
-20	14	2	127	127	10
-17	14	2	233	240	9
-14	14	2	275	283	5
-11	14	2	35	22	-21
-8	14	2	70	89	9
-5	14	2	105	124	8
-2	14	2	343	343	5
1	14	2	194	173	6
4	14	2	107	98	10
7	14	2	45	34	-29
10	14	2	79	71	19
13	14	2	58	43	-30
-25	15	2	27	36	-48
-22	15	2	44	32	-30
-19	15	2	86	71	18
-16	15	2	208	185	9
-13	15	2	103	90	11
-10	15	2	19	7	-33
-7	15	2	235	250	6
-4	15	2	230	230	10
-1	15	2	198	172	11
2	15	2	110	93	9
5	15	2	60	33	-19
8	15	2	38	29	-32
11	15	2	46	25	-33

Table 52. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-27	16	2	29	13	-51
-24	16	2	65	13	-22
-21	16	2	66	76	-17
-18	16	2	177	163	8
-15	16	2	204	187	6
-12	16	2	38	0	-21
-9	16	2	135	137	10
-6	16	2	223	225	6
-3	16	2	320	337	6
0	16	2	160	189	7
3	16	2	50	49	-23
6	16	2	53	2	-23
9	16	2	57	55	-34
-26	17	2	65	36	-24
-23	17	2	80	94	-26
-20	17	2	219	204	8
-17	17	2	340	353	12
-14	17	2	223	246	8
-11	17	2	21	27	-37
-8	17	2	50	49	-19
-5	17	2	92	82	9
-2	17	2	102	93	14
1	17	2	30	26	-34
4	17	2	36	26	-24
7	17	2	98	77	21
-25	18	2	58	57	-30
-22	18	2	85	100	-24
-19	18	2	128	137	11
-16	18	2	166	165	8
-13	18	2	164	140	12
-10	18	2	99	84	10
-7	18	2	94	84	14
-4	18	2	116	97	10
-1	18	2	37	28	-28
2	18	2	42	14	-28
5	18	2	60	32	-22
8	18	2	54	29	-31
-24	19	2	63	2	-27
-21	19	2	53	41	-24
-18	19	2	131	133	12
-15	19	2	88	74	12
-12	19	2	23	47	-40
-9	19	2	54	7	-17
-6	19	2	23	49	-40
-3	19	2	36	53	-31
0	19	2	38	4	-29
3	19	2	44	10	-32
6	19	2	27	43	-48
-26	20	2	29	31	-51
-23	20	2	91	88	16
-20	20	2	150	157	9
-17	20	2	205	204	12
-14	20	2	131	125	12
-11	20	2	32	44	-32
-8	20	2	23	38	-41
-5	20	2	46	31	-22
-2	20	2	25	13	-44
1	20	2	54	2	-26
4	20	2	81	53	-22
-25	21	2	59	43	-29
-22	21	2	67	64	-19
-19	21	2	61	44	-28
-16	21	2	71	73	16
-13	21	2	95	90	12
-10	21	2	43	19	-29
-7	21	2	66	32	-19
-4	21	2	55	27	-22
-1	21	2	43	2	-31
2	21	2	27	33	-47
-24	22	2	63	21	-22
-21	22	2	55	64	-27
-18	22	2	85	100	15
-15	22	2	25	29	-44
-12	22	2	54	18	-22
-9	22	2	25	2	-44
-6	22	2	64	2	-26
-3	22	2	62	9	-28
0	22	2	47	21	-28
-23	23	2	85	75	15
-20	23	2	89	89	18
-17	23	2	88	90	18
-14	23	2	44	43	-31
-11	23	2	51	27	-24
-8	23	2	36	31	-37
-5	23	2	60	30	-24
-2	23	2	43	34	-34
1	23	2	40	11	-38
-22	24	2	48	22	-30
-19	24	2	43	2	-35
-16	24	2	32	13	-39
-13	24	2	46	13	-32
-10	24	2	75	73	-21

Table 52. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-7	24	2	99	76	14
-4	24	2	79	54	20
-1	24	2	53	11	-33
-21	25	2	59	44	-27
-18	25	2	85	55	-29
-15	25	2	27	38	-47
-12	25	2	64	34	-26
-9	25	2	66	54	-21
-6	25	2	65	44	-24
-20	26	2	39	31	-41
-17	26	2	70	36	-19
-14	26	2	47	13	-30
-11	26	2	27	25	-48
-8	26	2	45	28	-35
-16	27	2	28	13	-49
-13	27	2	48	43	-32
0	0	3	41	10	-11
1	1	3	2057	2135	80
-1	2	3	1968	2130	95
2	2	3	1674	1623	42
-3	3	3	28	7	-11
0	3	3	27	13	-12
3	3	3	64	48	7
-5	4	3	1442	1453	44
-2	4	3	1611	1628	42
1	4	3	778	817	10
4	4	3	278	286	10
-7	5	3	924	864	18
-4	5	3	1415	1460	17
-1	5	3	776	801	7
2	5	3	451	419	5
5	5	3	76	106	6
-9	6	3	410	342	9
-6	6	3	13	7	-20
-3	6	3	64	50	8
0	6	3	37	6	-10
3	6	3	354	343	5
6	6	3	157	190	7
-11	7	3	185	205	8
-8	7	3	165	150	5
-5	7	3	912	859	3
-2	7	3	456	423	6
1	7	3	330	316	5
4	7	3	245	220	7
7	7	3	18	1	-31
-13	8	3	464	404	8
-10	8	3	34	39	-14
-7	8	3	167	161	5
-4	8	3	277	277	7
-1	8	3	333	323	6
2	8	3	96	96	6
5	8	3	122	95	7
8	8	3	444	444	10
-15	9	3	450	472	9
-12	9	3	16	28	-29
-9	9	3	31	2	-12
-6	9	3	410	335	4
-3	9	3	353	337	5
0	9	3	26	10	-16
3	9	3	271	274	5
6	9	3	290	295	7
9	9	3	383	371	16
-17	10	3	21	0	-36
-14	10	3	29	11	-24
-11	10	3	78	63	11
-8	10	3	20	53	-21
-5	10	3	72	98	7
-2	10	3	100	97	6
1	10	3	52	36	10
4	10	3	28	45	-24
7	10	3	62	47	13
10	10	3	41	3	-25
-19	11	3	302	309	12
-16	11	3	445	435	11
-13	11	3	78	58	9
-10	11	3	77	60	8
-7	11	3	195	205	5
-4	11	3	249	224	4
-1	11	3	57	45	8
2	11	3	137	135	6
5	11	3	226	223	6
8	11	3	325	324	7
11	11	3	152	153	9
-21	12	3	194	206	11
-18	12	3	300	298	13
-15	12	3	220	223	6
-12	12	3	18	4	-27
-9	12	3	42	16	-14
-6	12	3	157	203	6
-3	12	3	264	265	6
0	12	3	31	4	-16
3	12	3	171	163	9

Table 52. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
6	12	3	232	229	6
9	12	3	188	201	25
12	12	3	101	110	19
-23	13	3	58	37	-27
-20	13	3	23	2	-40
-17	13	3	80	67	20
-14	13	3	119	111	7
-11	13	3	77	45	8
-8	13	3	462	395	8
-5	13	3	124	98	7
-2	13	3	133	143	6
1	13	3	129	128	11
4	13	3	54	24	-17
7	13	3	56	61	-22
10	13	3	52	17	-22
13	13	3	45	33	-31
-25	14	3	27	44	-47
-22	14	3	100	106	19
-19	14	3	180	192	8
-16	14	3	130	131	8
-13	14	3	118	112	11
-10	14	3	29	5	-23
-7	14	3	27	9	-23
-4	14	3	38	42	-16
-1	14	3	139	122	6
2	14	3	154	164	8
5	14	3	222	220	13
8	14	3	157	155	12
11	14	3	33	46	-41
-27	15	3	66	33	-25
-24	15	3	71	79	-20
-21	15	3	92	81	16
-18	15	3	65	9	14
-15	15	3	33	3	-22
-12	15	3	209	217	10
-9	15	3	456	473	6
-6	15	3	295	296	8
-3	15	3	171	163	7
0	15	3	33	5	-22
3	15	3	140	151	9
6	15	3	90	113	13
9	15	3	77	85	17
12	15	3	80	43	-26
-26	16	3	36	9	-39
-23	16	3	52	12	-26
-20	16	3	127	107	10
-17	16	3	159	154	9
-14	16	3	127	134	14
-11	16	3	448	435	8
-8	16	3	445	437	8
-5	16	3	224	228	10
-2	16	3	153	165	10
1	16	3	48	26	-25
4	16	3	24	32	-42
7	16	3	26	12	-45
10	16	3	69	30	-22
-25	17	3	62	54	-25
-22	17	3	104	91	18
-19	17	3	106	117	11
-16	17	3	157	151	9
-13	17	3	75	75	12
-10	17	3	21	1	-36
-7	17	3	54	43	-16
-4	17	3	28	24	-30
-1	17	3	47	22	-25
2	17	3	111	94	10
5	17	3	77	69	18
8	17	3	56	27	-28
-24	18	3	55	53	-24
-21	18	3	48	18	-26
-18	18	3	42	0	-23
-15	18	3	23	8	-40
-12	18	3	312	298	6
-9	18	3	370	373	10
-6	18	3	234	231	6
-3	18	3	149	154	9
0	18	3	49	3	-25
3	18	3	51	15	-26
6	18	3	78	15	-29
-26	19	3	49	1	-34
-23	19	3	27	8	-47
-20	19	3	65	48	-18
-17	19	3	101	114	12
-14	19	3	173	199	8
-11	19	3	300	310	6
-8	19	3	321	326	7
-5	19	3	235	224	7
-2	19	3	100	92	12
1	19	3	72	63	-19
4	19	3	26	30	-46
7	19	3	28	11	-50
-25	20	3	54	25	-31

Table 52. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-22	20	3	70	16	-25
-19	20	3	56	47	-23
-16	20	3	108	109	15
-13	20	3	60	8	-24
-10	20	3	30	4	-34
-7	20	3	68	63	16
-4	20	3	34	32	-34
-1	20	3	83	60	15
2	20	3	36	34	-37
5	20	3	34	4	-41
-24	21	3	42	18	-34
-21	21	3	26	1	-40
-18	21	3	38	13	-34
-15	21	3	73	81	16
-12	21	3	197	203	16
-9	21	3	182	199	10
-6	21	3	102	114	15
-3	21	3	46	15	-25
0	21	3	26	1	-40
3	21	3	27	4	-48
-23	22	3	45	22	-34
-20	22	3	56	11	-30
-17	22	3	101	90	16
-14	22	3	106	108	17
-11	22	3	153	148	18
-8	22	3	148	156	11
-5	22	3	68	69	-19
-2	22	3	49	33	-36
1	22	3	72	5	-21
-22	23	3	58	22	-27
-19	23	3	56	7	-29
-16	23	3	65	11	-28
-13	23	3	34	36	-36
-10	23	3	34	16	-36
-7	23	3	65	12	-31
-4	23	3	43	30	-34
-1	23	3	51	4	-31
-21	24	3	47	15	-34
-18	24	3	83	53	-28
-15	24	3	64	81	-21
-12	24	3	105	107	16
-9	24	3	83	86	16
-6	24	3	50	15	-28
-3	24	3	27	4	-47
-20	25	3	57	24	-31
-17	25	3	46	55	-30
-14	25	3	46	43	-33
-11	25	3	76	46	-23
-8	25	3	33	28	-40
-5	25	3	42	4	-36
-19	26	3	45	1	-36
-16	26	3	51	11	-32
-13	26	3	60	32	-23
-10	26	3	40	31	-43
-7	26	3	60	11	-28
-15	27	3	38	33	-42
-12	27	3	55	43	-29
-1	1	4	391	542	6
-3	2	4	412	213	8
0	2	4	1255	1051	31
-5	3	4	264	185	8
-2	3	4	400	201	6
1	3	4	522	656	9
-7	4	4	537	583	18
-4	4	4	176	252	3
-1	4	4	522	653	10
2	4	4	575	505	12
-9	5	4	486	447	10
-6	5	4	582	533	12
-3	5	4	261	192	4
0	5	4	558	446	8
3	5	4	18	12	-21
-11	6	4	429	395	11
-8	6	4	334	365	10
-5	6	4	575	529	3
-2	6	4	574	501	8
1	6	4	430	426	4
4	6	4	522	549	11
-13	7	4	380	369	4
-10	7	4	1051	1007	25
-7	7	4	999	987	19
-4	7	4	529	584	4
-1	7	4	431	424	5
2	7	4	289	256	8
5	7	4	39	20	-18
-15	8	4	88	89	10
-12	8	4	143	146	6
-9	8	4	667	691	13
-6	8	4	336	355	5
-3	8	4	45	26	11
0	8	4	326	318	5
3	8	4	172	155	8

Table 52. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
6	8	4	124	109	8
-17	9	4	55	33	-16
-14	9	4	206	193	6
-11	9	4	609	648	8
-8	9	4	661	707	6
-5	9	4	482	458	9
-2	9	4	293	275	5
1	9	4	273	270	10
4	9	4	125	135	7
7	9	4	125	128	10
-19	10	4	139	143	9
-16	10	4	242	258	9
-13	10	4	678	637	15
-10	10	4	1406	1341	28
-7	10	4	1041	1020	6
-4	10	4	521	555	5
-1	10	4	280	268	10
2	10	4	100	86	7
5	10	4	116	111	7
8	10	4	158	152	10
-21	11	4	44	32	-26
-18	11	4	179	173	7
-15	11	4	295	308	8
-12	11	4	444	483	14
-9	11	4	606	644	6
-6	11	4	429	411	6
-3	11	4	164	163	9
0	11	4	100	114	9
3	11	4	107	112	8
6	11	4	122	109	15
9	11	4	35	15	-31
-23	12	4	25	19	-45
-20	12	4	24	24	-42
-17	12	4	63	67	-17
-14	12	4	55	50	-16
-11	12	4	440	470	11
-8	12	4	138	142	5
-5	12	4	29	8	-18
-2	12	4	96	94	7
1	12	4	55	13	-15
4	12	4	80	74	12
7	12	4	45	16	-26
10	12	4	37	9	-33
-25	13	4	57	38	-29
-22	13	4	37	27	-34
-19	13	4	71	75	14
-16	13	4	159	173	7
-13	13	4	471	447	4
-10	13	4	672	631	11
-7	13	4	370	379	11
-4	13	4	132	129	6
-1	13	4	24	10	-27
2	13	4	129	120	9
5	13	4	121	118	11
8	13	4	59	42	-26
11	13	4	36	8	-38
-24	14	4	48	46	-32
-21	14	4	57	49	-19
-18	14	4	126	122	9
-15	14	4	207	197	6
-12	14	4	32	54	-24
-9	14	4	208	196	5
-6	14	4	129	117	10
-3	14	4	103	112	8
0	14	4	170	179	6
3	14	4	224	225	6
6	14	4	95	101	16
9	14	4	60	35	-25
12	14	4	91	10	-29
-26	15	4	28	13	-49
-23	15	4	53	17	-22
-20	15	4	54	37	-22
-17	15	4	22	4	-39
-14	15	4	191	195	10
-11	15	4	296	295	10
-8	15	4	89	91	12
-5	15	4	115	107	7
-2	15	4	126	122	7
1	15	4	122	116	12
4	15	4	67	75	16
7	15	4	49	28	-29
10	15	4	69	26	-22
-25	16	4	49	41	-29
-22	16	4	44	48	-31
-19	16	4	59	77	-19
-16	16	4	145	171	7
-13	16	4	156	171	9
-10	16	4	247	254	10
-7	16	4	122	128	8
-4	16	4	88	79	16
-1	16	4	111	112	9
2	16	4	134	130	9

Table 52. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
5	16	4	80	70	20
8	16	4	41	13	-35
-24	17	4	71	68	-19
-21	17	4	46	46	-27
-18	17	4	76	76	14
-15	17	4	45	7	-22
-12	17	4	58	67	-16
-9	17	4	30	27	-29
-6	17	4	106	108	9
-3	17	4	220	228	5
0	17	4	273	267	12
3	17	4	181	189	10
6	17	4	59	71	-23
9	17	4	27	27	-48
-26	18	4	40	26	-38
-23	18	4	54	16	-29
-20	18	4	52	52	-25
-17	18	4	78	84	-26
-14	18	4	125	124	9
-11	18	4	174	173	5
-8	18	4	154	156	8
-5	18	4	120	113	10
-2	18	4	143	133	8
1	18	4	95	111	15
4	18	4	67	58	-22
7	18	4	65	36	-30
-25	19	4	47	35	-29
-22	19	4	26	11	-46
-19	19	4	101	101	20
-16	19	4	77	82	15
-13	19	4	75	79	-23
-10	19	4	144	144	8
-7	19	4	23	18	-40
-4	19	4	83	76	-26
-1	19	4	100	109	15
2	19	4	72	84	-19
5	19	4	58	15	-24
-24	20	4	27	29	-47
-21	20	4	26	6	-45
-18	20	4	66	50	-18
-15	20	4	62	40	-23
-12	20	4	68	27	-25
-9	20	4	54	16	-25
-6	20	4	87	98	14
-3	20	4	186	191	13
0	20	4	191	188	13
3	20	4	76	90	-23
-23	21	4	65	12	-28
-20	21	4	44	5	-33
-17	21	4	25	43	-45
-14	21	4	46	50	-29
-11	21	4	62	32	-20
-8	21	4	57	44	-27
-5	21	4	71	68	-18
-2	21	4	85	86	-25
1	21	4	81	61	18
4	21	4	76	48	-23
-22	22	4	39	17	-33
-19	22	4	26	13	-46
-16	22	4	57	45	-24
-13	22	4	35	25	-35
-10	22	4	44	8	-30
-7	22	4	61	25	-22
-4	22	4	61	59	-23
-1	22	4	82	61	21
2	22	4	39	5	-38
-21	23	4	48	12	-30
-18	23	4	45	13	-30
-15	23	4	76	21	-25
-12	23	4	52	16	-29
-9	23	4	48	33	-31
-6	23	4	63	68	-23
-3	23	4	79	91	17
0	23	4	46	53	-33
-20	24	4	39	28	-36
-17	24	4	74	67	-29
-14	24	4	72	48	18
-11	24	4	39	10	-31
-8	24	4	64	11	-29
-5	24	4	81	14	-27
-2	24	4	74	6	-28
-19	25	4	57	36	-26
-16	25	4	54	39	-25
-13	25	4	52	38	-33
-10	25	4	27	27	-47
-7	25	4	55	35	-30
-4	25	4	79	50	-25
-18	26	4	58	25	-30
-15	26	4	27	15	-48
-12	26	4	27	10	-48
-9	26	4	68	27	-29
0	1	5	16	26	-15

Table 52. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-2	2	5	26	59	-11
1	2	5	672	665	17
-4	3	5	747	625	21
-1	3	5	664	683	18
2	3	5	286	239	8
-6	4	5	405	454	4
-3	4	5	736	624	13
0	4	5	15	1	-17
3	4	5	163	194	4
-8	5	5	827	774	1
-5	5	5	47	27	-15
-2	5	5	283	250	4
1	5	5	312	371	8
4	5	5	800	795	10
-10	6	5	89	45	8
-7	6	5	343	297	5
-4	6	5	399	472	4
-1	6	5	306	339	3
2	6	5	842	798	1
5	6	5	592	608	14
-12	7	5	371	322	8
-9	7	5	277	251	6
-6	7	5	335	294	3
-3	7	5	158	190	6
0	7	5	34	11	-13
3	7	5	163	179	8
6	7	5	70	85	9
-14	8	5	36	46	-18
-11	8	5	55	87	11
-8	8	5	27	8	-14
-5	8	5	795	779	8
-2	8	5	823	810	8
1	8	5	995	988	12
4	8	5	707	672	8
7	8	5	86	77	9
-16	9	5	108	107	10
-13	9	5	160	173	13
-10	9	5	179	191	5
-7	9	5	273	271	5
-4	9	5	792	780	6
-1	9	5	998	984	13
2	9	5	783	783	9
5	9	5	315	338	16
8	9	5	167	180	12
-18	10	5	57	57	-19
-15	10	5	20	17	-35
-12	10	5	183	144	10
-9	10	5	175	193	5
-6	10	5	92	47	7
-3	10	5	157	180	5
0	10	5	45	3	-13
3	10	5	79	63	13
6	10	5	135	139	7
9	10	5	47	32	-24
-20	11	5	60	49	-20
-17	11	5	127	131	8
-14	11	5	115	88	13
-11	11	5	18	4	-27
-8	11	5	54	97	10
-5	11	5	593	617	7
-2	11	5	785	789	14
1	11	5	642	626	11
4	11	5	190	200	12
7	11	5	80	75	15
10	11	5	24	11	-43
-22	12	5	25	8	-44
-19	12	5	92	75	12
-16	12	5	158	152	7
-13	12	5	19	12	-34
-10	12	5	169	152	5
-7	12	5	372	322	5
-4	12	5	711	670	9
-1	12	5	645	638	7
2	12	5	369	364	5
5	12	5	204	212	20
8	12	5	24	30	-42
11	12	5	63	43	-27
-24	13	5	33	43	-40
-21	13	5	69	27	-24
-18	13	5	24	35	-51
-15	13	5	202	188	6
-12	13	5	28	20	-24
-9	13	5	153	178	6
-6	13	5	75	92	9
-3	13	5	78	67	12
0	13	5	40	4	-18
3	13	5	100	103	14
6	13	5	23	26	-41
9	13	5	25	38	-44
12	13	5	33	11	-41
-26	14	5	70	23	-22
-23	14	5	26	21	-45

Table 52. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-20	14	5	46	38	-33
-17	14	5	73	63	15
-14	14	5	28	8	-25
-11	14	5	119	90	7
-8	14	5	26	43	-26
-5	14	5	325	329	9
-2	14	5	370	366	10
1	14	5	172	183	7
4	14	5	77	78	17
7	14	5	30	19	-37
10	14	5	80	22	-27
-25	15	5	38	26	-39
-22	15	5	55	58	-24
-19	15	5	142	145	10
-16	15	5	317	314	6
-13	15	5	197	198	7
-10	15	5	20	27	-35
-7	15	5	76	65	11
-4	15	5	192	201	8
-1	15	5	180	189	10
2	15	5	139	151	10
5	15	5	63	26	-22
8	15	5	32	57	-40
11	15	5	28	40	-49
-24	16	5	38	65	-38
-21	16	5	95	101	13
-18	16	5	214	214	15
-15	16	5	301	310	11
-12	16	5	152	160	9
-9	16	5	116	112	10
-6	16	5	133	139	10
-3	16	5	107	107	18
0	16	5	23	3	-34
3	16	5	50	20	-26
6	16	5	60	39	-27
9	16	5	47	39	-34
-26	17	5	28	12	-49
-23	17	5	43	29	-34
-20	17	5	59	33	15
-17	17	5	63	1	-23
-14	17	5	78	63	18
-11	17	5	130	136	8
-8	17	5	171	173	8
-5	17	5	203	211	7
-2	17	5	155	152	8
1	17	5	76	73	14
4	17	5	45	12	-30
7	17	5	36	18	-38
-25	18	5	41	36	-36
-22	18	5	73	68	-21
-19	18	5	165	164	9
-16	18	5	214	210	13
-13	18	5	44	39	-25
-10	18	5	39	52	-26
-7	18	5	65	73	16
-4	18	5	82	76	16
-1	18	5	78	75	17
2	18	5	60	29	-26
5	18	5	57	51	-27
8	18	5	82	54	20
-24	19	5	66	71	-21
-21	19	5	131	132	11
-18	19	5	163	164	9
-15	19	5	141	144	10
-12	19	5	68	83	-18
-9	19	5	32	32	-32
-6	19	5	49	32	-21
-3	19	5	59	22	-19
0	19	5	25	2	-38
3	19	5	27	24	-47
6	19	5	67	44	-27
-23	20	5	46	32	-30
-20	20	5	40	1	-26
-17	20	5	35	31	-25
-14	20	5	24	38	-42
-11	20	5	71	50	18
-8	20	5	24	30	-42
-5	20	5	40	27	-30
-2	20	5	47	30	-27
1	20	5	35	23	-38
4	20	5	55	5	-31
-22	21	5	75	82	19
-19	21	5	122	129	11
-16	21	5	95	99	18
-13	21	5	60	31	-21
-10	21	5	25	14	-43
-7	21	5	45	18	-26
-4	21	5	56	12	-21
-1	21	5	44	25	-32
2	21	5	27	10	-47
-24	22	5	67	62	-25
-21	22	5	100	83	19

Table 52. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-18	22	5	76	67	17
-15	22	5	60	58	-24
-12	22	5	25	9	-44
-9	22	5	43	38	-27
-6	22	5	25	37	-44
-3	22	5	48	25	-27
0	22	5	55	0	-23
-23	23	5	42	0	-35
-20	23	5	63	31	-23
-17	23	5	51	29	-28
-14	23	5	44	24	-32
-11	23	5	55	41	-29
-8	23	5	63	57	-23
-5	23	5	58	51	-29
-2	23	5	27	8	-48
-22	24	5	83	62	-25
-19	24	5	69	70	-20
-16	24	5	69	66	-23
-13	24	5	50	45	-33
-10	24	5	43	21	-35
-7	24	5	27	18	-47
-4	24	5	81	3	-28
-18	25	5	76	36	-27
-15	25	5	50	25	-33
-12	25	5	27	10	-47
-9	25	5	28	39	-49
-6	25	5	63	45	-23
-17	26	5	68	12	-23
-14	26	5	49	24	-29
-11	26	5	48	40	-34
-8	26	5	29	55	-51
0	0	6	526	782	22
1	1	6	743	547	16
-1	2	6	732	556	18
2	2	6	1337	1181	36
-3	3	6	1324	1411	33
0	3	6	1468	1596	33
3	3	6	1059	1029	1
-5	4	6	422	363	9
-2	4	6	1314	1166	35
1	4	6	398	335	8
4	4	6	222	222	8
-7	5	6	403	412	8
-4	5	6	416	342	10
-1	5	6	398	303	11
2	5	6	315	306	6
5	5	6	151	139	5
-9	6	6	114	107	8
-6	6	6	326	310	5
-3	6	6	1020	1035	15
0	6	6	565	546	7
3	6	6	142	139	6
6	6	6	29	45	-21
-11	7	6	78	71	8
-8	7	6	36	22	-11
-5	7	6	399	393	4
-2	7	6	319	304	7
1	7	6	46	13	-16
4	7	6	112	70	9
7	7	6	366	384	12
-13	8	6	189	174	5
-10	8	6	54	20	11
-7	8	6	48	26	-12
-4	8	6	214	195	4
-1	8	6	35	2	-17
2	8	6	155	137	12
5	8	6	175	146	8
8	8	6	207	199	13
-15	9	6	197	190	17
-12	9	6	42	23	-16
-9	9	6	128	183	6
-6	9	6	111	104	9
-3	9	6	143	148	6
0	9	6	92	106	6
3	9	6	27	24	-24
6	9	6	217	206	12
9	9	6	222	222	7
-17	10	6	388	387	14
-14	10	6	285	287	10
-11	10	6	50	11	12
-8	10	6	35	3	-15
-5	10	6	150	147	9
-2	10	6	157	135	6
1	10	6	40	16	-16
4	10	6	287	314	7
7	10	6	420	408	6
10	10	6	204	213	11
-19	11	6	66	90	-18
-16	11	6	134	132	8
-13	11	6	168	183	6
-10	11	6	41	7	-15
-7	11	6	71	72	8

Table 52. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-4	11	6	112	84	9
-1	11	6	33	12	-17
2	11	6	196	181	8
5	11	6	186	181	7
8	11	6	91	110	19
11	11	6	79	111	16
-21	12	6	83	71	14
-18	12	6	188	198	7
-15	12	6	114	100	9
-12	12	6	72	35	9
-9	12	6	28	25	-22
-6	12	6	37	56	-16
-3	12	6	30	33	-21
0	12	6	127	133	7
3	12	6	68	70	13
6	12	6	182	188	15
9	12	6	76	54	17
12	12	6	77	29	-27
-23	13	6	133	127	12
-20	13	6	176	176	8
-17	13	6	208	208	9
-14	13	6	80	75	14
-11	13	6	162	177	7
-8	13	6	193	186	7
-5	13	6	174	148	7
-2	13	6	194	188	6
1	13	6	38	37	-22
4	13	6	214	213	7
7	13	6	163	164	12
10	13	6	115	120	17
13	13	6	73	44	-29
-25	14	6	68	47	-21
-22	14	6	69	79	-18
-19	14	6	58	7	-20
-16	14	6	36	4	-26
-13	14	6	80	77	12
-10	14	6	284	292	7
-7	14	6	366	380	5
-4	14	6	286	308	15
-1	14	6	51	43	-15
2	14	6	27	24	-33
5	14	6	29	14	-36
8	14	6	65	87	-23
11	14	6	41	47	-33
-24	15	6	75	33	-22
-21	15	6	80	79	16
-18	15	6	134	138	17
-15	15	6	113	110	7
-12	15	6	104	110	9
-9	15	6	198	186	6
-6	15	6	216	210	7
-3	15	6	63	67	16
0	15	6	66	50	12
3	15	6	124	134	10
6	15	6	67	59	-20
9	15	6	27	24	-48
-26	16	6	28	36	-50
-23	16	6	84	89	-25
-20	16	6	83	81	18
-17	16	6	87	75	13
-14	16	6	49	7	-23
-11	16	6	127	135	8
-8	16	6	197	199	11
-5	16	6	197	179	10
-2	16	6	22	30	-39
1	16	6	61	60	-20
4	16	6	63	62	-19
7	16	6	95	83	20
10	16	6	69	36	-31
-25	17	6	45	25	-34
-22	17	6	38	14	-32
-19	17	6	69	38	16
-16	17	6	73	76	15
-13	17	6	211	214	7
-10	17	6	392	383	6
-7	17	6	411	411	14
-4	17	6	219	215	8
-1	17	6	68	62	16
2	17	6	73	56	15
5	17	6	40	18	-34
8	17	6	61	29	-23
-24	18	6	27	32	-47
-21	18	6	61	50	-24
-18	18	6	78	84	17
-15	18	6	144	145	9
-12	18	6	194	198	9
-9	18	6	225	224	8
-6	18	6	185	193	9
-3	18	6	118	131	14
0	18	6	85	92	13
3	18	6	83	46	-22
6	18	6	44	27	-34

Table 52. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
-23	19	6	65	28	-23	-21	24	6	28	7	-50
-20	19	6	26	23	-46	-18	24	6	46	31	-31
-17	19	6	47	40	-26	-15	24	6	27	35	-47
-14	19	6	31	6	-34	-12	24	6	71	31	-27
-11	19	6	90	85	12	-9	24	6	58	23	-27
-8	19	6	103	108	11	-6	24	6	34	27	-42
-5	19	6	66	15	-18	-3	24	6	64	1	-22
-2	19	6	63	52	-26	-17	25	6	35	25	-41
1	19	6	59	17	-23	-14	25	6	48	45	-31
4	19	6	49	32	-29	-11	25	6	40	46	-37
-22	20	6	47	9	-29	-8	25	6	55	29	-31
-19	20	6	25	21	-44	-16	26	6	28	36	-50
-16	20	6	61	83	-24	-13	26	6	39	43	-40
-13	20	6	179	172	14	-10	26	6	40	35	-38
-10	20	6	211	212	16	-1	1	7	29	2	-12
-7	20	6	159	168	11	-3	2	7	339	370	10
-4	20	6	79	63	-21	0	2	7	20	24	-15
-1	20	6	26	21	-46	-5	3	7	213	193	7
2	20	6	47	0	-33	-2	3	7	334	354	11
-24	21	6	57	7	-28	1	3	7	339	296	6
-21	21	6	27	14	-41	-7	4	7	39	67	-15
-18	21	6	90	50	16	-4	4	7	37	25	9
-15	21	6	83	79	14	-1	4	7	334	311	10
-12	21	6	76	72	13	2	4	7	276	327	8
-9	21	6	57	56	-18	-9	5	7	721	721	18
-6	21	6	72	60	-24	-6	5	7	428	457	11
-3	21	6	62	47	-20	-3	5	7	213	189	8
0	21	6	48	2	-29	0	5	7	25	16	-14
3	21	6	92	0	-30	3	5	7	572	522	9
-23	22	6	39	2	-39	-11	6	7	514	524	10
-20	22	6	46	10	-34	-8	6	7	683	672	17
-17	22	6	37	16	-36	-5	6	7	424	448	8
-14	22	6	90	76	22	-2	6	7	277	335	8
-11	22	6	99	109	18	1	6	7	250	241	5
-8	22	6	87	87	-24	4	6	7	52	26	11
-5	22	6	34	16	-39	-13	7	7	43	33	-15
-2	22	6	34	1	-39	-10	7	7	82	93	8
1	22	6	51	5	-33	-7	7	7	15	17	-23
-22	23	6	43	4	-36	-4	7	7	53	66	8
-19	23	6	27	28	-47	-1	7	7	253	235	5
-16	23	6	87	90	16	2	7	7	156	162	5
-13	23	6	118	127	12	5	7	7	276	261	5
-10	23	6	103	120	14	-15	8	7	68	62	13
-7	23	6	61	82	-25	-12	8	7	565	533	16
-4	23	6	27	32	-48	-9	8	7	805	795	18
-1	23	6	62	5	-24	-6	8	7	674	651	11

Table 52. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-3	8	7	567	546	9
0	8	7	23	11	-19
3	8	7	56	48	-14
6	8	7	88	92	13
-17	9	7	147	146	10
-14	9	7	325	330	5
-11	9	7	597	610	13
-8	9	7	793	801	5
-5	9	7	716	733	5
-2	9	7	153	160	6
1	9	7	125	121	14
4	9	7	141	130	11
7	9	7	95	108	10
-19	10	7	46	30	-28
-16	10	7	135	135	8
-13	10	7	56	14	-16
-10	10	7	27	6	-21
-7	10	7	95	104	10
-4	10	7	50	18	-17
-1	10	7	120	120	7
2	10	7	82	77	11
5	10	7	49	4	-23
8	10	7	40	41	-29
-21	11	7	61	5	-22
-18	11	7	38	46	-29
-15	11	7	183	189	7
-12	11	7	480	462	10
-9	11	7	580	585	5
-6	11	7	507	524	6
-3	11	7	50	58	-14
0	11	7	19	4	-29
3	11	7	61	69	-16
6	11	7	135	127	9
9	11	7	59	44	-22
-23	12	7	26	25	-46
-20	12	7	37	14	-33
-17	12	7	179	173	8
-14	12	7	308	311	9
-11	12	7	467	462	11
-8	12	7	556	540	8
-5	12	7	270	258	5
-2	12	7	87	77	8
1	12	7	32	10	-26
4	12	7	117	119	7
7	12	7	75	72	15
10	12	7	61	12	-23
-25	13	7	57	15	-32
-22	13	7	31	26	-39
-19	13	7	42	21	-29
-16	13	7	58	54	-18
-13	13	7	44	2	-17
-10	13	7	19	7	-42
-7	13	7	50	25	-13
-4	13	7	139	133	9
-1	13	7	26	7	-29
2	13	7	166	160	9
5	13	7	46	12	-24
8	13	7	25	15	-44
11	13	7	35	23	-39
-24	14	7	51	6	-32
-21	14	7	25	5	-44
-18	14	7	63	79	-17
-15	14	7	196	201	5
-12	14	7	305	300	6
-9	14	7	321	328	5
-6	14	7	99	93	11
-3	14	7	73	70	14
0	14	7	39	0	-21
3	14	7	84	73	13
6	14	7	63	57	13
9	14	7	73	2	-28
-23	15	7	33	37	-39
-20	15	7	45	27	-30
-17	15	7	138	135	9
-14	15	7	192	195	6
-11	15	7	194	189	10
-8	15	7	57	61	14
-5	15	7	29	10	-28
-2	15	7	158	161	9
1	15	7	267	275	7
4	15	7	142	136	17
7	15	7	51	61	-32
10	15	7	68	24	-23
-25	16	7	84	37	-29
-22	16	7	65	13	-27
-19	16	7	25	20	-43
-16	16	7	39	3	-25
-13	16	7	33	50	-30
-10	16	7	127	136	8
-7	16	7	115	111	12
-4	16	7	113	121	8
-1	16	7	270	277	7

Table 52. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
2	16	7	170	181	13
5	16	7	79	79	17
8	16	7	42	52	-36
-24	17	7	44	14	-34
-21	17	7	33	7	-39
-18	17	7	32	55	-37
-15	17	7	128	134	16
-12	17	7	173	175	7
-9	17	7	140	154	9
-6	17	7	130	127	15
-3	17	7	76	73	19
0	17	7	45	0	-23
3	17	7	39	16	-33
6	17	7	42	18	-35
-23	18	7	53	37	-28
-20	18	7	26	13	-45
-17	18	7	48	50	-29
-14	18	7	81	82	20
-11	18	7	86	50	12
-8	18	7	29	41	-34
-5	18	7	58	12	-25
-2	18	7	180	181	8
1	18	7	128	142	16
4	18	7	71	57	-18
7	18	7	39	33	-40
-22	19	7	27	11	-47
-19	19	7	26	3	-39
-16	19	7	51	19	-25
-13	19	7	42	17	-26
-10	19	7	56	32	-26
-7	19	7	64	70	-20
-4	19	7	136	138	16
-1	19	7	144	142	13
2	19	7	101	104	13
5	19	7	47	59	-32
-24	20	7	58	5	-31
-21	20	7	27	5	-48
-18	20	7	37	14	-33
-15	20	7	25	28	-44
-12	20	7	38	16	-32
-9	20	7	75	42	-26
-6	20	7	75	58	14
-3	20	7	42	16	-31
0	20	7	45	0	-26
3	20	7	27	28	-48
-23	21	7	39	10	-36
-20	21	7	42	2	-35
-17	21	7	56	6	-30
-14	21	7	63	8	-22
-11	21	7	25	3	-43
-8	21	7	59	13	-27
-5	21	7	83	79	19
-2	21	7	105	103	13
1	21	7	70	59	-25
-22	22	7	49	1	-31
-19	22	7	74	8	-28
-16	22	7	35	13	-38
-13	22	7	50	25	-27
-10	22	7	73	10	-27
-7	22	7	92	61	20
-4	22	7	90	57	-29
-1	22	7	28	59	-60
-21	23	7	28	10	-49
-18	23	7	68	34	-25
-15	23	7	54	34	-26
-12	23	7	65	26	-24
-9	23	7	27	2	-57
-6	23	7	72	17	-29
-3	23	7	58	27	-31
-20	24	7	28	5	-50
-17	24	7	37	11	-39
-14	24	7	50	5	-30
-11	24	7	63	21	-23
-8	24	7	59	51	-25
-5	24	7	84	58	19
-16	25	7	54	37	-28
-13	25	7	36	18	-45
-10	25	7	27	22	-48
-7	25	7	28	32	-49
0	1	8	171	235	4
-2	2	8	223	162	3
1	2	8	154	134	4
-4	3	8	244	272	11
-1	3	8	152	123	4
2	3	8	54	81	-15
-6	4	8	221	223	7
-3	4	8	237	272	4
0	4	8	450	451	8
3	4	8	472	428	12
-8	5	8	157	168	11
-5	5	8	217	220	4
-2	5	8	49	67	9

Table 52. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
1	5	8	323	377	5
4	5	8	217	229	5
-10	6	8	292	282	11
-7	6	8	261	244	4
-4	6	8	217	215	8
-1	6	8	322	380	7
2	6	8	245	281	6
5	6	8	311	287	9
-12	7	8	33	4	-22
-9	7	8	50	64	-13
-6	7	8	261	258	5
-3	7	8	460	455	9
0	7	8	857	796	16
3	7	8	654	627	9
6	7	8	230	246	18
-14	8	8	124	104	8
-11	8	8	163	164	7
-8	8	8	322	340	8
-5	8	8	159	168	5
-2	8	8	241	275	5
1	8	8	420	463	5
4	8	8	115	119	8
7	8	8	66	56	-17
-16	9	8	111	114	12
-13	9	8	100	108	9
-10	9	8	161	147	9
-7	9	8	65	58	9
-4	9	8	213	220	6
-1	9	8	425	455	13
2	9	8	388	384	6
5	9	8	159	152	8
8	9	8	61	58	-17
-18	10	8	65	67	16
-15	10	8	81	80	16
-12	10	8	94	104	10
-9	10	8	152	145	6
-6	10	8	287	294	6
-3	10	8	654	633	9
0	10	8	909	887	6
3	10	8	422	431	8
6	10	8	195	195	10
9	10	8	81	87	15
-20	11	8	59	22	-16
-17	11	8	53	60	-21
-14	11	8	84	91	11
-11	11	8	60	58	12
-8	11	8	168	167	6
-5	11	8	308	284	8
-2	11	8	387	390	10
1	11	8	321	327	6
4	11	8	203	210	16
7	11	8	100	98	15
10	11	8	25	27	-44
-22	12	8	35	9	-38
-19	12	8	24	18	-43
-16	12	8	65	45	-20
-13	12	8	20	14	-36
-10	12	8	93	97	10
-7	12	8	19	3	-33
-4	12	8	129	109	7
-1	12	8	330	318	6
2	12	8	61	38	14
5	12	8	39	25	-29
8	12	8	49	7	-29
11	12	8	27	18	-47
-24	13	8	76	5	-28
-21	13	8	64	22	-25
-18	13	8	61	39	-26
-15	13	8	88	86	15
-12	13	8	21	20	-36
-9	13	8	96	104	9
-6	13	8	224	237	6
-3	13	8	419	424	9
0	13	8	323	321	7
3	13	8	128	127	9
6	13	8	68	42	-22
9	13	8	54	22	-29
12	13	8	48	29	-35
-23	14	8	59	24	-25
-20	14	8	87	81	18
-17	14	8	148	144	9
-14	14	8	120	125	9
-11	14	8	94	92	9
-8	14	8	114	95	8
-5	14	8	170	148	9
-2	14	8	31	39	-29
1	14	8	128	137	9
4	14	8	70	74	-19
7	14	8	55	32	-22
10	14	8	58	33	-26
-25	15	8	49	18	-33
-22	15	8	27	26	-47

Table 52. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-19	15	8	85	80	11
-16	15	8	64	71	-23
-13	15	8	80	83	17
-10	15	8	76	86	17
-7	15	8	58	59	-18
-4	15	8	211	210	11
-1	15	8	122	137	10
2	15	8	55	4	-26
5	15	8	50	24	-24
8	15	8	26	11	-46
-24	16	8	40	6	-35
-21	16	8	70	43	-20
-18	16	8	66	71	-19
-15	16	8	74	75	14
-12	16	8	40	43	-29
-9	16	8	107	110	13
-6	16	8	186	193	7
-3	16	8	126	127	9
0	16	8	99	121	11
3	16	8	70	52	-20
6	16	8	46	32	-30
9	16	8	60	30	-25
-23	17	8	40	50	-37
-20	17	8	133	141	14
-17	17	8	155	163	10
-14	17	8	136	144	9
-11	17	8	73	66	-20
-8	17	8	74	56	14
-5	17	8	32	24	-33
-2	17	8	44	4	-23
1	17	8	70	53	-18
4	17	8	27	33	-47
7	17	8	71	49	-22
-22	18	8	84	47	21
-19	18	8	84	82	17
-16	18	8	76	68	16
-13	18	8	56	43	-18
-10	18	8	51	68	-23
-7	18	8	88	100	14
-4	18	8	64	73	-16
-1	18	8	75	52	18
2	18	8	51	42	-27
5	18	8	67	17	-19
-24	19	8	56	9	-27
-21	19	8	71	67	-22
-18	19	8	100	83	20
-15	19	8	81	80	12
-12	19	8	49	22	-25
-9	19	8	94	85	12
-6	19	8	38	43	-30
-3	19	8	42	51	-29
0	19	8	84	74	16
3	19	8	33	1	-40
-23	20	8	42	71	-36
-20	20	8	133	144	14
-17	20	8	152	141	11
-14	20	8	77	87	19
-11	20	8	37	24	-23
-8	20	8	32	5	-37
-5	20	8	50	24	-23
-2	20	8	43	41	-33
1	20	8	43	5	-34
-22	21	8	52	49	-33
-19	21	8	59	68	-31
-16	21	8	62	46	-28
-13	21	8	52	23	-29
-10	21	8	42	28	-29
-7	21	8	69	29	-22
-4	21	8	26	34	-46
-1	21	8	52	8	-28
-21	22	8	28	44	-49
-18	22	8	49	43	-29
-15	22	8	60	28	-22
-12	22	8	61	10	-29
-9	22	8	41	21	-35
-6	22	8	27	30	-47
-3	22	8	36	1	-38
0	22	8	41	6	-35
-20	23	8	69	67	-24
-17	23	8	65	50	-26
-14	23	8	61	24	-30
-11	23	8	57	19	-29
-8	23	8	46	9	-33
-5	23	8	27	19	-47
-19	24	8	29	10	-50
-16	24	8	38	5	-43
-13	24	8	26	5	-46
-10	24	8	68	31	-28
-7	24	8	59	49	-28
-15	25	8	28	17	-49
-12	25	8	59	28	-29
-9	25	8	83	29	-29

Table 52. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
0	0	9	30	13	-24
1	1	9	985	986	27
-1	2	9	967	972	26
2	2	9	729	702	17
-3	3	9	16	9	-24
0	3	9	36	9	-15
3	3	9	154	167	7
-5	4	9	369	352	5
-2	4	9	722	703	20
1	4	9	532	530	17
4	4	9	168	153	7
-7	5	9	254	231	7
-4	5	9	363	346	9
-1	5	9	532	535	10
2	5	9	399	390	11
5	5	9	25	3	-26
-9	6	9	106	105	6
-6	6	9	28	0	-15
-3	6	9	157	161	9
0	6	9	26	1	-18
3	6	9	129	130	6
6	6	9	160	164	7
-11	7	9	151	149	11
-8	7	9	252	238	7
-5	7	9	246	226	7
-2	7	9	397	387	9
1	7	9	156	156	7
4	7	9	58	39	12
7	7	9	44	19	-22
-13	8	9	132	126	7
-10	8	9	55	58	12
-7	8	9	249	237	11
-4	8	9	168	154	14
-1	8	9	150	158	6
2	8	9	60	69	12
5	8	9	229	243	9
8	8	9	230	241	7
-15	9	9	142	148	6
-12	9	9	126	143	8
-9	9	9	23	7	-25
-6	9	9	102	99	7
-3	9	9	128	137	6
0	9	9	48	4	-17
3	9	9	86	78	11
6	9	9	264	259	7
9	9	9	214	220	13
-17	10	9	63	26	-23
-14	10	9	34	14	-27
-11	10	9	59	43	-18
-8	10	9	59	57	13
-5	10	9	41	11	-15
-2	10	9	80	74	13
1	10	9	69	82	12
4	10	9	39	10	-26
7	10	9	34	14	-32
10	10	9	32	7	-38
-19	11	9	201	196	11
-16	11	9	135	139	9
-13	11	9	124	114	8
-10	11	9	44	44	-19
-7	11	9	146	156	10
-4	11	9	61	35	-20
-1	11	9	80	84	13
2	11	9	30	23	-30
5	11	9	190	212	10
8	11	9	172	173	16
11	11	9	109	102	13
-21	12	9	136	131	15
-18	12	9	147	134	12
-15	12	9	75	67	13
-12	12	9	28	4	-30
-9	12	9	129	139	8
-6	12	9	155	164	7
-3	12	9	88	80	17
0	12	9	39	0	-19
3	12	9	122	116	10
6	12	9	171	177	15
9	12	9	129	133	11
12	12	9	78	61	-30
-23	13	9	33	2	-40
-20	13	9	25	38	-45
-17	13	9	24	27	-42
-14	13	9	118	109	9
-11	13	9	120	117	9
-8	13	9	118	123	19
-5	13	9	222	239	6
-2	13	9	44	25	-21
1	13	9	64	41	14
4	13	9	24	24	-43
7	13	9	31	13	-39
10	13	9	27	17	-47
-22	14	9	106	106	18

Table 52. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
-19	14	9	131	136	14	-12	18	9	126	134	10
-16	14	9	98	108	17	-9	18	9	218	218	9
-13	14	9	112	112	12	-6	18	9	168	178	9
-10	14	9	46	13	-26	-3	18	9	50	20	-22
-7	14	9	53	19	-17	0	18	9	31	1	-35
-4	14	9	40	9	-25	3	18	9	64	16	-28
-1	14	9	47	42	-20	-23	19	9	58	27	-27
2	14	9	55	59	-20	-20	19	9	73	43	-19
5	14	9	102	99	17	-17	19	9	45	64	-29
8	14	9	75	68	-19	-14	19	9	134	138	11
-24	15	9	72	45	-29	-11	19	9	202	197	12
-21	15	9	84	71	-27	-8	19	9	178	173	13
-18	15	9	92	90	11	-5	19	9	104	101	13
-15	15	9	57	2	-21	-2	19	9	60	60	-24
-12	15	9	70	65	16	1	19	9	27	21	-47
-9	15	9	144	146	6	4	19	9	28	4	-50
-6	15	9	266	261	6	-22	20	9	54	25	-30
-3	15	9	127	121	11	-19	20	9	49	44	-29
0	15	9	24	1	-36	-16	20	9	43	26	-33
3	15	9	25	16	-31	-13	20	9	59	39	-22
6	15	9	62	57	-24	-10	20	9	37	4	-35
9	15	9	36	41	-40	-7	20	9	62	13	-21
-23	16	9	27	20	-48	-4	20	9	55	45	-24
-20	16	9	50	23	-27	-1	20	9	43	21	-35
-17	16	9	41	20	-31	2	20	9	64	9	-34
-14	16	9	105	108	18	-21	21	9	28	1	-42
-11	16	9	138	138	10	-18	21	9	47	10	-28
-8	16	9	227	240	12	-15	21	9	59	71	-24
-5	16	9	199	213	8	-12	21	9	128	130	13
-2	16	9	46	64	-23	-9	21	9	121	132	13
1	16	9	83	69	16	-6	21	9	40	58	-33
4	16	9	56	45	-22	-3	21	9	59	18	-29
7	16	9	48	9	-33	0	21	9	58	0	-29
-22	17	9	56	48	-29	-20	22	9	57	25	-31
-19	17	9	52	58	-26	-17	22	9	27	50	-48
-16	17	9	25	22	-43	-14	22	9	93	107	17
-13	17	9	36	26	-32	-11	22	9	104	105	14
-10	17	9	44	28	-24	-8	22	9	80	68	17
-7	17	9	23	13	-41	-5	22	9	74	54	-24
-4	17	9	60	24	-21	-2	22	9	44	10	-32
-1	17	9	56	69	-24	-19	23	9	28	27	-50
2	17	9	89	56	-28	-16	23	9	48	22	-28
5	17	9	60	52	-24	-13	23	9	44	2	-35
-21	18	9	60	9	-24	-10	23	9	44	13	-33
-18	18	9	26	1	-39	-7	23	9	77	10	-27
-15	18	9	92	92	12	-4	23	9	41	3	-34

Table 52. (cont).
F(obs), F(calc), and σ_F

($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-15	24	9	53	42	-26
-12	24	9	66	59	-25
-9	24	9	52	39	-29
-1	1	10	30	37	-17
-3	2	10	69	102	8
0	2	10	300	266	7
-5	3	10	154	174	9
-2	3	10	65	102	10
1	3	10	41	20	-14
-7	4	10	476	474	15
-4	4	10	517	496	14
-1	4	10	37	21	-14
2	4	10	33	38	-18
-9	5	10	146	135	6
-6	5	10	293	292	11
-3	5	10	153	174	13
0	5	10	68	25	8
3	5	10	247	264	11
-11	6	10	136	137	13
-8	6	10	355	354	10
-5	6	10	290	295	10
-2	6	10	17	43	-30
1	6	10	54	15	-18
4	6	10	206	210	7
-13	7	10	278	279	8
-10	7	10	456	469	7
-7	7	10	691	718	13
-4	7	10	468	478	14
-1	7	10	61	23	11
2	7	10	72	78	12
5	7	10	125	111	10
-15	8	10	132	132	12
-12	8	10	301	290	6
-9	8	10	284	278	9
-6	8	10	348	357	5
-3	8	10	246	267	7
0	8	10	79	86	9
3	8	10	93	96	10
6	8	10	60	53	12
-17	9	10	24	2	-42
-14	9	10	45	57	-24
-11	9	10	144	127	8
-8	9	10	283	274	5
-5	9	10	149	136	7
-2	9	10	87	75	10
1	9	10	27	10	-28
4	9	10	90	94	12
7	9	10	98	84	22
-19	10	10	25	2	-45
-16	10	10	118	125	10
-13	10	10	332	327	6
-10	10	10	376	388	6
-7	10	10	442	471	10
-4	10	10	202	216	6
-1	10	10	53	4	-21
2	10	10	31	7	-28
5	10	10	36	48	-28
8	10	10	36	36	-33
-21	11	10	55	20	-29
-18	11	10	75	38	-26
-15	11	10	125	127	11
-12	11	10	204	194	7
-9	11	10	148	130	7
-6	11	10	138	137	8
-3	11	10	97	98	11
0	11	10	49	39	-17
3	11	10	45	16	-25
6	11	10	49	8	-27
9	11	10	39	26	-35
-23	12	10	27	15	-48
-20	12	10	36	26	-36
-17	12	10	48	36	-25
-14	12	10	157	150	9
-11	12	10	198	192	7
-8	12	10	286	288	12
-5	12	10	121	110	8
-2	12	10	21	6	-37
1	12	10	42	40	-25
4	12	10	59	16	-25
7	12	10	25	16	-44
10	12	10	76	21	-25
-22	13	10	49	3	-33
-19	13	10	31	21	-38
-16	13	10	172	172	8
-13	13	10	310	309	8
-10	13	10	330	331	11
-7	13	10	280	280	6
-4	13	10	90	97	12
-1	13	10	41	41	-23
2	13	10	76	69	18
5	13	10	65	67	-21
8	13	10	72	54	-21

Table 52. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
11	13	10	41	1	-38
-24	14	10	60	34	-28
-21	14	10	27	21	-47
-18	14	10	71	51	-20
-15	14	10	107	98	11
-12	14	10	159	153	12
-9	14	10	74	60	16
-6	14	10	54	53	14
-3	14	10	22	16	-39
0	14	10	136	146	10
3	14	10	134	116	10
6	14	10	63	74	-22
9	14	10	82	18	-25
-23	15	10	45	13	-34
-20	15	10	58	25	-24
-17	15	10	52	37	-25
-14	15	10	89	92	14
-11	15	10	118	123	9
-8	15	10	110	128	12
-5	15	10	62	51	-19
-2	15	10	77	69	-21
1	15	10	67	75	-20
4	15	10	59	41	-24
7	15	10	47	7	-33
-22	16	10	27	4	-48
-19	16	10	54	18	-29
-16	16	10	95	92	10
-13	16	10	165	169	14
-10	16	10	125	124	10
-7	16	10	96	82	13
-4	16	10	58	16	-19
-1	16	10	99	78	18
2	16	10	77	73	17
5	16	10	67	47	-24
-21	17	10	39	11	-34
-18	17	10	33	14	-38
-15	17	10	70	38	-21
-12	17	10	63	35	-25
-9	17	10	30	1	-35
-6	17	10	48	11	-28
-3	17	10	123	117	10
0	17	10	140	156	9
3	17	10	92	107	16
6	17	10	57	46	-30
-23	18	10	29	15	-51
-20	18	10	38	5	-37
-17	18	10	25	16	-44
-14	18	10	47	50	-26
-11	18	10	49	36	-25
-8	18	10	24	36	-43
-5	18	10	50	71	-26
-2	18	10	82	73	16
1	18	10	71	64	-22
4	18	10	76	42	-20
-22	19	10	28	3	-50
-19	19	10	48	2	-29
-16	19	10	37	18	-35
-13	19	10	25	20	-54
-10	19	10	50	1	-29
-7	19	10	45	14	-30
-4	19	10	67	41	-29
-1	19	10	46	63	-31
2	19	10	62	32	-26
-21	20	10	44	2	-36
-18	20	10	27	9	-47
-15	20	10	40	27	-32
-12	20	10	53	27	-27
-9	20	10	56	27	-28
-6	20	10	79	77	18
-3	20	10	105	105	14
0	20	10	86	83	17
-20	21	10	59	3	-31
-17	21	10	27	15	-47
-14	21	10	26	24	-46
-11	21	10	26	22	-46
-8	21	10	73	55	-23
-5	21	10	70	49	-19
-2	21	10	27	32	-48
-19	22	10	28	5	-50
-16	22	10	49	1	-32
-13	22	10	69	8	-23
-10	22	10	51	23	-30
-7	22	10	27	8	-48
-4	22	10	44	40	-31
-18	23	10	65	17	-23
-15	23	10	44	16	-35
-12	23	10	54	18	-27
-9	23	10	37	17	-37
-6	23	10	62	46	-30
-14	24	10	29	34	-50
-11	24	10	28	1	-50
0	1	11	20	1	-23

Table 52. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-2	2	11	30	8	-19
1	2	11	18	23	-32
-4	3	11	158	175	8
-1	3	11	41	26	-16
2	3	11	311	324	7
-6	4	11	157	150	6
-3	4	11	158	176	7
0	4	11	19	4	-33
3	4	11	85	91	9
-8	5	11	51	37	-15
-5	5	11	37	2	-17
-2	5	11	303	319	5
1	5	11	531	536	13
4	5	11	298	291	7
-10	6	11	131	128	9
-7	6	11	192	197	6
-4	6	11	158	143	6
-1	6	11	518	544	10
2	6	11	427	438	13
5	6	11	206	197	6
-12	7	11	168	168	7
-9	7	11	155	159	7
-6	7	11	188	198	6
-3	7	11	87	90	9
0	7	11	46	2	-19
3	7	11	26	24	-32
6	7	11	22	7	-39
-14	8	11	128	131	19
-11	8	11	53	59	-18
-8	8	11	37	3	-17
-5	8	11	42	36	-17
-2	8	11	419	441	9
1	8	11	419	416	10
4	8	11	224	222	7
7	8	11	133	147	9
-16	9	11	42	17	-26
-13	9	11	22	18	-38
-10	9	11	50	38	-23
-7	9	11	152	154	7
-4	9	11	299	295	8
-1	9	11	413	418	8
2	9	11	345	348	9
5	9	11	207	212	7
8	9	11	30	49	-37
-18	10	11	41	3	-32
-15	10	11	67	50	-18
-12	10	11	42	8	-20
-9	10	11	45	38	-26
-6	10	11	112	130	8
-3	10	11	36	24	-31
0	10	11	22	1	-33
3	10	11	56	61	-20
6	10	11	24	1	-41
9	10	11	67	30	-23
-20	11	11	40	22	-35
-17	11	11	25	5	-43
-14	11	11	68	41	-21
-11	11	11	36	3	-16
-8	11	11	60	59	-16
-5	11	11	208	198	7
-2	11	11	343	345	6
1	11	11	255	255	8
4	11	11	153	146	10
7	11	11	34	14	-35
10	11	11	46	6	-34
-22	12	11	27	16	-47
-19	12	11	68	40	-20
-16	12	11	37	30	-33
-13	12	11	57	67	-18
-10	12	11	30	6	-31
-7	12	11	165	170	11
-4	12	11	220	223	6
-1	12	11	266	256	8
2	12	11	210	215	8
5	12	11	76	69	12
8	12	11	41	16	-34
11	12	11	43	3	-35
-21	13	11	27	15	-48
-18	13	11	83	69	-22
-15	13	11	49	55	-24
-12	13	11	74	69	17
-9	13	11	22	16	-39
-6	13	11	30	6	-32
-3	13	11	53	58	-18
0	13	11	23	2	-36
3	13	11	33	8	-34
6	13	11	52	25	-26
9	13	11	37	2	-37
-23	14	11	36	9	-42
-20	14	11	41	7	-34
-17	14	11	47	19	-30
-14	14	11	40	0	-23

Table 52. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-11	14	11	42	39	-25
-8	14	11	130	130	9
-5	14	11	206	209	8
-2	14	11	210	208	9
1	14	11	140	137	10
4	14	11	39	26	-34
7	14	11	27	10	-47
-22	15	11	66	33	-28
-19	15	11	88	85	16
-16	15	11	84	78	17
-13	15	11	52	58	-23
-10	15	11	59	49	-17
-7	15	11	151	147	8
-4	15	11	150	145	9
-1	15	11	144	137	20
2	15	11	67	64	-27
5	15	11	42	10	-36
8	15	11	57	23	-28
-21	16	11	95	58	-30
-18	16	11	122	105	14
-15	16	11	78	77	16
-12	16	11	41	29	-30
-9	16	11	48	16	-23
-6	16	11	24	1	-42
-3	16	11	48	4	-22
0	16	11	25	1	-39
3	16	11	26	5	-46
6	16	11	48	11	-33
-20	17	11	38	4	-39
-17	17	11	41	2	-28
-14	17	11	31	24	-38
-11	17	11	40	9	-28
-8	17	11	73	48	-25
-5	17	11	84	66	11
-2	17	11	62	62	-24
1	17	11	46	31	-30
4	17	11	27	8	-48
-22	18	11	59	49	-33
-19	18	11	105	106	14
-16	18	11	97	110	15
-13	18	11	69	75	-20
-10	18	11	33	9	-36
-7	18	11	60	10	-27
-4	18	11	48	26	-29
-1	18	11	26	29	-46
2	18	11	27	12	-47
-21	19	11	96	72	23
-18	19	11	124	108	18
-15	19	11	78	88	17
-12	19	11	48	45	-31
-9	19	11	62	37	-23
-6	19	11	43	26	-31
-3	19	11	49	5	-30
0	19	11	27	2	-42
-20	20	11	28	2	-43
-17	20	11	27	6	-47
-14	20	11	62	9	-24
-11	20	11	79	24	-27
-8	20	11	45	18	-33
-5	20	11	46	12	-37
-2	20	11	50	13	-37
-19	21	11	59	69	-26
-16	21	11	73	56	-21
-13	21	11	27	15	-47
-10	21	11	27	8	-47
-7	21	11	41	8	-36
-4	21	11	41	10	-42
-18	22	11	81	49	-22
-15	22	11	27	33	-48
-12	22	11	51	18	-29
-9	22	11	55	3	-24
-6	22	11	63	11	-28
-14	23	11	28	10	-49
-11	23	11	40	3	-35
-8	23	11	28	20	-50
0	0	12	979	958	33
1	1	12	381	418	5
-1	2	12	368	412	15
2	2	12	66	81	12
-3	3	12	546	524	9
0	3	12	508	482	14
3	3	12	225	210	6
-5	4	12	238	246	9
-2	4	12	79	87	10
1	4	12	222	226	10
4	4	12	123	110	11
-7	5	12	36	3	-24
-4	5	12	238	251	13
-1	5	12	218	227	8
2	5	12	61	24	15
5	5	12	88	85	13
-9	6	12	100	101	9

Table 52. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-6	6	12	275	279	8
-3	6	12	213	211	8
0	6	12	221	214	6
3	6	12	119	113	10
6	6	12	79	79	18
-11	7	12	93	92	9
-8	7	12	120	117	8
-5	7	12	45	5	-18
-2	7	12	49	31	-22
1	7	12	101	97	11
4	7	12	103	110	7
7	7	12	141	148	10
-13	8	12	51	33	-22
-10	8	12	48	48	-18
-7	8	12	125	117	8
-4	8	12	122	114	9
-1	8	12	102	94	15
2	8	12	125	121	8
5	8	12	65	66	15
8	8	12	81	82	17
-15	9	12	77	95	19
-12	9	12	61	55	15
-9	9	12	119	138	9
-6	9	12	99	99	10
-3	9	12	106	111	18
0	9	12	156	165	8
3	9	12	32	6	-32
6	9	12	68	60	-25
9	9	12	80	76	16
-17	10	12	173	166	9
-14	10	12	107	103	12
-11	10	12	22	4	-39
-8	10	12	48	47	-18
-5	10	12	90	85	10
-2	10	12	127	123	10
1	10	12	43	11	-30
4	10	12	72	78	-20
7	10	12	155	138	9
10	10	12	124	141	14
-19	11	12	85	79	16
-16	11	12	64	54	15
-13	11	12	23	9	-41
-10	11	12	30	2	-31
-7	11	12	93	89	9
-4	11	12	100	110	8
-1	11	12	38	9	-24
2	11	12	23	5	-41
5	11	12	71	52	-18
8	11	12	64	74	-21
11	11	12	28	40	-49
-21	12	12	87	56	-26
-18	12	12	81	71	-21
-15	12	12	89	59	-25
-12	12	12	62	32	-17
-9	12	12	64	55	15
-6	12	12	77	80	-23
-3	12	12	33	5	-30
0	12	12	59	40	-21
3	12	12	35	41	-33
6	12	12	83	49	-27
9	12	12	73	59	-24
-20	13	12	88	103	16
-17	13	12	111	94	18
-14	13	12	51	32	-25
-11	13	12	40	13	-28
-8	13	12	42	27	-24
-5	13	12	65	67	16
-2	13	12	24	3	-42
1	13	12	65	39	-20
4	13	12	68	76	-24
7	13	12	102	102	14
-22	14	12	27	16	-48
-19	14	12	48	23	-27
-16	14	12	63	9	-26
-13	14	12	36	28	-32
-10	14	12	115	96	12
-7	14	12	146	144	9
-4	14	12	87	75	-25
-1	14	12	40	38	-27
2	14	12	41	17	-30
5	14	12	27	42	-47
8	14	12	28	17	-50
-21	15	12	81	51	-29
-18	15	12	42	52	-35
-15	15	12	54	30	-25
-12	15	12	69	55	17
-9	15	12	90	91	17
-6	15	12	70	53	-22
-3	15	12	48	40	-24
0	15	12	48	32	-23
3	15	12	49	24	-31
6	15	12	40	44	-38

Table 52. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-20	16	12	61	42	-29
-17	16	12	61	29	-25
-14	16	12	25	11	-44
-11	16	12	61	54	-16
-8	16	12	82	86	16
-5	16	12	75	56	14
-2	16	12	51	20	-26
1	16	12	37	25	-37
4	16	12	63	50	-25
-19	17	12	58	20	-25
-16	17	12	26	34	-46
-13	17	12	90	96	17
-10	17	12	162	169	9
-7	17	12	153	138	11
-4	17	12	75	80	17
-1	17	12	41	30	-34
2	17	12	50	11	-30
-18	18	12	36	50	-41
-15	18	12	41	54	-30
-12	18	12	57	76	-21
-9	18	12	98	76	17
-6	18	12	54	50	-30
-3	18	12	67	28	-26
0	18	12	53	20	-22
-20	19	12	28	19	-50
-17	19	12	52	18	-33
-14	19	12	48	21	-31
-11	19	12	85	78	18
-8	19	12	73	73	-20
-5	19	12	52	42	-26
-2	19	12	27	13	-47
1	19	12	46	17	-37
-19	20	12	28	18	-50
-16	20	12	56	44	-26
-13	20	12	101	107	15
-10	20	12	127	141	12
-7	20	12	106	103	19
-4	20	12	73	54	-26
-1	20	12	50	17	-35
-15	21	12	57	55	-29
-12	21	12	55	60	-25
-9	21	12	60	62	-24
-6	21	12	63	47	-31
-14	22	12	28	13	-49
-11	22	12	49	35	-33
-8	22	12	59	13	-30
-1	1	13	35	4	-22
-3	2	13	69	61	12
0	2	13	42	5	-19
-5	3	13	225	225	8
-2	3	13	61	67	14
1	3	13	82	74	12
-7	4	13	21	18	-37
-4	4	13	32	1	-24
-1	4	13	72	82	12
2	4	13	88	99	13
-9	5	13	147	149	5
-6	5	13	291	296	8
-3	5	13	226	225	16
0	5	13	39	2	-19
3	5	13	84	74	14
-11	6	13	134	130	9
-8	6	13	299	298	11
-5	6	13	281	301	11
-2	6	13	98	97	11
1	6	13	102	110	15
4	6	13	41	34	-24
-13	7	13	38	13	-30
-10	7	13	40	37	-25
-7	7	13	53	3	-17
-4	7	13	34	19	-26
-1	7	13	105	110	13
2	7	13	100	112	11
5	7	13	94	99	13
-15	8	13	82	95	11
-12	8	13	166	164	11
-9	8	13	302	303	6
-6	8	13	295	299	13
-3	8	13	71	74	13
0	8	13	22	3	-34
3	8	13	99	79	11
6	8	13	90	82	19
-17	9	13	47	52	-27
-14	9	13	118	127	13
-11	9	13	282	276	7
-8	9	13	298	304	6
-5	9	13	149	147	7
-2	9	13	105	112	10
1	9	13	23	19	-40
4	9	13	67	39	-22
7	9	13	62	2	-26
-19	10	13	64	29	-21

Table 52. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-16	10	13	46	13	-30
-13	10	13	55	36	-27
-10	10	13	49	1	-25
-7	10	13	55	39	-24
-4	10	13	44	34	-25
-1	10	13	31	18	-32
2	10	13	29	11	-35
5	10	13	40	18	-31
8	10	13	27	6	-47
-21	11	13	44	9	-32
-18	11	13	54	19	-31
-15	11	13	82	84	14
-12	11	13	220	225	10
-9	11	13	269	280	7
-6	11	13	124	133	10
-3	11	13	86	85	12
0	11	13	45	3	-22
3	11	13	52	56	-28
6	11	13	32	14	-39
9	11	13	68	33	-23
-20	12	13	48	27	-30
-17	12	13	77	63	18
-14	12	13	155	160	9
-11	12	13	221	228	10
-8	12	13	169	166	10
-5	12	13	100	105	18
-2	12	13	23	16	-41
1	12	13	43	61	-27
4	12	13	60	49	-21
7	12	13	41	40	-33
-19	13	13	33	29	-40
-16	13	13	48	47	-25
-13	13	13	41	5	-21
-10	13	13	58	32	-21
-7	13	13	24	17	-41
-4	13	13	40	37	-27
-1	13	13	63	60	-18
2	13	13	50	40	-23
5	13	13	42	55	-36
8	13	13	27	5	-48
-21	14	13	28	2	-49
-18	14	13	27	1	-57
-15	14	13	52	68	-24
-12	14	13	137	157	10
-9	14	13	119	122	13
-6	14	13	78	82	17
-3	14	13	57	56	-19
0	14	13	38	2	-30
3	14	13	44	4	-33
6	14	13	27	11	-48
-20	15	13	41	4	-36
-17	15	13	71	45	-28
-14	15	13	68	70	-18
-11	15	13	77	82	16
-8	15	13	96	94	9
-5	15	13	41	20	-27
-2	15	13	25	42	-45
1	15	13	44	51	-32
4	15	13	70	64	-26
-19	16	13	27	7	-48
-16	16	13	27	0	-40
-13	16	13	58	45	-23
-10	16	13	56	10	-27
-7	16	13	31	3	-38
-4	16	13	60	51	-22
-1	16	13	40	50	-35
2	16	13	94	67	-28
-18	17	13	63	26	-30
-15	17	13	77	47	19
-12	17	13	73	59	-19
-9	17	13	56	48	-23
-6	17	13	44	14	-32
-3	17	13	34	7	-36
0	17	13	33	1	-34
3	17	13	29	12	-50
-17	18	13	38	25	-37
-14	18	13	47	1	-29
-11	18	13	27	17	-47
-8	18	13	43	3	-29
-5	18	13	82	59	19
-2	18	13	57	68	-25
1	18	13	88	74	18
-16	19	13	27	12	-48
-13	19	13	59	31	-24
-10	19	13	59	31	-26
-7	19	13	74	46	-26
-4	19	13	91	66	15
-1	19	13	87	74	-25
-15	20	13	74	8	-21
-12	20	13	72	30	-28
-9	20	13	49	37	-32
-6	20	13	57	13	-25

Table 52. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-3	20	13	45	13	-36
-14	21	13	28	2	-49
-11	21	13	27	13	-48
-8	21	13	60	6	-22
0	1	14	41	6	-22
-2	2	14	37	23	-21
1	2	14	37	23	-22
-4	3	14	51	43	-18
-1	3	14	37	27	-25
2	3	14	122	116	10
-6	4	14	42	12	-20
-3	4	14	45	48	-20
0	4	14	162	166	9
3	4	14	218	223	9
-8	5	14	102	107	11
-5	5	14	48	34	-18
-2	5	14	128	119	8
1	5	14	101	101	10
4	5	14	96	85	-27
-10	6	14	137	146	18
-7	6	14	48	36	-25
-4	6	14	36	13	-20
-1	6	14	109	96	10
2	6	14	179	173	8
5	6	14	109	109	13
-12	7	14	24	33	-42
-9	7	14	43	2	-27
-6	7	14	37	34	-26
-3	7	14	216	219	11
0	7	14	291	287	7
3	7	14	260	261	7
6	7	14	143	138	9
-14	8	14	53	37	-25
-11	8	14	88	64	17
-8	8	14	42	4	-22
-5	8	14	104	106	15
-2	8	14	177	175	8
1	8	14	132	117	9
4	8	14	122	116	13
7	8	14	68	51	-20
-16	9	14	53	19	-28
-13	9	14	53	22	-17
-10	9	14	38	4	-31
-7	9	14	38	4	-27
-4	9	14	89	85	14
-1	9	14	112	119	12
2	9	14	99	105	14
5	9	14	49	45	-25
8	9	14	32	14	-41
-18	10	14	53	21	-30
-15	10	14	63	12	-24
-12	10	14	35	47	-35
-9	10	14	23	9	-41
-6	10	14	156	147	8
-3	10	14	255	261	7
0	10	14	201	208	7
3	10	14	161	168	16
6	10	14	52	50	-30
9	10	14	56	4	-31
-20	11	14	65	4	-26
-17	11	14	27	5	-47
-14	11	14	43	17	-31
-11	11	14	48	24	-23
-8	11	14	51	66	-24
-5	11	14	118	112	10
-2	11	14	116	106	10
1	11	14	91	82	11
4	11	14	54	52	-25
7	11	14	61	24	-28
-19	12	14	34	17	-41
-16	12	14	49	6	-31
-13	12	14	25	18	-45
-10	12	14	25	46	-43
-7	12	14	29	33	-37
-4	12	14	118	115	21
-1	12	14	82	80	12
2	12	14	98	79	20
5	12	14	57	13	-25
8	12	14	59	4	-31
-18	13	14	44	35	-34
-15	13	14	26	18	-45
-12	13	14	48	21	-25
-9	13	14	53	24	-19
-6	13	14	141	140	12
-3	13	14	160	167	14
0	13	14	126	143	11
3	13	14	80	78	16
6	13	14	27	17	-48
-20	14	14	58	26	-29
-17	14	14	94	65	-25
-14	14	14	76	70	18
-11	14	14	62	15	-27

Table 52. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-8	14	14	45	39	-30
-5	14	14	69	47	-25
-2	14	14	100	82	18
1	14	14	57	42	-22
4	14	14	36	28	-46
-19	15	14	27	18	-48
-16	15	14	54	48	-30
-13	15	14	35	15	-37
-10	15	14	53	13	-29
-7	15	14	63	48	-21
-4	15	14	66	46	-25
-1	15	14	48	38	-31
2	15	14	34	18	-38
-18	16	14	59	42	-27
-15	16	14	55	51	-25
-12	16	14	65	12	-27
-9	16	14	45	16	-28
-6	16	14	59	45	-21
-3	16	14	84	75	21
0	16	14	59	41	-24
3	16	14	28	14	-49
-17	17	14	85	97	17
-14	17	14	68	69	-22
-11	17	14	66	12	-28
-8	17	14	26	19	-56
-5	17	14	57	12	-26
-2	17	14	62	17	-29
1	17	14	60	8	-33
-16	18	14	66	43	-30
-13	18	14	48	37	-32
-10	18	14	46	27	-33
-7	18	14	36	26	-38
-4	18	14	54	28	-31
-1	18	14	28	10	-50
-15	19	14	55	17	-31
-12	19	14	27	16	-48
-9	19	14	27	4	-48
-6	19	14	50	17	-33
-3	19	14	53	16	-30
-14	20	14	38	26	-41
-11	20	14	28	7	-49
-8	20	14	54	5	-31
0	0	15	23	3	-49
1	1	15	280	272	12
-1	2	15	264	276	10
2	2	15	231	231	10
-3	3	15	47	1	-21
0	3	15	23	0	-35
3	3	15	36	22	-28
-5	4	15	223	221	8
-2	4	15	229	231	7
1	4	15	185	178	7
4	4	15	76	76	-24
-7	5	15	132	121	10
-4	5	15	215	224	9
-1	5	15	178	178	8
2	5	15	78	80	13
5	5	15	70	21	15
-9	6	15	53	39	-25
-6	6	15	56	1	-16
-3	6	15	51	23	-20
0	6	15	52	0	-20
3	6	15	41	25	-30
6	6	15	43	25	-26
-11	7	15	53	30	-22
-8	7	15	33	23	-33
-5	7	15	116	120	10
-2	7	15	80	80	13
1	7	15	55	55	-22
4	7	15	39	35	-31
7	7	15	50	5	-26
-13	8	15	84	66	-23
-10	8	15	43	0	-29
-7	8	15	58	25	-20
-4	8	15	82	76	16
-1	8	15	57	52	-21
2	8	15	62	8	-26
5	8	15	25	22	-45
8	8	15	107	99	21
-15	9	15	90	101	15
-12	9	15	51	16	-27
-9	9	15	24	2	-37
-6	9	15	23	39	-41
-3	9	15	45	27	-28
0	9	15	56	0	-26
3	9	15	60	37	-25
6	9	15	70	72	-21
9	9	15	80	79	-21
-17	10	15	42	7	-36
-14	10	15	52	2	-30
-11	10	15	73	2	-26
-8	10	15	65	3	-25

Table 52. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-5	10	15	54	20	-26
-2	10	15	46	7	-29
1	10	15	54	10	-22
4	10	15	59	22	-28
7	10	15	50	9	-32
-19	11	15	53	67	-31
-16	11	15	84	91	20
-13	11	15	62	13	-27
-10	11	15	78	0	-26
-7	11	15	44	29	-30
-4	11	15	25	34	-43
-1	11	15	47	8	-25
2	11	15	33	19	-38
5	11	15	67	55	-20
8	11	15	72	69	-23
-18	12	15	81	59	18
-15	12	15	68	50	-28
-12	12	15	26	2	-39
-9	12	15	25	10	-44
-6	12	15	62	24	-20
-3	12	15	58	35	-27
0	12	15	25	2	-39
3	12	15	57	45	-25
6	12	15	51	53	-33
-17	13	15	60	23	-25
-14	13	15	53	16	-29
-11	13	15	26	9	-45
-8	13	15	70	61	-19
-5	13	15	25	19	-44
-2	13	15	71	16	-22
1	13	15	74	0	-27
4	13	15	27	1	-48
-16	14	15	34	32	-40
-13	14	15	57	17	-22
-10	14	15	48	3	-29
-7	14	15	38	10	-34
-4	14	15	36	25	-36
-1	14	15	48	0	-31
2	14	15	27	26	-47
-18	15	15	56	1	-29
-15	15	15	41	2	-29
-12	15	15	64	51	-20
-9	15	15	97	102	14
-6	15	15	54	73	-26
-3	15	15	55	46	-25
0	15	15	53	1	-29
3	15	15	69	28	-25
-17	16	15	28	39	-50
-14	16	15	59	36	-29
-11	16	15	101	93	14
-8	16	15	85	98	19
-5	16	15	76	55	-27
-2	16	15	51	28	-29
1	16	15	55	4	-35
-16	17	15	73	38	-19
-13	17	15	38	26	-37
-10	17	15	27	7	-47
-7	17	15	45	7	-31
-4	17	15	26	1	-46
-1	17	15	42	3	-37
-15	18	15	55	1	-32
-12	18	15	56	59	-26
-9	18	15	81	79	17
-6	18	15	68	54	-30
-3	18	15	59	31	-27
-11	19	15	81	69	-21
-8	19	15	66	70	-25
-1	1	16	59	46	-16
-3	2	16	62	18	-22
0	2	16	93	89	10
-5	3	16	57	37	-22
-2	3	16	24	16	-41
1	3	16	65	68	-20
-7	4	16	109	105	11
-4	4	16	61	76	-17
-1	4	16	75	68	17
2	4	16	78	51	14
-9	5	16	91	83	10
-6	5	16	45	61	-30
-3	5	16	45	38	-26
0	5	16	41	48	-22
3	5	16	57	12	-22
-11	6	16	59	70	-21
-8	6	16	67	62	-17
-5	6	16	62	63	-18
-2	6	16	57	51	-20
1	6	16	47	49	-26
4	6	16	83	91	-27
-13	7	16	90	63	14
-10	7	16	169	168	10
-7	7	16	148	159	11
-4	7	16	120	109	10

Table 52. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
-1	7	16	61	49	-19	-16	13	16	81	33	-28
2	7	16	50	47	-25	-13	13	16	62	77	-21
5	7	16	53	14	-24	-10	13	16	102	105	19
-15	8	16	26	28	-46	-7	13	16	64	62	-23
-12	8	16	56	43	-24	-4	13	16	26	16	-45
-9	8	16	99	101	14	-1	13	16	26	4	-46
-6	8	16	65	60	-17	2	13	16	67	20	-23
-3	8	16	47	13	-28	-15	14	16	56	33	-30
0	8	16	54	19	14	-12	14	16	56	12	-27
3	8	16	70	26	-26	-9	14	16	49	29	-28
6	8	16	67	14	-21	-6	14	16	26	14	-46
-17	9	16	41	3	-37	-3	14	16	72	15	-22
-14	9	16	50	29	-30	0	14	16	51	35	-32
-11	9	16	120	103	12	3	14	16	29	43	-50
-8	9	16	96	103	13	-14	15	16	43	34	-32
-5	9	16	99	87	10	-11	15	16	66	54	-23
-2	9	16	59	49	-18	-8	15	16	72	27	-27
1	9	16	33	31	-37	-5	15	16	26	16	-46
4	9	16	26	14	-46	-2	15	16	51	19	-28
7	9	16	27	21	-48	1	15	16	65	22	-28
-16	10	16	45	43	-34	-13	16	16	65	33	-24
-13	10	16	96	109	16	-10	16	16	33	41	-41
-10	10	16	209	211	8	-7	16	16	58	19	-25
-7	10	16	166	171	11	-4	16	16	45	11	-34
-4	10	16	97	97	13	-1	16	16	43	24	-36
-1	10	16	25	35	-45	-12	17	16	45	13	-32
2	10	16	38	2	-35	-9	17	16	44	5	-34
5	10	16	55	15	-23	-6	17	16	27	23	-48
8	10	16	70	31	-24	-3	17	16	45	45	-33
-18	11	16	41	33	-39	-11	18	16	67	34	-29
-15	11	16	39	58	-34	-8	18	16	29	34	-51
-12	11	16	81	78	20	0	1	17	24	1	-37
-9	11	16	104	106	13	-2	2	17	51	3	-18
-6	11	16	76	73	16	1	2	17	87	68	14
-3	11	16	44	30	-32	-4	3	17	76	53	18
0	11	16	43	20	-25	-1	3	17	75	66	15
3	11	16	26	15	-46	2	3	17	60	51	-16
6	11	16	52	20	-28	-6	4	17	81	59	-26
-17	12	16	28	13	-49	-3	4	17	63	56	-21
-14	12	16	26	10	-46	0	4	17	24	1	-37
-11	12	16	68	71	-20	3	4	17	62	16	-25
-8	12	16	26	39	-46	-8	5	17	81	85	15
-5	12	16	34	14	-36	-5	5	17	47	1	-25
-2	12	16	51	2	-29	-2	5	17	56	49	-16
1	12	16	51	3	-31	1	5	17	60	67	-20
4	12	16	43	9	-34	4	5	17	111	99	27

Table 52. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-10	6	17	46	4	-31
-7	6	17	88	7	-27
-4	6	17	70	59	-18
-1	6	17	81	63	17
2	6	17	111	108	19
5	6	17	58	69	-23
-12	7	17	39	46	-44
-9	7	17	83	43	18
-6	7	17	32	7	-36
-3	7	17	64	16	-19
0	7	17	34	2	-30
3	7	17	45	20	-33
6	7	17	53	20	-30
-14	8	17	47	4	-29
-11	8	17	27	13	-47
-8	8	17	63	3	-24
-5	8	17	76	88	16
-2	8	17	106	109	12
1	8	17	140	142	10
4	8	17	108	98	13
7	8	17	27	19	-48
-16	9	17	43	8	-36
-13	9	17	45	24	-33
-10	9	17	48	33	-31
-7	9	17	66	49	-21
-4	9	17	90	102	15
-1	9	17	129	142	11
2	9	17	102	113	23
5	9	17	58	43	-31
-15	10	17	26	1	-46
-12	10	17	63	22	-24
-9	10	17	48	33	-29
-6	10	17	41	7	-33
-3	10	17	43	22	-33
0	10	17	44	1	-31
3	10	17	71	6	-28
6	10	17	35	16	-41
-14	11	17	27	5	-47
-11	11	17	69	2	-21
-8	11	17	38	15	-36
-5	11	17	90	68	-24
-2	11	17	102	110	17
1	11	17	111	97	14
4	11	17	28	29	-49
-13	12	17	27	4	-48
-10	12	17	53	20	-30
-7	12	17	54	48	-29
-4	12	17	106	98	17
-1	12	17	111	98	13
2	12	17	74	55	-24
-15	13	17	41	28	-38
-12	13	17	26	2	-46
-9	13	17	47	23	-28
-6	13	17	26	22	-47
-3	13	17	33	10	-40
0	13	17	47	2	-30
-14	14	17	44	2	-32
-11	14	17	27	8	-48
-8	14	17	27	3	-47
-5	14	17	62	39	-23
-2	14	17	55	52	-31
-13	15	17	28	30	-50
-10	15	17	44	4	-34
-7	15	17	60	16	-30
-4	15	17	38	28	-37
-9	16	17	28	12	-49
-6	16	17	28	17	-49
0	0	18	131	139	15
1	1	18	68	70	-21
-1	2	18	81	72	20
2	2	18	102	89	13
-3	3	18	150	142	10
0	3	18	154	153	11
3	3	18	94	100	15
-5	4	18	35	42	-35
-2	4	18	80	89	17
1	4	18	70	54	-28
4	4	18	26	26	-45
-7	5	18	49	33	-26
-4	5	18	33	37	-37
-1	5	18	69	49	-21
2	5	18	46	30	-28
5	5	18	27	6	-47
-9	6	18	51	17	-26
-6	6	18	70	47	-20
-3	6	18	88	94	16
0	6	18	79	66	14
3	6	18	70	16	-24
6	6	18	78	3	-20
-11	7	18	56	2	-25
-8	7	18	26	1	-46
-5	7	18	72	33	-25

Table 52. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-2	7	18	62	30	-24
1	7	18	60	14	-26
4	7	18	54	7	-30
7	7	18	45	48	-36
-13	8	18	61	24	-30
-10	8	18	48	8	-32
-7	8	18	52	4	-27
-4	8	18	50	23	-34
-1	8	18	26	16	-46
2	8	18	27	10	-47
5	8	18	47	18	-33
-12	9	18	45	3	-34
-9	9	18	26	2	-40
-6	9	18	39	18	-32
-3	9	18	26	16	-46
0	9	18	26	2	-40
3	9	18	46	0	-33
-14	10	18	60	33	-31
-11	10	18	34	7	-40
-8	10	18	48	5	-32
-5	10	18	47	6	-33
-2	10	18	33	12	-40
1	10	18	52	2	-33
4	10	18	75	40	-30
-13	11	18	65	15	-21
-10	11	18	43	4	-33
-7	11	18	27	1	-47
-4	11	18	26	9	-46
-1	11	18	54	5	-30
2	11	18	45	24	-35
-12	12	18	55	2	-25
-9	12	18	52	5	-31
-6	12	18	27	1	-47
-3	12	18	66	2	-23
0	12	18	45	24	-29
-11	13	18	38	15	-38
-8	13	18	55	26	-32
-5	13	18	39	21	-38
-2	13	18	57	25	-28
-10	14	18	85	34	21
-7	14	18	43	48	-36
-4	14	18	28	40	-49
-1	1	19	26	1	-40
-3	2	19	26	22	-45
0	2	19	26	3	-45
-5	3	19	51	30	-27
-2	3	19	56	21	-26
1	3	19	26	9	-45
-7	4	19	47	2	-32
-4	4	19	41	2	-30
-1	4	19	37	11	-36
2	4	19	85	24	-27
-9	5	19	92	67	20
-6	5	19	71	59	-19
-3	5	19	56	30	-24
0	5	19	62	1	-23
3	5	19	57	42	-30
-11	6	19	69	53	-23
-8	6	19	79	71	-22
-5	6	19	51	57	-26
-2	6	19	35	25	-38
1	6	19	26	14	-46
4	6	19	44	2	-34
-10	7	19	52	4	-30
-7	7	19	27	2	-41
-4	7	19	60	1	-29
-1	7	19	39	14	-37
2	7	19	27	11	-48
5	7	19	64	24	-26
-12	8	19	80	49	-22
-9	8	19	72	79	-27
-6	8	19	87	73	21
-3	8	19	45	45	-38
0	8	19	74	2	19
3	8	19	68	2	-29
-11	9	19	76	62	-21
-8	9	19	99	79	14
-5	9	19	72	70	-28
-2	9	19	27	16	-47
1	9	19	61	10	-30
-10	10	19	36	2	-35
-7	10	19	34	6	-41
-4	10	19	62	4	-24
-1	10	19	59	10	-23
-9	11	19	71	59	-30
-6	11	19	69	52	-23
-3	11	19	34	4	-41
-8	12	19	83	48	-27
-5	12	19	61	25	-25
0	1	20	36	7	-33
-2	2	20	42	2	-28
1	2	20	27	16	-47

Table 52. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
-4	3	20	27	15	-47	0	4	20	68	43	-22
-1	3	20	27	14	-47	3	4	20	67	42	-29
2	3	20	41	10	-35	-8	5	20	50	20	-30
-6	4	20	53	13	-31	-5	5	20	64	13	-20
-3	4	20	26	12	-46	-2	5	20	59	10	-29

APPENDIX E

TABLE 53

Table 53. Cis-p-Menthane Thiourea Host/Guest Adduct (subcell)

F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-1	2	0	681	924	11
0	3	0	3050	2913	30
-2	4	0	1233	805	10
-4	5	0	1178	1172	25
-1	5	0	1188	1035	12
-3	6	0	106	89	3
0	6	0	622	648	11
-5	7	0	332	310	2
-2	7	0	333	398	3
-7	8	0	435	455	4
-4	8	0	430	379	4
-1	8	0	443	445	3
-6	9	0	112	94	6
-3	9	0	117	126	5
0	9	0	612	538	8
-8	10	0	191	253	12
-5	10	0	234	272	5
-2	10	0	190	268	7
-10	11	0	157	43	9
-7	11	0	629	565	10
-4	11	0	628	522	7
-1	11	0	155	46	5
-9	12	0	87	169	10
-6	12	0	311	420	8
-3	12	0	91	197	9
0	12	0	73	148	8
-11	13	0	153	105	10
-8	13	0	79	147	9
-5	13	0	75	155	9
-2	13	0	149	79	8
-13	14	0	168	108	7
-10	14	0	392	320	4
-7	14	0	616	540	5
-4	14	0	390	296	4
-1	14	0	160	96	5
-12	15	0	143	177	11
-9	15	0	201	243	7
-6	15	0	201	258	6
-3	15	0	148	185	6
0	15	0	76	66	12
-14	16	0	36	11	-25
-11	16	0	85	91	10
-8	16	0	163	213	6
-5	16	0	68	102	11
-2	16	0	21	20	-36
-16	17	0	21	25	-37
-13	17	0	194	193	9
-10	17	0	361	354	16
-7	17	0	358	361	6
-4	17	0	199	192	7
-1	17	0	31	34	-29
-15	18	0	77	33	-22
-12	18	0	130	110	7
-9	18	0	155	123	8
-6	18	0	127	115	10
-3	18	0	64	40	-17
0	18	0	46	13	-21
-17	19	0	66	40	-19
-14	19	0	132	118	13
-11	19	0	192	205	14
-8	19	0	193	207	7
-5	19	0	121	113	10
-2	19	0	62	41	-17
-19	20	0	53	8	-22
-16	20	0	73	96	14
-13	20	0	203	238	26
-10	20	0	289	307	18
-7	20	0	209	239	15
-4	20	0	86	98	16
-1	20	0	52	5	-26
-18	21	0	24	22	-42
-15	21	0	73	79	18
-12	21	0	136	120	9
-9	21	0	126	117	14
-6	21	0	82	80	14
-3	21	0	61	19	-23
0	21	0	42	2	-26
-20	22	0	24	9	-42
-17	22	0	24	5	-42
-14	22	0	43	35	-28
-11	22	0	71	65	15
-8	22	0	60	36	-21
-5	22	0	50	3	-26
-2	22	0	57	9	-26
-19	23	0	50	13	-28
-16	23	0	72	29	-24
-13	23	0	94	77	-25
-10	23	0	80	77	19
-7	23	0	45	32	-29
-4	23	0	47	13	-25

Table 53. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-18	24	0	25	0	-43
-15	24	0	47	10	-25
-12	24	0	38	8	-31
-9	24	0	24	10	-42
-6	24	0	48	0	-28
-14	25	0	62	24	-26
-11	25	0	50	24	-25
-1	1	1	36	35	3
-3	2	1	230	218	6
0	2	1	45	48	3
-5	3	1	1775	1467	13
-2	3	1	223	204	6
1	3	1	1450	1377	12
-7	4	1	171	67	8
-4	4	1	26	24	-12
-1	4	1	1442	1453	29
2	4	1	93	113	4
-9	5	1	565	550	6
-6	5	1	2073	2027	24
-3	5	1	1762	1455	10
0	5	1	36	24	9
3	5	1	108	69	6
-11	6	1	385	379	6
-8	6	1	1633	1399	15
-5	6	1	2086	1912	16
-2	6	1	94	132	7
1	6	1	650	611	8
4	6	1	359	297	6
-13	7	1	53	17	12
-10	7	1	197	234	3
-7	7	1	19	54	-20
-4	7	1	169	135	9
-1	7	1	658	610	4
2	7	1	319	347	3
5	7	1	268	305	5
-15	8	1	265	263	5
-12	8	1	370	367	6
-9	8	1	1156	1077	16
-6	8	1	1609	1358	42
-3	8	1	110	86	4
0	8	1	35	35	-11
3	8	1	121	127	5
6	8	1	223	265	16
-17	9	1	62	25	15
-14	9	1	314	333	4
-11	9	1	866	897	9
-8	9	1	1163	1127	28
-5	9	1	561	629	9
-2	9	1	320	320	4
1	9	1	31	43	-20
4	9	1	210	193	5
7	9	1	24	19	-29
-19	10	1	63	16	-21
-16	10	1	54	54	-17
-13	10	1	171	176	5
-10	10	1	37	17	-16
-7	10	1	199	241	4
-4	10	1	359	281	3
-1	10	1	28	54	-20
2	10	1	116	124	10
5	10	1	56	36	-15
8	10	1	60	49	-16
-21	11	1	66	30	-21
-18	11	1	21	6	-36
-15	11	1	244	223	5
-12	11	1	591	596	11
-9	11	1	869	848	17
-6	11	1	386	389	5
-3	11	1	123	119	5
0	11	1	18	4	-27
3	11	1	126	127	6
6	11	1	58	44	13
9	11	1	30	18	-32
-23	12	1	48	15	-24
-20	12	1	40	32	-28
-17	12	1	25	33	-31
-14	12	1	399	421	11
-11	12	1	596	587	13
-8	12	1	364	369	22
-5	12	1	267	291	4
-2	12	1	120	133	6
1	12	1	344	330	7
4	12	1	160	129	8
7	12	1	79	75	15
10	12	1	42	19	-20
-25	13	1	67	51	-21
-22	13	1	46	17	-21
-19	13	1	44	2	-24
-16	13	1	20	31	-35
-13	13	1	33	12	-19
-10	13	1	172	152	5
-7	13	1	56	27	12

Table 53. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-4	13	1	215	167	5
-1	13	1	342	332	4
2	13	1	205	202	9
5	13	1	205	198	7
8	13	1	72	66	-19
11	13	1	36	19	-32
-24	14	1	33	6	-34
-21	14	1	45	40	-23
-18	14	1	63	25	-21
-15	14	1	199	216	9
-12	14	1	396	425	10
-9	14	1	323	354	12
-6	14	1	224	281	4
-3	14	1	129	128	6
0	14	1	24	1	-26
3	14	1	60	82	-18
6	14	1	23	40	-40
9	14	1	43	11	-28
-23	15	1	82	61	18
-20	15	1	53	58	-25
-17	15	1	30	58	-30
-14	15	1	198	211	7
-11	15	1	242	229	11
-8	15	1	270	253	4
-5	15	1	51	37	-13
-2	15	1	209	216	8
1	15	1	164	165	7
4	15	1	144	142	11
7	15	1	54	53	-26
10	15	1	38	28	-32
-25	16	1	60	70	-29
-22	16	1	60	41	-21
-19	16	1	36	8	-28
-16	16	1	48	0	-20
-13	16	1	20	26	-35
-10	16	1	38	56	-18
-7	16	1	36	18	-23
-4	16	1	161	130	7
-1	16	1	169	165	7
2	16	1	207	208	10
5	16	1	115	110	8
8	16	1	32	8	-35
-24	17	1	25	1	-43
-21	17	1	37	30	-30
-18	17	1	39	5	-24
-15	17	1	61	55	14
-12	17	1	60	43	-20
-9	17	1	44	24	-20
-6	17	1	58	37	13
-3	17	1	59	84	-19
0	17	1	46	3	-17
3	17	1	24	2	-41
6	17	1	44	13	-29
-23	18	1	58	53	-20
-20	18	1	46	25	-17
-17	18	1	45	7	-22
-14	18	1	57	21	-16
-11	18	1	29	7	-27
-8	18	1	56	47	-18
-5	18	1	202	194	6
-2	18	1	205	203	9
1	18	1	175	184	8
4	18	1	113	96	16
-22	19	1	46	21	-29
-19	19	1	39	0	-18
-16	19	1	36	5	-28
-13	19	1	22	2	-38
-10	19	1	22	12	-38
-7	19	1	85	76	11
-4	19	1	146	136	8
-1	19	1	181	185	9
2	19	1	128	122	14
5	19	1	51	23	-28
-21	20	1	59	12	-26
-18	20	1	63	28	-16
-15	20	1	52	57	-22
-12	20	1	23	34	-40
-9	20	1	32	18	-31
-6	20	1	31	40	-32
-3	20	1	58	1	-24
0	20	1	24	0	-37
3	20	1	25	6	-43
-20	21	1	24	12	-42
-17	21	1	69	31	-24
-14	21	1	30	42	-33
-11	21	1	58	30	-24
-8	21	1	71	66	-18
-5	21	1	113	105	12
-2	21	1	113	120	17
1	21	1	84	75	15
-22	22	1	30	0	-33
-19	22	1	24	21	-42

Table 53. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
-16	22	1	50	38	-24	3	7	2	1109	1041	14
-13	22	1	39	17	-19	6	7	2	487	514	5
-10	22	1	50	18	-16	-14	8	2	60	59	-19
-7	22	1	70	50	-22	-11	8	2	75	90	8
-4	22	1	100	93	14	-8	8	2	151	120	7
-1	22	1	79	75	17	-5	8	2	613	557	8
-18	23	1	61	52	-18	1	8	2	591	611	16
-15	23	1	81	62	17	4	8	2	504	529	30
-12	23	1	37	16	-29	7	8	2	193	181	5
-9	23	1	36	8	-31	-16	9	2	32	36	-23
-6	23	1	24	12	-42	-13	9	2	77	60	9
-3	23	1	48	4	-28	-10	9	2	91	112	6
-17	24	1	38	2	-30	-7	9	2	101	80	5
-14	24	1	41	6	-30	-4	9	2	349	379	4
-11	24	1	58	18	-18	-1	9	2	586	582	8
-8	24	1	25	7	-43	2	9	2	297	287	6
-5	24	1	36	24	-32	5	9	2	103	101	7
-16	25	1	75	70	17	8	9	2	57	43	14
-13	25	1	74	51	-26	-18	10	2	30	1	-29
-10	25	1	45	29	-30	-15	10	2	41	10	-22
0	1	2	206	268	2	-12	10	2	83	48	9
-2	2	2	968	761	13	-9	10	2	97	127	8
1	2	2	331	304	3	-6	10	2	511	502	3
-4	3	2	193	160	3	-3	10	2	1109	1007	15
-1	3	2	335	338	7	0	10	2	780	733	3
2	3	2	699	614	4	3	10	2	536	544	9
-6	4	2	117	115	3	6	10	2	117	126	11
-3	4	2	194	180	5	9	10	2	79	86	13
0	4	2	1463	1362	16	-20	11	2	42	45	-23
3	4	2	1337	1104	18	-17	11	2	41	51	-19
-8	5	2	609	590	9	-14	11	2	119	72	6
-5	5	2	155	196	3	-11	11	2	271	194	6
-2	5	2	703	603	15	-8	11	2	60	97	11
1	5	2	834	788	9	-5	11	2	353	317	4
4	5	2	349	363	5	-2	11	2	299	271	3
-10	6	2	516	497	6	1	11	2	286	304	9
-7	6	2	79	75	11	4	11	2	147	131	8
-4	6	2	117	84	5	7	11	2	35	27	-26
-1	6	2	835	796	11	10	11	2	51	39	-25
2	6	2	981	934	7	-22	12	2	27	16	-26
5	6	2	351	319	5	-19	12	2	61	34	-17
-12	7	2	198	208	4	-16	12	2	76	89	10
-9	7	2	100	46	5	-13	12	2	130	159	8
-6	7	2	87	35	11	-10	12	2	91	43	10
-3	7	2	1190	1159	211	-7	12	2	199	221	12
0	7	2	1825	1571	30	-4	12	2	520	512	5

Table 53. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-1	12	2	286	293	6
2	12	2	246	261	5
5	12	2	87	77	10
8	12	2	38	31	-27
11	12	2	75	33	-25
-24	13	2	50	31	-24
-21	13	2	24	32	-41
-18	13	2	89	66	17
-15	13	2	60	79	13
-12	13	2	135	161	6
-9	13	2	81	52	12
-6	13	2	483	492	6
-3	13	2	526	557	3
0	13	2	420	466	8
3	13	2	186	216	6
6	13	2	39	36	-27
9	13	2	54	35	-26
12	13	2	73	19	-26
-23	14	2	24	15	-41
-20	14	2	100	101	11
-17	14	2	229	233	9
-14	14	2	333	323	6
-11	14	2	120	84	6
-8	14	2	48	49	-18
-5	14	2	105	98	7
-2	14	2	248	254	9
1	14	2	104	107	9
4	14	2	22	8	-38
7	14	2	37	24	-30
10	14	2	94	70	13
-25	15	2	25	13	-43
-22	15	2	39	24	-30
-19	15	2	90	92	15
-16	15	2	184	186	6
-13	15	2	75	76	14
-10	15	2	36	16	-22
-7	15	2	193	179	5
-4	15	2	146	134	6
-1	15	2	96	109	10
2	15	2	86	71	10
5	15	2	35	32	-30
8	15	2	24	25	-42
-24	16	2	38	5	-32
-21	16	2	69	48	14
-18	16	2	146	120	8
-15	16	2	188	182	6
-12	16	2	91	82	9
-9	16	2	53	33	-14
-6	16	2	106	127	11
-3	16	2	186	216	12
0	16	2	74	96	12
3	16	2	37	31	-29
6	16	2	63	30	-17
-23	17	2	53	52	-22
-20	17	2	155	165	10
-17	17	2	289	311	6
-14	17	2	222	232	7
-11	17	2	56	57	-15
-8	17	2	47	39	-16
-5	17	2	80	77	11
-2	17	2	77	66	13
1	17	2	54	19	-19
4	17	2	38	9	-30
7	17	2	91	64	19
-22	18	2	77	65	-23
-19	18	2	111	117	18
-16	18	2	151	122	8
-13	18	2	86	65	17
-10	18	2	44	1	-22
-7	18	2	30	26	-29
-4	18	2	22	5	-38
-1	18	2	55	13	-24
2	18	2	40	38	-22
5	18	2	53	14	-27
-21	19	2	25	34	-43
-18	19	2	95	115	16
-15	19	2	90	91	17
-12	19	2	48	39	-24
-9	19	2	83	85	12
-6	19	2	35	35	-28
-3	19	2	51	27	-20
0	19	2	88	68	10
3	19	2	42	25	-30
-23	20	2	50	49	-29
-20	20	2	131	124	9
-17	20	2	142	165	10
-14	20	2	96	103	17
-11	20	2	39	44	-28
-8	20	2	40	28	-24
-5	20	2	54	28	-22
-2	20	2	49	38	-19
1	20	2	25	17	-43

Table 53. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-22	21	2	33	40	-35
-19	21	2	72	35	-20
-16	21	2	59	48	13
-13	21	2	50	29	-25
-10	21	2	70	39	17
-7	21	2	23	26	-40
-4	21	2	34	10	-32
-1	21	2	25	22	-43
-21	22	2	58	42	-22
-18	22	2	47	66	-26
-15	22	2	77	26	-25
-12	22	2	47	18	-19
-9	22	2	24	37	-42
-6	22	2	34	32	-33
-3	22	2	31	30	-36
-20	23	2	56	52	-21
-17	23	2	67	54	-18
-14	23	2	24	15	-42
-11	23	2	24	31	-42
-8	23	2	42	24	-29
-5	23	2	55	11	-27
-16	24	2	24	5	-42
-13	24	2	58	29	-22
-10	24	2	67	69	-23
-7	24	2	85	63	15
-15	25	2	35	12	-34
-12	25	2	41	18	-31
0	0	3	62	72	6
1	1	3	2326	2125	18
-1	2	3	2317	2278	104
2	2	3	1741	1451	7
-3	3	3	21	71	-14
0	3	3	40	10	-12
3	3	3	107	77	7
-5	4	3	1531	1384	14
-2	4	3	1744	1417	57
1	4	3	934	911	15
4	4	3	259	334	5
-7	5	3	718	593	7
-4	5	3	1546	1457	28
-1	5	3	939	982	19
2	5	3	284	239	9
5	5	3	86	96	7
-9	6	3	200	228	1
-6	6	3	30	14	-15
-3	6	3	111	64	7
0	6	3	29	69	-13
3	6	3	285	306	4
6	6	3	233	228	4
-11	7	3	246	239	6
-8	7	3	50	32	10
-5	7	3	723	644	14
-2	7	3	293	192	12
1	7	3	170	146	3
4	7	3	134	104	7
7	7	3	43	45	-18
-13	8	3	463	426	4
-10	8	3	117	119	5
-7	8	3	78	39	-25
-4	8	3	255	307	3
-1	8	3	167	220	7
2	8	3	122	86	6
5	8	3	263	211	12
8	8	3	434	423	5
-15	9	3	451	449	4
-12	9	3	84	98	8
-9	9	3	17	20	-25
-6	9	3	199	188	10
-3	9	3	289	257	6
0	9	3	17	38	-25
3	9	3	280	287	6
6	9	3	320	314	7
9	9	3	330	331	12
-17	10	3	21	4	-36
-14	10	3	59	54	15
-11	10	3	95	106	16
-8	10	3	113	132	8
-5	10	3	88	64	15
-2	10	3	134	146	14
1	10	3	45	83	-16
4	10	3	46	22	-17
7	10	3	52	31	-15
10	10	3	23	4	-39
-19	11	3	241	264	11
-16	11	3	386	397	8
-13	11	3	132	129	6
-10	11	3	87	88	9
-7	11	3	249	234	6
-4	11	3	134	140	5
-1	11	3	42	44	-15
2	11	3	213	203	4
5	11	3	246	228	12

Table 53. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
8	11	3	261	259	13
11	11	3	122	105	17
-21	12	3	155	160	26
-18	12	3	284	278	7
-15	12	3	246	238	5
-12	12	3	29	5	-22
-9	12	3	88	90	9
-6	12	3	237	219	7
-3	12	3	280	257	6
0	12	3	35	0	-20
3	12	3	179	171	6
6	12	3	201	208	11
9	12	3	141	152	9
12	12	3	26	61	-44
-23	13	3	24	31	-42
-20	13	3	35	18	-29
-17	13	3	61	24	-20
-14	13	3	62	66	12
-11	13	3	128	137	6
-8	13	3	453	437	17
-5	13	3	261	236	7
-2	13	3	216	229	4
1	13	3	107	104	7
4	13	3	35	9	-24
7	13	3	23	27	-39
10	13	3	57	9	-18
-25	14	3	50	12	-27
-22	14	3	61	56	-17
-19	14	3	127	136	12
-16	14	3	80	91	11
-13	14	3	65	62	12
-10	14	3	60	46	11
-7	14	3	30	43	-24
-4	14	3	40	31	-16
-1	14	3	112	116	14
2	14	3	142	131	6
5	14	3	147	145	9
8	14	3	106	99	13
11	14	3	38	19	-33
-24	15	3	31	37	-37
-21	15	3	67	55	12
-18	15	3	45	30	-22
-15	15	3	29	1	-24
-12	15	3	242	237	9
-9	15	3	460	441	12
-6	15	3	305	305	4
-3	15	3	175	179	8
0	15	3	21	5	-31
3	15	3	121	126	10
6	15	3	99	85	11
9	15	3	63	41	-23
-23	16	3	24	4	-42
-20	16	3	62	51	-19
-17	16	3	72	69	14
-14	16	3	88	95	14
-11	16	3	385	389	6
-8	16	3	436	427	6
-5	16	3	240	236	12
-2	16	3	133	134	8
1	16	3	45	16	-22
4	16	3	23	16	-40
7	16	3	46	3	-28
-22	17	3	53	29	-22
-19	17	3	65	47	15
-16	17	3	87	69	13
-13	17	3	22	26	-37
-10	17	3	28	8	-30
-7	17	3	47	32	-18
-4	17	3	29	6	-29
-1	17	3	22	13	-38
2	17	3	37	27	-30
5	17	3	44	22	-29
-24	18	3	48	19	-25
-21	18	3	53	3	-22
-18	18	3	30	2	-29
-15	18	3	54	30	-19
-12	18	3	292	273	8
-9	18	3	328	329	15
-6	18	3	185	209	12
-3	18	3	119	131	13
0	18	3	53	2	-23
3	18	3	62	15	-17
6	18	3	25	8	-43
-23	19	3	33	9	-35
-20	19	3	44	6	-24
-17	19	3	54	45	-25
-14	19	3	116	135	10
-11	19	3	248	261	17
-8	19	3	247	260	6
-5	19	3	142	147	9
-2	19	3	45	26	-23
1	19	3	43	3	-27

Table 53. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
4	19	3	41	4	-27
-22	20	3	62	21	-20
-19	20	3	63	7	-21
-16	20	3	60	48	-18
-13	20	3	57	15	-24
-10	20	3	44	5	-26
-7	20	3	35	25	-30
-4	20	3	33	21	-32
-1	20	3	51	1	-26
2	20	3	32	6	-36
-21	21	3	46	1	-26
-18	21	3	46	4	-29
-15	21	3	73	54	-19
-12	21	3	148	158	14
-9	21	3	151	153	14
-6	21	3	86	88	12
-3	21	3	43	15	-28
0	21	3	41	1	-27
-20	22	3	36	23	-32
-17	22	3	81	25	17
-14	22	3	52	56	-20
-11	22	3	97	105	13
-8	22	3	89	101	15
-5	22	3	36	21	-32
-2	22	3	39	6	-29
-19	23	3	25	11	-43
-16	23	3	24	6	-42
-13	23	3	49	31	-27
-10	23	3	36	10	-32
-7	23	3	30	1	-35
-4	23	3	41	3	-29
-18	24	3	44	19	-27
-15	24	3	25	38	-44
-12	24	3	85	61	-27
-9	24	3	39	44	-30
-6	24	3	33	7	-35
-14	25	3	25	13	-43
-11	25	3	25	20	-43
-1	1	4	337	584	3
-3	2	4	331	205	6
0	2	4	1638	1257	43
-5	3	4	308	285	3
-2	3	4	330	250	5
1	3	4	743	689	10
-7	4	4	763	675	4
-4	4	4	360	401	4
-1	4	4	751	733	16
2	4	4	534	538	3
-9	5	4	600	624	3
-6	5	4	481	477	9
-3	5	4	309	349	5
0	5	4	432	431	5
3	5	4	103	52	11
-11	6	4	379	387	9
-8	6	4	355	346	13
-5	6	4	481	516	7
-2	6	4	539	509	14
1	6	4	497	447	6
4	6	4	532	531	5
-13	7	4	223	257	10
-10	7	4	1033	971	5
-7	7	4	1066	887	8
-4	7	4	769	652	15
-1	7	4	498	454	3
2	7	4	377	406	3
5	7	4	111	94	10
-15	8	4	46	32	-17
-12	8	4	187	175	5
-9	8	4	640	656	1
-6	8	4	358	396	4
-3	8	4	98	48	6
0	8	4	81	109	6
3	8	4	54	30	13
6	8	4	85	33	10
-17	9	4	21	6	-37
-14	9	4	238	215	9
-11	9	4	672	669	10
-8	9	4	628	655	30
-5	9	4	606	642	10
-2	9	4	378	410	8
1	9	4	197	197	5
4	9	4	28	18	-24
7	9	4	41	7	-20
-19	10	4	61	58	15
-16	10	4	94	147	12
-13	10	4	547	579	6
-10	10	4	1304	1262	16
-7	10	4	1037	994	16
-4	10	4	533	535	9
-1	10	4	200	197	5
2	10	4	130	113	6
5	10	4	99	62	8

Table 53. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
8	10	4	81	58	13
-21	11	4	57	28	-19
-18	11	4	83	87	15
-15	11	4	221	200	7
-12	11	4	412	391	6
-9	11	4	675	659	11
-6	11	4	382	354	8
-3	11	4	59	37	13
0	11	4	41	19	-16
3	11	4	163	188	5
6	11	4	123	133	10
9	11	4	52	5	-20
-23	12	4	30	3	-35
-20	12	4	23	24	-39
-17	12	4	64	64	12
-14	12	4	94	78	19
-11	12	4	413	388	5
-8	12	4	181	159	10
-5	12	4	118	96	8
-2	12	4	133	103	9
1	12	4	78	51	10
4	12	4	144	133	7
7	12	4	54	34	-18
10	12	4	55	24	-20
-22	13	4	47	52	-28
-19	13	4	22	8	-39
-16	13	4	51	84	-19
-13	13	4	347	364	6
-10	13	4	556	592	8
-7	13	4	228	274	13
-4	13	4	23	32	-28
-1	13	4	90	53	8
2	13	4	173	133	6
5	13	4	96	80	16
8	13	4	46	7	-26
11	13	4	55	23	-21
-24	14	4	61	59	-21
-21	14	4	92	82	9
-18	14	4	45	54	-22
-15	14	4	114	108	10
-12	14	4	90	78	9
-9	14	4	236	212	6
-6	14	4	73	27	10
-3	14	4	164	186	5
0	14	4	224	237	5
3	14	4	232	248	7
6	14	4	94	85	16
9	14	4	60	8	-23
-23	15	4	52	18	-26
-20	15	4	42	19	-27
-17	15	4	49	43	-24
-14	15	4	120	103	9
-11	15	4	216	199	5
-8	15	4	64	36	12
-5	15	4	107	67	7
-2	15	4	165	131	10
1	15	4	134	132	9
4	15	4	78	92	15
7	15	4	46	35	-24
-22	16	4	25	73	-43
-19	16	4	38	5	-29
-16	16	4	50	34	-20
-13	16	4	63	81	15
-10	16	4	121	144	8
-7	16	4	51	5	-19
-4	16	4	146	126	6
-1	16	4	152	129	7
2	16	4	123	118	13
5	16	4	54	37	-20
8	16	4	43	2	-29
-24	17	4	76	74	16
-21	17	4	89	76	16
-18	17	4	23	14	-40
-15	17	4	68	43	-22
-12	17	4	54	67	-16
-9	17	4	42	5	-19
-6	17	4	116	137	18
-3	17	4	226	240	6
0	17	4	239	242	6
3	17	4	154	153	8
6	17	4	64	42	-26
-23	18	4	31	16	-37
-20	18	4	55	31	-21
-17	18	4	37	20	-26
-14	18	4	55	57	-16
-11	18	4	95	91	17
-8	18	4	72	59	13
-5	18	4	99	78	10
-2	18	4	116	117	13
1	18	4	85	91	9
4	18	4	63	46	-22
-22	19	4	61	32	-20

Table 53. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-19	19	4	59	30	-16
-16	19	4	40	0	-28
-13	19	4	38	9	-28
-10	19	4	64	58	-20
-7	19	4	36	34	-26
-4	19	4	66	88	16
-1	19	4	95	91	10
2	19	4	72	61	-18
-21	20	4	36	12	-32
-18	20	4	60	31	-25
-15	20	4	44	22	-26
-12	20	4	22	24	-39
-9	20	4	52	4	-24
-6	20	4	95	83	12
-3	20	4	152	150	8
0	20	4	130	134	9
-20	21	4	44	16	-28
-17	21	4	95	75	13
-14	21	4	92	84	9
-11	21	4	41	28	-28
-8	21	4	23	9	-41
-5	21	4	41	37	-30
-2	21	4	66	60	-25
1	21	4	60	38	-22
-19	22	4	44	35	-26
-16	22	4	90	73	21
-13	22	4	72	54	-24
-10	22	4	36	26	-31
-7	22	4	47	34	-24
-4	22	4	33	44	-35
-1	22	4	54	40	-21
-18	23	4	65	13	-26
-15	23	4	24	17	-42
-12	23	4	45	2	-24
-9	23	4	24	7	-42
-6	23	4	67	41	-20
-17	24	4	85	73	18
-14	24	4	70	60	-19
-11	24	4	43	24	-30
-8	24	4	25	2	-43
0	1	5	38	36	9
-2	2	5	44	42	9
1	2	5	867	866	11
-4	3	5	876	850	12
-1	3	5	875	795	26
2	3	5	386	384	3
-6	4	5	520	499	2
-3	4	5	872	829	16
0	4	5	26	1	-15
3	4	5	255	226	3
-8	5	5	969	942	5
-5	5	5	25	2	-13
-2	5	5	385	305	7
1	5	5	348	303	4
4	5	5	808	762	5
-10	6	5	228	204	5
-7	6	5	386	384	7
-4	6	5	520	470	11
-1	6	5	349	315	6
2	6	5	853	832	6
5	6	5	594	607	5
-12	7	5	236	201	5
-9	7	5	187	206	5
-6	7	5	394	362	5
-3	7	5	258	218	4
0	7	5	35	25	-14
3	7	5	143	187	5
6	7	5	63	79	-19
-14	8	5	72	49	9
-11	8	5	143	152	9
-8	8	5	23	35	-21
-5	8	5	970	947	20
-2	8	5	855	805	19
1	8	5	1073	1054	17
4	8	5	733	715	21
7	8	5	35	17	-24
-16	9	5	93	74	9
-13	9	5	90	83	7
-10	9	5	46	51	-19
-7	9	5	182	146	5
-4	9	5	807	791	12
-1	9	5	1073	1039	17
2	9	5	762	769	10
5	9	5	227	253	5
8	9	5	56	66	-17
-18	10	5	47	10	-25
-15	10	5	142	145	6
-12	10	5	44	46	-14
-9	10	5	66	82	9
-6	10	5	233	189	7
-3	10	5	142	176	6
0	10	5	19	13	-29

Table 53. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
3	10	5	75	86	17	1	14	5	76	99	12
6	10	5	111	108	8	4	14	5	47	20	-20
9	10	5	40	2	-23	7	14	5	49	11	-25
-20	11	5	23	12	-40	10	14	5	25	26	-43
-17	11	5	30	18	-29	-22	15	5	71	23	-18
-14	11	5	122	113	7	-19	15	5	143	146	10
-11	11	5	38	23	-15	-16	15	5	312	310	7
-8	11	5	140	165	12	-13	15	5	239	239	5
-5	11	5	602	608	8	-10	15	5	136	139	6
-2	11	5	759	743	8	-7	15	5	39	16	-23
1	11	5	626	624	13	-4	15	5	158	167	6
4	11	5	166	165	9	-1	15	5	84	86	10
7	11	5	52	13	-19	2	15	5	42	57	-23
10	11	5	38	1	-19	5	15	5	51	31	-23
-22	12	5	24	34	-42	8	15	5	93	85	18
-19	12	5	42	41	-24	-24	16	5	45	42	-27
-16	12	5	164	161	6	-21	16	5	75	85	15
-13	12	5	35	27	-23	-18	16	5	208	212	9
-10	12	5	59	36	11	-15	16	5	314	313	11
-7	12	5	241	218	6	-12	16	5	165	169	7
-4	12	5	734	711	7	-9	16	5	91	84	9
-1	12	5	623	604	5	-6	16	5	107	108	8
2	12	5	260	271	5	-3	16	5	65	71	16
5	12	5	113	124	8	0	16	5	30	2	-27
8	12	5	71	32	16	3	16	5	49	9	-23
11	12	5	71	69	-20	6	16	5	55	55	-21
-24	13	5	25	28	-43	-23	17	5	59	33	-22
-21	13	5	53	17	-15	-20	17	5	24	22	-41
-18	13	5	78	92	12	-17	17	5	23	2	-35
-15	13	5	242	231	7	-14	17	5	49	36	-21
-12	13	5	19	34	-34	-11	17	5	36	21	-26
-9	13	5	80	92	-20	-8	17	5	65	57	-17
-6	13	5	60	71	15	-5	17	5	113	123	13
-3	13	5	85	101	9	-2	17	5	61	52	-18
0	13	5	28	2	-24	1	17	5	40	19	-25
3	13	5	73	74	15	4	17	5	57	7	-25
6	13	5	37	4	-27	-22	18	5	52	43	-24
9	13	5	79	64	-26	-19	18	5	160	147	9
-23	14	5	43	36	-25	-16	18	5	210	212	13
-20	14	5	39	7	-26	-13	18	5	84	96	11
-17	14	5	30	39	-32	-10	18	5	45	12	-21
-14	14	5	21	4	-31	-7	18	5	22	12	-38
-11	14	5	114	116	10	-4	18	5	22	18	-39
-8	14	5	76	58	11	-1	18	5	53	15	-22
-5	14	5	232	252	6	2	18	5	24	15	-42
-2	14	5	247	274	5	5	18	5	77	62	-20

Table 53. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-21	19	5	99	94	19
-18	19	5	150	149	9
-15	19	5	152	145	8
-12	19	5	49	48	-19
-9	19	5	22	2	-39
-6	19	5	22	7	-38
-3	19	5	23	10	-40
0	19	5	43	1	-26
3	19	5	33	29	-36
-20	20	5	34	1	-30
-17	20	5	24	21	-42
-14	20	5	23	8	-40
-11	20	5	43	11	-24
-8	20	5	44	32	-23
-5	20	5	40	31	-26
-2	20	5	68	17	-24
1	20	5	42	3	-30
-19	21	5	94	94	14
-16	21	5	98	84	11
-13	21	5	45	19	-17
-10	21	5	54	2	-17
-7	21	5	33	12	-33
-4	21	5	50	8	-27
-1	21	5	30	4	-37
-18	22	5	58	42	-22
-15	22	5	70	22	-25
-12	22	5	33	34	-32
-9	22	5	81	64	-22
-6	22	5	67	54	-20
-3	22	5	25	29	-43
-17	23	5	43	34	-30
-14	23	5	53	38	-28
-11	23	5	80	68	18
-8	23	5	92	85	16
-5	23	5	70	62	-20
-16	24	5	67	45	-24
-13	24	5	60	30	-22
-10	24	5	25	25	-43
0	0	6	978	986	4
1	1	6	546	456	9
-1	2	6	546	535	11
2	2	6	1512	1190	9
-3	3	6	1726	1598	29
0	3	6	1875	1741	55
3	3	6	1131	1126	6
-5	4	6	325	261	4
-2	4	6	1499	1298	37
1	4	6	386	273	7
4	4	6	141	118	4
-7	5	6	491	425	15
-4	5	6	327	288	10
-1	5	6	387	338	8
2	5	6	435	399	4
5	5	6	117	128	6
-9	6	6	17	16	-30
-6	6	6	279	320	4
-3	6	6	1135	1023	30
0	6	6	444	480	4
3	6	6	54	17	13
6	6	6	92	75	7
-11	7	6	26	21	-25
-8	7	6	133	127	5
-5	7	6	493	454	1
-2	7	6	436	426	5
1	7	6	82	76	7
4	7	6	37	25	-22
7	7	6	386	403	4
-13	8	6	174	165	7
-10	8	6	73	70	8
-7	8	6	136	140	7
-4	8	6	146	117	4
-1	8	6	87	78	8
2	8	6	158	168	6
5	8	6	145	126	6
8	8	6	196	202	6
-15	9	6	233	224	5
-12	9	6	87	83	8
-9	9	6	353	334	7
-6	9	6	43	9	-17
-3	9	6	46	48	-18
0	9	6	309	296	3
3	9	6	91	88	10
6	9	6	250	246	5
9	9	6	227	238	12
-17	10	6	394	400	5
-14	10	6	353	342	6
-11	10	6	160	152	7
-8	10	6	74	96	10
-5	10	6	119	125	7
-2	10	6	163	176	6
1	10	6	118	116	7
4	10	6	364	356	8

Table 53. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
7	10	6	417	434	16
10	10	6	195	194	11
-19	11	6	89	82	17
-16	11	6	163	174	8
-13	11	6	159	165	6
-10	11	6	160	147	6
-7	11	6	18	22	-32
-4	11	6	33	23	-20
-1	11	6	125	108	7
2	11	6	186	193	6
5	11	6	207	209	6
8	11	6	106	104	13
11	11	6	70	96	-21
-21	12	6	63	49	-17
-18	12	6	162	171	9
-15	12	6	98	93	11
-12	12	6	42	37	-17
-9	12	6	84	72	10
-6	12	6	99	74	7
-3	12	6	93	85	9
0	12	6	66	64	10
3	12	6	49	45	-16
6	12	6	157	162	7
9	12	6	58	31	-19
12	12	6	25	10	-43
-23	13	6	68	84	-18
-20	13	6	131	131	12
-17	13	6	205	210	7
-14	13	6	115	107	7
-11	13	6	163	158	6
-8	13	6	162	151	11
-5	13	6	149	136	6
-2	13	6	184	181	6
1	13	6	45	60	-17
4	13	6	205	209	7
7	13	6	136	126	11
10	13	6	91	80	16
-22	14	6	64	58	-24
-19	14	6	31	20	-32
-16	14	6	49	42	-18
-13	14	6	120	101	7
-10	14	6	351	338	9
-7	14	6	386	406	4
-4	14	6	360	358	5
-1	14	6	68	64	14
2	14	6	67	65	13
5	14	6	58	20	-23
8	14	6	77	69	15
-24	15	6	33	14	-35
-21	15	6	59	32	-23
-18	15	6	98	89	10
-15	15	6	72	79	12
-12	15	6	106	90	10
-9	15	6	232	223	6
-6	15	6	255	241	7
-3	15	6	65	53	16
0	15	6	46	18	-22
3	15	6	100	81	18
6	15	6	24	18	-42
9	15	6	44	7	-29
-23	16	6	47	42	-26
-20	16	6	64	38	-22
-17	16	6	73	57	-23
-14	16	6	35	43	-28
-8	16	6	200	203	12
-5	16	6	209	212	6
-2	16	6	71	64	17
1	16	6	52	43	-25
4	16	6	35	21	-32
7	16	6	47	43	-27
-22	17	6	46	14	-28
-19	17	6	49	18	-21
-16	17	6	66	59	-20
-13	17	6	200	207	9
-10	17	6	397	404	20
-7	17	6	416	430	5
-4	17	6	204	214	6
-1	17	6	54	42	-20
2	17	6	42	32	-26
5	17	6	25	18	-43
-21	18	6	37	4	-32
-18	18	6	38	46	-18
-15	18	6	82	93	12
-12	18	6	173	173	9
-9	18	6	228	240	8
-6	18	6	150	164	8
-3	18	6	86	79	15
0	18	6	59	47	12
3	18	6	24	2	-42
-20	19	6	24	0	-41
-17	19	6	37	19	-30
-14	19	6	22	17	-39

Table 53. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-11	19	6	75	83	17
-8	19	6	83	104	14
-5	19	6	23	26	-40
-2	19	6	44	30	-28
1	19	6	52	7	-23
-19	20	6	24	1	-42
-16	20	6	62	35	-17
-13	20	6	136	128	9
-10	20	6	204	193	7
-7	20	6	133	129	9
-4	20	6	56	25	-22
-1	20	6	37	3	-31
-21	21	6	57	23	-20
-18	21	6	36	2	-32
-15	21	6	62	31	-17
-12	21	6	60	47	-23
-9	21	6	63	34	-22
-6	21	6	44	18	-29
-3	21	6	37	1	-31
0	21	6	51	34	-23
-17	22	6	33	15	-34
-14	22	6	60	58	-20
-11	22	6	79	96	14
-8	22	6	82	70	-27
-5	22	6	69	18	-25
-16	23	6	59	41	-25
-13	23	6	80	82	15
-10	23	6	81	81	15
-7	23	6	67	42	-23
-15	24	6	25	13	-43
-12	24	6	25	9	-43
-9	24	6	25	6	-43
-1	1	7	27	28	-15
-3	2	7	467	446	11
0	2	7	22	26	-17
-5	3	7	366	314	7
-2	3	7	465	477	13
1	3	7	409	364	2
-7	4	7	63	59	10
-4	4	7	45	5	-14
-1	4	7	412	428	10
2	4	7	330	363	1
-9	5	7	748	754	3
-6	5	7	524	511	7
-3	5	7	365	346	10
0	5	7	34	2	-14
3	5	7	724	674	5
-11	6	7	601	575	8
-8	6	7	817	768	8
-5	6	7	525	500	10
-2	6	7	337	305	10
1	6	7	291	322	9
4	6	7	115	123	8
-13	7	7	27	46	-25
-10	7	7	108	101	7
-7	7	7	34	11	-15
-4	7	7	68	33	10
-1	7	7	291	262	5
2	7	7	88	78	12
5	7	7	201	205	5
-15	8	7	50	22	-17
-12	8	7	583	587	14
-9	8	7	903	884	10
-6	8	7	819	819	19
-3	8	7	733	717	13
0	8	7	18	19	-27
3	8	7	102	80	7
6	8	7	45	27	-22
-17	9	7	52	64	-18
-14	9	7	270	292	8
-11	9	7	643	641	10
-8	9	7	889	891	28
-5	9	7	751	716	16
-2	9	7	83	81	10
1	9	7	19	5	-32
4	9	7	68	58	11
7	9	7	100	89	12
-19	10	7	43	4	-27
-16	10	7	108	111	8
-13	10	7	52	23	-15
-10	10	7	35	0	-20
-7	10	7	117	103	8
-4	10	7	112	106	11
-1	10	7	19	16	-32
2	10	7	19	13	-34
5	10	7	99	89	8
8	10	7	22	8	-38
-21	11	7	42	3	-28
-18	11	7	31	1	-31
-15	11	7	167	170	6
-12	11	7	468	472	5
-9	11	7	648	648	13

Table 53. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-6	11	7	605	582	13
-3	11	7	107	106	10
0	11	7	44	2	-18
3	11	7	88	103	10
6	11	7	49	46	-19
9	11	7	44	3	-21
-23	12	7	70	51	-19
-20	12	7	64	39	15
-17	12	7	91	100	13
-14	12	7	228	244	7
-11	12	7	481	480	12
-8	12	7	581	583	21
-5	12	7	204	203	6
-2	12	7	19	9	-34
1	12	7	67	57	16
4	12	7	121	135	11
7	12	7	38	45	-29
10	12	7	38	25	-31
-22	13	7	33	53	-35
-19	13	7	42	1	-26
-16	13	7	67	23	-22
-13	13	7	49	3	-20
-10	13	7	31	18	-24
-7	13	7	39	33	-19
-4	13	7	63	59	13
-1	13	7	64	53	14
2	13	7	216	218	9
5	13	7	70	59	14
8	13	7	24	7	-41
-21	14	7	45	15	-25
-18	14	7	27	32	-34
-15	14	7	111	122	10
-12	14	7	227	250	7
-9	14	7	270	292	5
-6	14	7	30	36	-27
-3	14	7	96	95	19
0	14	7	30	2	-25
3	14	7	66	45	-17
6	14	7	46	31	-27
9	14	7	43	17	-27
-23	15	7	80	64	-21
-20	15	7	35	25	-32
-17	15	7	67	46	-24
-14	15	7	116	122	15
-11	15	7	172	163	11
-8	15	7	50	23	-21
-5	15	7	98	94	10
-2	15	7	216	211	6
1	15	7	284	294	9
4	15	7	136	134	8
7	15	7	48	29	-29
-22	16	7	76	32	-24
-19	16	7	47	7	-27
-16	16	7	42	1	-22
-13	16	7	24	28	-29
-10	16	7	105	109	8
-7	16	7	92	89	10
-4	16	7	109	134	13
-1	16	7	299	293	6
2	16	7	189	192	8
5	16	7	81	68	16
-21	17	7	68	23	-25
-18	17	7	37	4	-21
-15	17	7	53	50	-20
-12	17	7	73	103	-26
-9	17	7	56	70	-19
-6	17	7	53	45	-17
-3	17	7	59	48	-19
0	17	7	30	1	-31
3	17	7	24	15	-42
-20	18	7	50	32	-24
-17	18	7	32	3	-23
-14	18	7	44	28	-23
-11	18	7	40	2	-23
-8	18	7	56	8	-22
-5	18	7	68	58	14
-2	18	7	183	194	8
1	18	7	135	136	11
4	18	7	51	37	-29
-19	19	7	45	1	-24
-16	19	7	32	6	-33
-13	19	7	43	1	-26
-10	19	7	59	5	-23
-7	19	7	55	44	-19
-4	19	7	141	136	10
-1	19	7	133	134	10
2	19	7	87	82	14
-21	20	7	34	22	-35
-18	20	7	40	31	-31
-15	20	7	43	27	-26
-12	20	7	76	36	-21
-9	20	7	41	3	-20

Table 53. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-6	20	7	41	32	-25
-3	20	7	55	15	-21
0	20	7	25	0	-37
-20	21	7	49	21	-23
-17	21	7	34	24	-33
-14	21	7	49	18	-26
-11	21	7	47	5	-23
-8	21	7	31	5	-34
-5	21	7	72	69	18
-2	21	7	69	81	-19
-16	22	7	57	33	-26
-13	22	7	56	51	-20
-10	22	7	24	26	-42
-7	22	7	48	29	-29
-4	22	7	89	37	-27
-15	23	7	26	65	-44
-12	23	7	78	53	15
-9	23	7	25	16	-43
0	1	8	257	215	4
-2	2	8	213	249	4
1	2	8	187	223	3
-4	3	8	305	329	8
-1	3	8	188	233	4
2	3	8	185	178	4
-6	4	8	313	262	5
-3	4	8	302	313	8
0	4	8	626	573	10
3	4	8	572	606	3
-8	5	8	192	134	6
-5	5	8	267	208	7
-2	5	8	188	194	8
1	5	8	506	498	3
4	5	8	345	307	4
-10	6	8	313	332	4
-7	6	8	247	293	8
-4	6	8	311	286	10
-1	6	8	505	506	5
2	6	8	375	327	10
5	6	8	298	256	4
-12	7	8	66	44	12
-9	7	8	127	71	7
-6	7	8	243	282	5
-3	7	8	578	567	11
0	7	8	975	956	11
3	7	8	710	732	9
6	7	8	217	216	5
-14	8	8	58	67	14
-11	8	8	80	76	13
-8	8	8	251	249	4
-5	8	8	201	174	9
-2	8	8	379	369	11
1	8	8	541	511	15
4	8	8	156	150	10
7	8	8	45	9	-24
-16	9	8	22	22	-37
-13	9	8	58	61	14
-10	9	8	129	144	10
-7	9	8	130	99	10
-4	9	8	347	340	8
-1	9	8	546	525	12
2	9	8	436	417	5
5	9	8	164	164	6
8	9	8	64	45	-22
-18	10	8	59	12	-18
-15	10	8	69	66	13
-12	10	8	124	118	8
-9	10	8	125	133	6
-6	10	8	309	303	5
-3	10	8	712	704	12
0	10	8	935	953	10
3	10	8	432	448	4
6	10	8	108	121	9
9	10	8	23	24	-41
-20	11	8	31	18	-34
-17	11	8	100	96	11
-14	11	8	176	162	6
-11	11	8	69	66	16
-8	11	8	75	70	9
-5	11	8	300	273	4
-2	11	8	439	428	11
1	11	8	324	326	5
4	11	8	155	153	6
7	11	8	49	34	-21
10	11	8	24	17	-42
-22	12	8	74	26	18
-19	12	8	74	71	17
-16	12	8	97	109	10
-13	12	8	68	63	15
-10	12	8	117	118	8
-7	12	8	48	42	-18
-4	12	8	155	160	7
-1	12	8	323	329	4

Table 53. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
2	12	8	68	65	12
5	12	8	22	25	-39
8	12	8	29	10	-35
11	12	8	53	4	-26
-21	13	8	52	10	-24
-18	13	8	52	24	-19
-15	13	8	113	101	13
-12	13	8	66	55	17
-9	13	8	49	56	-19
-6	13	8	209	217	5
-3	13	8	432	442	6
0	13	8	301	324	5
3	13	8	81	79	13
6	13	8	24	10	-29
9	13	8	59	43	-26
-23	14	8	43	9	-30
-20	14	8	101	89	19
-17	14	8	176	182	10
-14	14	8	195	197	6
-11	14	8	178	172	6
-8	14	8	59	56	-16
-5	14	8	173	160	6
-2	14	8	76	63	-21
1	14	8	91	98	12
4	14	8	52	29	-21
7	14	8	74	65	16
-22	15	8	58	37	-22
-19	15	8	101	106	15
-16	15	8	113	107	16
-13	15	8	122	106	12
-10	15	8	66	60	13
-7	15	8	21	12	-36
-4	15	8	151	158	7
-1	15	8	96	101	12
2	15	8	23	18	-40
5	15	8	36	15	-32
-21	16	8	33	27	-35
-18	16	8	84	68	15
-15	16	8	107	99	18
-12	16	8	104	103	16
-9	16	8	36	23	-26
-6	16	8	112	122	12
-3	16	8	74	80	17
0	16	8	57	52	-18
3	16	8	37	0	-31
6	16	8	73	55	-19
-20	17	8	121	131	11
-17	17	8	168	175	8
-14	17	8	145	184	-48
-11	17	8	113	95	15
-8	17	8	52	41	-19
-5	17	8	48	30	-20
-2	17	8	23	20	-40
1	17	8	57	19	-25
4	17	8	76	57	18
-19	18	8	74	78	17
-16	18	8	95	70	21
-13	18	8	34	23	-29
-10	18	8	36	9	-29
-7	18	8	47	34	-22
-4	18	8	29	29	-34
-1	18	8	24	16	-42
2	18	8	43	27	-30
-21	19	8	71	59	17
-18	19	8	94	81	18
-15	19	8	117	107	10
-12	19	8	82	70	20
-9	19	8	23	21	-40
-6	19	8	50	12	-19
-3	19	8	24	3	-41
0	19	8	52	31	-23
-20	20	8	133	123	9
-17	20	8	140	136	14
-14	20	8	91	90	13
-11	20	8	75	17	-25
-8	20	8	42	7	-29
-5	20	8	40	10	-27
-2	20	8	49	26	-24
-19	21	8	81	59	15
-16	21	8	25	29	-43
-13	21	8	40	8	-30
-10	21	8	31	17	-36
-7	21	8	66	64	-21
-4	21	8	71	56	-23
-15	22	8	66	38	-21
-12	22	8	48	26	-26
-9	22	8	62	45	-18
-6	22	8	56	56	-23
-14	23	8	42	10	-30
-11	23	8	34	4	-34
0	0	9	49	13	-23
1	1	9	1300	1264	25

Table 53. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-1	2	9	1294	1279	31
2	2	9	914	865	24
-3	3	9	30	17	-19
0	3	9	42	15	-14
3	3	9	182	178	4
-5	4	9	430	383	7
-2	4	9	910	886	14
1	4	9	583	578	9
4	4	9	106	96	6
-7	5	9	257	229	5
-4	5	9	423	380	11
-1	5	9	588	576	14
2	5	9	412	394	8
5	5	9	128	119	7
-9	6	9	167	182	5
-6	6	9	36	14	-17
-3	6	9	189	189	4
0	6	9	37	15	-15
3	6	9	46	42	-18
6	6	9	257	268	6
-11	7	9	86	85	9
-8	7	9	212	191	7
-5	7	9	257	235	4
-2	7	9	409	395	5
1	7	9	155	152	5
4	7	9	78	87	11
7	7	9	54	39	-17
-13	8	9	254	251	7
-10	8	9	39	40	-22
-7	8	9	212	207	5
-4	8	9	111	122	6
-1	8	9	152	170	5
2	8	9	37	5	-22
5	8	9	346	341	4
8	8	9	293	284	5
-15	9	9	191	207	6
-12	9	9	193	198	5
-9	9	9	39	1	-17
-6	9	9	166	151	6
-3	9	9	48	70	-13
0	9	9	25	6	-24
3	9	9	118	119	7
6	9	9	293	298	5
9	9	9	239	246	15
-17	10	9	51	10	-20
-14	10	9	37	46	-26
-11	10	9	37	28	-23
-8	10	9	48	44	-15
-5	10	9	116	124	6
-2	10	9	26	11	-27
1	10	9	20	8	-35
4	10	9	43	49	-21
7	10	9	31	23	-32
10	10	9	40	13	-30
-19	11	9	196	191	9
-16	11	9	178	175	8
-13	11	9	192	188	6
-10	11	9	48	20	-15
-7	11	9	82	90	10
-4	11	9	85	84	10
-1	11	9	20	23	-35
2	11	9	89	87	13
5	11	9	248	242	6
8	11	9	194	182	7
11	11	9	100	91	15
-21	12	9	120	122	16
-18	12	9	150	154	9
-15	12	9	83	86	11
-12	12	9	33	4	-23
-9	12	9	196	196	5
-6	12	9	264	260	5
-3	12	9	124	117	7
0	12	9	21	3	-31
3	12	9	135	135	8
6	12	9	201	205	15
9	12	9	132	130	13
-20	13	9	40	22	-27
-17	13	9	57	18	-19
-14	13	9	135	143	8
-11	13	9	194	195	8
-8	13	9	242	255	7
-5	13	9	346	345	6
-2	13	9	88	93	10
1	13	9	29	19	-30
4	13	9	39	1	-28
7	13	9	24	25	-42
-22	14	9	93	87	13
-19	14	9	132	122	11
-16	14	9	117	115	16
-13	14	9	138	138	13
-10	14	9	67	53	-18
-7	14	9	47	56	-20

Table 53. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-4	14	9	66	53	16
-1	14	9	47	22	-19
2	14	9	54	50	-19
5	14	9	94	93	14
8	14	9	65	54	-20
-21	15	9	82	70	19
-18	15	9	98	98	13
-15	15	9	29	3	-28
-12	15	9	86	82	12
-9	15	9	198	203	7
-6	15	9	295	299	6
-3	15	9	134	135	11
0	15	9	32	1	-26
3	15	9	61	38	-19
6	15	9	74	57	-22
-20	16	9	54	9	-27
-17	16	9	43	5	-25
-14	16	9	125	107	9
-11	16	9	175	173	8
-8	16	9	290	288	8
-5	16	9	248	245	12
-2	16	9	46	50	-23
1	16	9	56	20	-26
4	16	9	25	15	-43
-19	17	9	32	25	-35
-16	17	9	33	6	-33
-13	17	9	23	14	-40
-10	17	9	60	15	-24
-7	17	9	23	18	-40
-4	17	9	31	0	-32
-1	17	9	55	19	-21
2	17	9	34	21	-32
-21	18	9	25	10	-43
-18	18	9	68	1	-24
-15	18	9	101	94	12
-12	18	9	144	152	17
-9	18	9	248	247	11
-6	18	9	204	206	7
-3	18	9	54	38	-23
0	18	9	25	2	-37
3	18	9	38	7	-30
-20	19	9	48	4	-29
-17	19	9	49	24	-28
-14	19	9	128	116	18
-11	19	9	206	192	9
-8	19	9	188	184	8
-5	19	9	91	93	16
-2	19	9	34	22	-34
1	19	9	32	5	-36
-19	20	9	40	1	-32
-16	20	9	38	9	-32
-13	20	9	65	19	-18
-10	20	9	34	14	-34
-7	20	9	34	27	-34
-4	20	9	24	15	-42
-1	20	9	25	7	-43
-18	21	9	32	12	-36
-15	21	9	50	69	-29
-12	21	9	124	124	14
-9	21	9	121	133	11
-6	21	9	76	57	-23
-3	21	9	42	8	-31
-14	22	9	90	87	14
-11	22	9	106	92	24
-8	22	9	52	54	-26
-1	1	10	70	80	10
-3	2	10	211	202	5
0	2	10	346	313	5
-5	3	10	246	214	6
-2	3	10	207	218	4
1	3	10	25	4	-24
-7	4	10	642	655	18
-4	4	10	760	715	17
-1	4	10	50	12	-16
2	4	10	67	60	14
-9	5	10	206	186	8
-6	5	10	499	456	13
-3	5	10	245	224	4
0	5	10	63	69	11
3	5	10	319	298	6
-11	6	10	149	138	7
-8	6	10	462	443	21
-5	6	10	503	448	9
-2	6	10	68	69	9
1	6	10	35	51	-21
4	6	10	253	250	4
-13	7	10	310	317	10
-10	7	10	605	593	3
-7	7	10	1024	1010	23
-4	7	10	648	663	14
-1	7	10	62	65	12
2	7	10	88	80	17

Table 53. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
5	7	10	159	162	6
-15	8	10	110	126	10
-12	8	10	342	349	5
-9	8	10	400	401	4
-6	8	10	458	459	11
-3	8	10	318	299	9
0	8	10	56	47	12
3	8	10	27	37	-28
6	8	10	22	40	-39
-17	9	10	23	4	-40
-14	9	10	57	60	-16
-11	9	10	138	132	7
-8	9	10	394	387	6
-5	9	10	205	183	7
-2	9	10	80	73	14
1	9	10	65	50	14
4	9	10	99	93	9
7	9	10	49	62	-22
-19	10	10	48	48	-28
-16	10	10	99	98	14
-13	10	10	362	354	11
-10	10	10	521	502	7
-7	10	10	607	593	17
-4	10	10	251	239	5
-1	10	10	53	53	-18
2	10	10	64	71	-18
5	10	10	64	68	-20
8	10	10	33	4	-24
-21	11	10	46	8	-29
-18	11	10	34	24	-22
-15	11	10	85	96	13
-12	11	10	222	227	5
-9	11	10	140	136	6
-6	11	10	139	139	7
-3	11	10	28	31	-27
0	11	10	195	187	5
3	11	10	101	96	9
6	11	10	35	36	-30
9	11	10	43	40	-29
-20	12	10	46	23	-28
-17	12	10	70	54	15
-14	12	10	140	154	8
-11	12	10	224	233	13
-8	12	10	329	356	7
-5	12	10	155	168	10
-2	12	10	66	74	12
1	12	10	93	105	10
4	12	10	65	39	16
7	12	10	24	36	-41
10	12	10	62	3	-26
-19	13	10	35	30	-33
-16	13	10	132	139	9
-13	13	10	322	328	5
-10	13	10	356	362	6
-7	13	10	314	319	7
-4	13	10	98	90	9
-1	13	10	95	98	10
2	13	10	78	73	13
5	13	10	58	37	-18
8	13	10	84	33	-23
-21	14	10	25	12	-43
-18	14	10	24	7	-42
-15	14	10	83	82	12
-12	14	10	144	152	8
-9	14	10	76	58	11
-6	14	10	28	38	-31
-3	14	10	93	97	16
0	14	10	208	214	7
3	14	10	154	142	7
6	14	10	91	81	13
-20	15	10	35	27	-33
-17	15	10	33	36	-33
-14	15	10	82	84	13
-11	15	10	87	107	16
-8	15	10	114	132	13
-5	15	10	70	67	14
-2	15	10	100	77	10
1	15	10	105	108	8
4	15	10	69	70	16
-19	16	10	55	31	-21
-16	16	10	63	63	-17
-13	16	10	121	143	10
-10	16	10	97	102	22
-7	16	10	80	66	15
-4	16	10	75	35	-24
-1	16	10	100	105	10
2	16	10	48	66	-24
5	16	10	26	44	-45
-18	17	10	24	11	-42
-15	17	10	54	37	-26
-12	17	10	36	52	-28
-9	17	10	44	3	-23

Table 53. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-6	17	10	43	33	-27
-3	17	10	150	143	6
0	17	10	193	179	9
3	17	10	119	114	13
-20	18	10	36	30	-34
-17	18	10	24	15	-42
-14	18	10	33	8	-34
-11	18	10	24	23	-29
-8	18	10	37	2	-23
-5	18	10	53	37	-26
-2	18	10	77	67	16
1	18	10	70	74	-18
-19	19	10	59	52	-22
-16	19	10	53	34	-27
-13	19	10	33	35	-33
-10	19	10	71	50	-20
-7	19	10	57	33	-22
-4	19	10	83	69	17
-1	19	10	79	73	16
-18	20	10	66	31	-26
-15	20	10	37	32	-33
-12	20	10	56	28	-25
-9	20	10	54	40	-22
-6	20	10	87	79	14
-3	20	10	115	113	12
-14	21	10	25	11	-43
-11	21	10	25	8	-43
-8	21	10	39	33	-30
-5	21	10	69	42	-19
-10	22	10	62	2	-26
0	1	11	38	6	-15
-2	2	11	19	10	-28
1	2	11	80	63	11
-4	3	11	249	243	5
-1	3	11	76	79	9
2	3	11	510	487	18
-6	4	11	211	219	8
-3	4	11	242	246	9
0	4	11	20	9	-29
3	4	11	131	122	6
-8	5	11	73	54	10
-5	5	11	23	3	-25
-2	5	11	510	485	10
1	5	11	838	823	10
4	5	11	414	420	4
-10	6	11	156	151	9
-7	6	11	236	227	7
-4	6	11	213	225	5
-1	6	11	839	835	17
2	6	11	663	659	10
5	6	11	270	279	5
-12	7	11	184	186	8
-9	7	11	166	164	8
-6	7	11	235	237	7
-3	7	11	131	121	7
0	7	11	44	7	-23
3	7	11	78	67	10
6	7	11	53	38	-17
-14	8	11	147	155	9
-11	8	11	53	55	-17
-8	8	11	25	2	-26
-5	8	11	57	58	13
-2	8	11	677	656	12
1	8	11	573	567	10
4	8	11	247	248	7
7	8	11	143	142	8
-16	9	11	63	18	-23
-13	9	11	53	56	-18
-10	9	11	31	14	-27
-7	9	11	156	162	6
-4	9	11	410	413	11
-1	9	11	573	571	11
2	9	11	440	449	4
5	9	11	213	224	6
8	9	11	23	9	-29
-18	10	11	58	46	-19
-15	10	11	23	23	-39
-12	10	11	81	77	13
-9	10	11	30	15	-28
-6	10	11	151	147	6
-3	10	11	71	68	-18
0	10	11	29	2	-27
3	10	11	73	77	-21
6	10	11	31	39	-35
9	10	11	47	4	-24
-20	11	11	46	27	-29
-17	11	11	53	41	-21
-14	11	11	34	30	-30
-11	11	11	49	0	-17
-8	11	11	54	55	-19
-5	11	11	271	270	6
-2	11	11	443	450	11

Table 53. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
1	11	11	317	312	5
4	11	11	154	163	12
7	11	11	53	9	-21
10	11	11	54	30	-25
-19	12	11	66	40	-21
-16	12	11	48	50	-22
-13	12	11	156	163	7
-10	12	11	90	75	18
-7	12	11	185	178	9
-4	12	11	253	245	6
-1	12	11	317	315	5
2	12	11	225	240	6
5	12	11	41	11	-28
8	12	11	38	35	-33
-21	13	11	47	45	-30
-18	13	11	130	114	12
-15	13	11	126	132	9
-12	13	11	157	168	11
-9	13	11	49	61	-18
-6	13	11	66	39	16
-3	13	11	88	83	12
0	13	11	23	1	-34
3	13	11	50	28	-18
6	13	11	53	9	-20
-20	14	11	61	25	-26
-17	14	11	50	58	-24
-14	14	11	47	4	-19
-11	14	11	49	37	-19
-8	14	11	152	155	13
-5	14	11	214	222	7
-2	14	11	232	240	6
1	14	11	154	163	10
4	14	11	24	9	-42
-19	15	11	90	84	14
-16	15	11	113	110	11
-13	15	11	124	126	9
-10	15	11	36	23	-26
-7	15	11	130	142	9
-4	15	11	167	157	10
-1	15	11	159	162	12
2	15	11	64	36	-24
5	15	11	50	26	-28
-18	16	11	134	136	10
-15	16	11	127	113	9
-12	16	11	74	52	16
-9	16	11	57	19	-18
-6	16	11	50	37	-25
-3	16	11	56	22	-16
0	16	11	55	2	-23
3	16	11	32	1	-35
-17	17	11	37	1	-26
-14	17	11	39	56	-31
-11	17	11	40	42	-27
-8	17	11	41	9	-22
-5	17	11	42	10	-28
-2	17	11	56	40	-21
1	17	11	34	3	-33
-16	18	11	148	139	10
-13	18	11	126	116	10
-10	18	11	65	47	-21
-7	18	11	31	11	-34
-4	18	11	60	7	-19
-1	18	11	25	4	-43
-15	19	11	94	88	13
-12	19	11	49	41	-28
-9	19	11	32	5	-34
-6	19	11	40	9	-29
-3	19	11	43	4	-27
-14	20	11	45	25	-27
-11	20	11	52	27	-27
-8	20	11	25	37	-43
-5	20	11	25	28	-44
-13	21	11	47	46	-30
-10	21	11	57	32	-27
0	0	12	1516	1473	27
1	1	12	596	618	13
-1	2	12	592	625	17
2	2	12	113	139	7
-3	3	12	845	804	13
0	3	12	797	753	8
3	3	12	291	281	9
-5	4	12	347	350	11
-2	4	12	111	140	8
1	4	12	303	310	6
4	4	12	77	98	10
-7	5	12	52	5	-17
-4	5	12	346	354	14
-1	5	12	303	307	13
2	5	12	43	22	-22
5	5	12	115	123	13
-9	6	12	70	57	14
-6	6	12	354	333	5

Table 53. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-3	6	12	295	271	10
0	6	12	297	277	7
3	6	12	93	90	9
6	6	12	167	181	10
-11	7	12	221	209	7
-8	7	12	118	131	9
-5	7	12	46	11	-19
-2	7	12	31	26	-25
1	7	12	92	95	9
4	7	12	240	236	6
7	7	12	273	270	6
-13	8	12	72	60	15
-10	8	12	50	56	-16
-7	8	12	120	132	7
-4	8	12	103	101	13
-1	8	12	88	103	12
2	8	12	134	164	7
5	8	12	91	107	11
8	8	12	114	121	7
-15	9	12	156	161	10
-12	9	12	130	147	10
-9	9	12	139	115	11
-6	9	12	60	45	14
-3	9	12	96	87	8
0	9	12	198	182	7
3	9	12	46	62	-21
6	9	12	100	104	11
9	9	12	100	79	12
-17	10	12	231	223	9
-14	10	12	190	186	9
-11	10	12	69	39	15
-8	10	12	44	52	-20
-5	10	12	115	120	14
-2	10	12	143	163	9
1	10	12	52	39	-19
4	10	12	152	141	7
7	10	12	192	182	13
10	10	12	184	167	9
-19	11	12	117	113	11
-16	11	12	72	69	15
-13	11	12	48	28	-23
-10	11	12	51	37	-19
-7	11	12	221	216	8
-4	11	12	238	230	13
-1	11	12	44	36	-23
2	11	12	23	12	-39
5	11	12	87	64	-26
8	11	12	83	103	15
-18	12	12	92	81	15
-15	12	12	101	110	9
-12	12	12	86	90	11
-9	12	12	136	148	9
-6	12	12	166	185	14
-3	12	12	54	67	-16
0	12	12	86	94	10
3	12	12	81	77	11
6	12	12	51	53	-22
-20	13	12	136	128	11
-17	13	12	131	122	9
-14	13	12	68	55	-18
-11	13	12	55	35	-24
-8	13	12	60	57	-16
-5	13	12	107	101	9
-2	13	12	60	12	-17
1	13	12	67	57	15
4	13	12	125	101	11
7	13	12	129	130	11
-19	14	12	66	47	-19
-16	14	12	32	8	-34
-13	14	12	58	50	-17
-10	14	12	192	184	8
-7	14	12	267	271	6
-4	14	12	150	138	9
-1	14	12	81	59	13
2	14	12	79	26	13
5	14	12	86	74	15
-18	15	12	56	41	-20
-15	15	12	45	38	-21
-12	15	12	107	108	8
-9	15	12	146	158	9
-6	15	12	101	110	10
-3	15	12	73	81	14
0	15	12	32	27	-29
3	15	12	42	2	-27
-17	16	12	50	22	-25
-14	16	12	24	6	-42
-11	16	12	81	67	17
-8	16	12	127	121	9
-5	16	12	65	63	-22
-2	16	12	55	28	-21
1	16	12	57	14	-25
-16	17	12	24	24	-42

Table 53. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-13	17	12	137	120	12
-10	17	12	230	221	9
-7	17	12	182	185	8
-4	17	12	119	104	18
-1	17	12	24	18	-42
-15	18	12	50	41	-24
-12	18	12	94	79	14
-9	18	12	83	78	18
-6	18	12	58	57	-22
-3	18	12	67	4	-19
-14	19	12	46	47	-31
-11	19	12	113	112	14
-8	19	12	97	105	23
-5	19	12	76	74	-20
-13	20	12	126	127	11
-10	20	12	164	167	9
-7	20	12	128	132	12
-1	1	13	33	2	-20
-3	2	13	136	147	9
0	2	13	36	1	-18
-5	3	13	389	388	14
-2	3	13	139	138	9
1	3	13	107	105	11
-7	4	13	62	54	14
-4	4	13	21	2	-31
-1	4	13	103	100	10
2	4	13	166	171	6
-9	5	13	258	255	6
-6	5	13	529	510	11
-3	5	13	389	379	9
0	5	13	24	0	-27
3	5	13	159	153	6
-11	6	13	220	214	6
-8	6	13	534	515	7
-5	6	13	524	511	15
-2	6	13	163	170	7
1	6	13	123	116	7
4	6	13	42	12	-25
-13	7	13	31	3	-32
-10	7	13	75	67	13
-7	7	13	49	2	-19
-4	7	13	68	47	17
-1	7	13	114	115	9
2	7	13	127	134	9
5	7	13	132	120	11
-15	8	13	115	111	10
-12	8	13	241	233	6
-9	8	13	507	502	5
-6	8	13	529	509	21
-3	8	13	168	153	19
0	8	13	21	7	-32
3	8	13	109	115	12
6	8	13	94	109	14
-17	9	13	35	34	-33
-14	9	13	138	158	9
-11	9	13	417	421	5
-8	9	13	501	497	6
-5	9	13	252	261	9
-2	9	13	136	132	8
1	9	13	55	33	-18
4	9	13	110	95	11
7	9	13	45	7	-28
-19	10	13	52	12	-24
-16	10	13	52	7	-27
-13	10	13	57	48	-25
-10	10	13	62	4	-22
-7	10	13	69	67	17
-4	10	13	43	15	-21
-1	10	13	46	35	-20
2	10	13	62	45	-18
5	10	13	51	10	-24
8	10	13	31	13	-36
-18	11	13	25	14	-43
-15	11	13	107	100	10
-12	11	13	324	321	5
-9	11	13	415	424	7
-6	11	13	215	221	11
-3	11	13	119	121	11
0	11	13	60	5	-16
3	11	13	45	67	-18
6	11	13	45	6	-29
-17	12	13	25	37	-43
-14	12	13	192	201	10
-11	12	13	325	316	9
-8	12	13	242	239	6
-5	12	13	126	127	12
-2	12	13	23	45	-40
1	12	13	139	146	7
4	12	13	82	86	14
7	12	13	55	43	-24
-16	13	13	36	43	-31
-13	13	13	52	0	-22

Table 53. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-10	13	13	58	49	-17
-7	13	13	35	3	-30
-4	13	13	96	94	11
-1	13	13	133	148	8
2	13	13	103	102	11
5	13	13	107	97	15
-18	14	13	60	21	-21
-15	14	13	92	74	-27
-12	14	13	191	197	9
-9	14	13	145	161	8
-6	14	13	94	114	15
-3	14	13	69	68	13
0	14	13	32	0	-29
3	14	13	40	27	-31
-17	15	13	61	22	-26
-14	15	13	85	72	19
-11	15	13	111	97	14
-8	15	13	106	112	13
-5	15	13	42	8	-26
-2	15	13	86	104	17
1	15	13	81	86	-27
-16	16	13	25	1	-37
-13	16	13	51	42	-23
-10	16	13	54	4	-26
-7	16	13	24	10	-42
-4	16	13	79	87	15
-1	16	13	81	87	14
-15	17	13	25	22	-44
-12	17	13	39	36	-29
-9	17	13	25	35	-43
-6	17	13	30	3	-36
-3	17	13	34	26	-35
-14	18	13	25	22	-43
-11	18	13	35	10	-34
-8	18	13	25	15	-43
-5	18	13	95	95	13
-10	19	13	33	15	-37
-7	19	13	61	45	-21
0	1	14	75	59	9
-2	2	14	96	93	11
1	2	14	54	51	-21
-4	3	14	133	124	7
-1	3	14	56	51	13
2	3	14	205	210	8
-6	4	14	62	56	14
-3	4	14	127	127	7
0	4	14	329	332	5
3	4	14	424	404	15
-8	5	14	150	156	9
-5	5	14	77	89	12
-2	5	14	205	219	5
1	5	14	192	201	6
4	5	14	181	176	7
-10	6	14	248	243	6
-7	6	14	77	78	16
-4	6	14	47	55	-17
-1	6	14	191	194	6
2	6	14	289	294	6
5	6	14	186	173	7
-12	7	14	72	61	14
-9	7	14	43	51	-26
-6	7	14	68	68	13
-3	7	14	413	402	7
0	7	14	529	519	15
3	7	14	459	448	6
6	7	14	189	192	6
-14	8	14	24	23	-41
-11	8	14	42	54	-24
-8	8	14	58	20	-20
-5	8	14	149	154	7
-2	8	14	298	296	6
1	8	14	216	224	6
4	8	14	166	169	13
7	8	14	76	54	-20
-16	9	14	24	15	-42
-13	9	14	33	6	-33
-10	9	14	59	8	-23
-7	9	14	57	49	-18
-4	9	14	183	180	14
-1	9	14	214	223	11
2	9	14	190	193	7
5	9	14	82	68	19
8	9	14	67	27	-26
-18	10	14	25	1	-43
-15	10	14	53	24	-26
-12	10	14	75	47	14
-9	10	14	23	3	-40
-6	10	14	252	240	12
-3	10	14	455	448	12
0	10	14	366	372	8
3	10	14	247	251	8
6	10	14	25	47	-43

Table 53. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-17	11	14	25	32	-43
-14	11	14	43	28	-26
-11	11	14	55	16	-22
-8	11	14	48	57	-21
-5	11	14	170	169	8
-2	11	14	190	192	12
1	11	14	120	129	10
4	11	14	37	54	-30
7	11	14	34	2	-34
-16	12	14	45	53	-30
-13	12	14	78	61	19
-10	12	14	66	43	13
-7	12	14	61	63	-16
-4	12	14	164	171	17
-1	12	14	120	129	12
2	12	14	111	114	11
5	12	14	35	24	-34
-15	13	14	64	31	-17
-12	13	14	75	57	-19
-9	13	14	43	1	-24
-6	13	14	190	189	5
-3	13	14	248	249	12
0	13	14	187	197	7
3	13	14	76	88	-20
-17	14	14	118	117	14
-14	14	14	138	141	8
-11	14	14	24	28	-42
-8	14	14	45	23	-25
-5	14	14	73	65	15
-2	14	14	110	111	12
1	14	14	25	43	-43
-16	15	14	91	88	14
-13	15	14	48	33	-23
-10	15	14	31	21	-35
-7	15	14	56	52	-21
-4	15	14	70	54	-20
-1	15	14	55	46	-20
-15	16	14	95	89	23
-12	16	14	64	53	-18
-9	16	14	25	16	-43
-6	16	14	63	43	-26
-3	16	14	89	87	16
-14	17	14	125	120	11
-11	17	14	62	38	-24
-8	17	14	45	29	-29
-5	17	14	25	21	-43
-10	18	14	25	4	-44
-7	18	14	25	2	-43
0	0	15	34	11	-35
1	1	15	527	529	11
-1	2	15	529	533	14
2	2	15	436	434	18
-3	3	15	55	1	-20
0	3	15	35	0	-26
3	3	15	105	98	12
-5	4	15	428	420	17
-2	4	15	430	444	7
1	4	15	374	365	8
4	4	15	130	135	9
-7	5	15	170	164	7
-4	5	15	434	421	15
-1	5	15	364	366	13
2	5	15	119	116	16
5	5	15	37	7	-30
-9	6	15	45	27	-25
-6	6	15	60	2	-17
-3	6	15	108	90	13
0	6	15	31	1	-29
3	6	15	77	59	-20
6	6	15	58	64	-20
-11	7	15	76	70	9
-8	7	15	38	9	-28
-5	7	15	172	168	10
-2	7	15	120	123	10
1	7	15	53	45	-19
4	7	15	66	26	12
7	7	15	25	3	-42
-13	8	15	150	146	9
-10	8	15	75	71	-20
-7	8	15	23	8	-39
-4	8	15	129	132	8
-1	8	15	23	44	-41
2	8	15	55	46	-20
5	8	15	92	83	13
8	8	15	180	190	9
-15	9	15	178	187	8
-12	9	15	54	52	-21
-9	9	15	60	0	-18
-6	9	15	42	28	-26
-3	9	15	66	57	-17
0	9	15	42	1	-25
3	9	15	96	88	23

Table 53. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
6	9	15	151	150	9
-14	10	15	33	7	-35
-11	10	15	49	57	-23
-8	10	15	77	74	17
-5	10	15	23	11	-40
-2	10	15	65	48	-21
1	10	15	33	16	-33
4	10	15	66	38	-22
-16	11	15	162	169	12
-13	11	15	74	70	-18
-10	11	15	64	59	-16
-7	11	15	78	76	10
-4	11	15	58	18	-19
-1	11	15	59	18	-25
2	11	15	42	57	-28
5	11	15	113	108	12
-15	12	15	105	109	15
-12	12	15	50	3	-23
-9	12	15	58	48	-24
-6	12	15	66	60	-18
-3	12	15	83	86	14
0	12	15	45	0	-24
3	12	15	80	96	16
-14	13	15	37	17	-33
-11	13	15	71	66	-20
-8	13	15	141	145	12
-5	13	15	79	86	17
-2	13	15	56	58	-19
1	13	15	45	4	-28
-13	14	15	33	15	-35
-10	14	15	58	8	-27
-7	14	15	53	6	-25
-4	14	15	25	35	-43
-1	14	15	25	3	-43
-12	15	15	114	108	13
-9	15	15	186	185	8
-6	15	15	148	150	12
-3	15	15	76	97	19
-11	16	15	171	169	8
-8	16	15	185	191	18
-5	16	15	111	111	11
-1	1	16	91	116	10
-3	2	16	60	30	-16
0	2	16	240	221	6
-5	3	16	111	107	9
-2	3	16	23	32	-40
1	3	16	161	165	7
-7	4	16	256	253	21
-4	4	16	159	185	10
-1	4	16	164	175	10
2	4	16	131	122	8
-9	5	16	214	214	9
-6	5	16	135	138	13
-3	5	16	114	114	9
0	5	16	108	108	8
3	5	16	24	5	-41
-11	6	16	131	125	10
-8	6	16	136	130	8
-5	6	16	133	129	9
-2	6	16	131	122	8
1	6	16	98	99	13
4	6	16	201	204	9
-13	7	16	114	113	12
-10	7	16	364	359	12
-7	7	16	328	328	13
-4	7	16	265	256	7
-1	7	16	104	96	12
2	7	16	154	147	13
5	7	16	46	55	-25
-15	8	16	54	36	-25
-12	8	16	83	82	14
-9	8	16	208	201	9
-6	8	16	141	134	6
-3	8	16	33	3	-33
0	8	16	41	20	-25
3	8	16	24	7	-42
6	8	16	49	5	-25
-14	9	16	74	63	19
-11	9	16	224	221	11
-8	9	16	206	201	8
-5	9	16	214	217	11
-2	9	16	146	147	18
1	9	16	24	42	-42
4	9	16	25	3	-43
-13	10	16	213	210	8
-10	10	16	418	414	13
-7	10	16	361	364	5
-4	10	16	206	206	9
-1	10	16	58	43	-23
2	10	16	57	16	-26
5	10	16	34	22	-35
-12	11	16	125	129	17

Table 53. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-9	11	16	222	222	9
-6	11	16	120	123	15
-3	11	16	24	7	-42
0	11	16	30	5	-32
3	11	16	69	61	-21
-14	12	16	37	34	-33
-11	12	16	106	128	13
-8	12	16	94	85	17
-5	12	16	34	59	-34
-2	12	16	24	18	-42
1	12	16	33	27	-35
-13	13	16	126	126	12
-10	13	16	207	210	9
-7	13	16	111	115	11
-4	13	16	25	2	-43
-1	13	16	31	23	-36
-12	14	16	37	33	-30
-9	14	16	64	61	-20
-6	14	16	61	6	-21
-3	14	16	25	59	-44
-8	15	16	32	38	-37
-5	15	16	51	24	-29
0	1	17	28	1	-30
-2	2	17	24	2	-35
1	2	17	192	192	7
-4	3	17	147	152	7
-1	3	17	180	192	9
2	3	17	130	147	7
-6	4	17	156	164	7
-3	4	17	147	150	5
0	4	17	47	2	-15
3	4	17	55	48	-27
-8	5	17	231	223	12
-5	5	17	52	0	-23
-2	5	17	133	142	6
1	5	17	152	168	17
4	5	17	219	219	12
-10	6	17	35	29	-35
-7	6	17	44	17	-25
-4	6	17	153	161	8
-1	6	17	165	167	8
2	6	17	266	261	13
5	6	17	153	159	10
-12	7	17	77	75	19
-9	7	17	89	87	13
-6	7	17	53	19	-26
-3	7	17	46	44	-25
0	7	17	49	2	-25
3	7	17	73	43	16
6	7	17	58	46	-20
-11	8	17	52	53	-23
-8	8	17	24	3	-37
-5	8	17	230	220	9
-2	8	17	255	255	8
1	8	17	326	327	10
4	8	17	212	219	7
-13	9	17	38	19	-30
-10	9	17	46	30	-26
-7	9	17	85	88	17
-4	9	17	215	218	8
-1	9	17	331	326	6
2	9	17	237	248	9
-12	10	17	47	16	-28
-9	10	17	55	26	-24
-6	10	17	47	28	-29
-3	10	17	72	46	-20
0	10	17	52	2	-21
-11	11	17	42	2	-28

APPENDIX F

TABLE 54

Table 54. Cis-p-Menthane Thiourea Host/Guest Adduct (supercell)

F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-1	2	0	2466	3183	84
0	3	0	11990	12490	623
-2	4	0	4513	3806	91
-4	5	0	4311	4228	99
-1	5	0	4334	4172	103
-3	6	0	409	541	24
0	6	0	2324	2571	30
-5	7	0	1219	1144	21
-2	7	0	1222	1292	21
-7	8	0	1614	1608	12
-4	8	0	1595	1434	13
-1	8	0	1624	1535	24
-6	9	0	431	447	24
-3	9	0	449	515	24
0	9	0	2279	2072	20
-8	10	0	717	894	27
-5	10	0	878	1012	19
-2	10	0	728	840	30
-10	11	0	580	351	22
-7	11	0	2331	2009	31
-4	11	0	2328	2051	23
-1	11	0	582	320	28
-9	12	0	332	655	34
-6	12	0	1149	1410	23
-3	12	0	337	615	30
0	12	0	280	546	33
-11	13	0	577	347	30
-8	13	0	314	511	36
-5	13	0	310	530	37
-2	13	0	552	359	26
-13	14	0	608	474	29
-10	14	0	1459	1217	15
-7	14	0	2321	2025	33
-4	14	0	1451	1196	13
-1	14	0	615	448	26
-12	15	0	558	684	39
-9	15	0	746	944	20
-6	15	0	751	912	18
-3	15	0	560	670	24
0	15	0	281	259	39
-14	16	0	166	103	-84
-11	16	0	327	388	36
-8	16	0	639	767	41
-5	16	0	307	411	55
-2	16	0	291	102	-89
-16	17	0	235	155	-98
-13	17	0	764	783	52
-10	17	0	1364	1371	47
-7	17	0	1359	1346	33
-4	17	0	748	746	29
-1	17	0	112	134	-107
-15	18	0	273	142	66
-12	18	0	499	456	30
-9	18	0	574	562	27
-6	18	0	498	452	38
-3	18	0	238	130	58
0	18	0	172	23	-89
-17	19	0	247	173	-82
-14	19	0	491	437	55
-11	19	0	728	703	39
-8	19	0	736	721	29
-5	19	0	452	441	43
-2	19	0	231	143	-73
-19	20	0	197	66	-93
-16	20	0	273	377	61
-13	20	0	755	880	113
-10	20	0	1075	1141	78
-7	20	0	776	850	66
-4	20	0	320	327	68
-1	20	0	193	7	-113
-18	21	0	90	72	-180
-15	21	0	270	269	76
-12	21	0	507	459	40
-9	21	0	468	443	61
-6	21	0	307	244	59
-3	21	0	226	41	-97
0	21	0	158	21	-114
-20	22	0	90	14	-181
-17	22	0	89	12	-179
-14	22	0	159	113	-121
-11	22	0	265	230	65
-8	22	0	221	131	-89
-5	22	0	186	5	-113
-2	22	0	212	26	-111
-19	23	0	185	20	-119
-16	23	0	269	94	-105
-13	23	0	350	285	-106
-10	23	0	296	274	80
-7	23	0	167	70	-123
-4	23	0	173	66	-108

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-18	24	0	92	20	-184
-15	24	0	176	30	-107
-12	24	0	140	8	-133
-9	24	0	90	4	-180
-6	24	0	177	41	-122
-14	25	0	230	101	-110
-11	25	0	184	113	-108
-1	1	1	52	884	-29
-3	2	1	76	159	-84
0	2	1	139	895	-45
-5	3	1	66	410	-132
-2	3	1	112	652	-69
1	3	1	68	322	-137
-7	4	1	170	469	-76
-4	4	1	94	639	-92
-1	4	1	68	454	-136
2	4	1	67	14	-134
-9	5	1	257	356	59
-6	5	1	67	210	-135
-3	5	1	67	202	-134
0	5	1	81	519	-99
3	5	1	73	350	-147
-11	6	1	140	243	-114
-8	6	1	136	325	-90
-5	6	1	68	159	-135
-2	6	1	67	132	-134
1	6	1	78	344	-190
4	6	1	74	222	-148
-13	7	1	229	228	-105
-10	7	1	119	337	-104
-7	7	1	72	266	-126
-4	7	1	225	165	50
-1	7	1	206	268	-69
2	7	1	154	91	-83
5	7	1	160	266	-112
-15	8	1	94	241	-188
-12	8	1	183	477	-86
-9	8	1	125	94	-112
-6	8	1	177	449	-95
-3	8	1	74	252	-147
0	8	1	73	331	-126
3	8	1	184	230	-84
6	8	1	197	332	-100
-17	9	1	337	253	-126
-14	9	1	234	335	-85
-11	9	1	250	113	-82
-8	9	1	78	9	-156
-5	9	1	203	119	-66
-2	9	1	112	308	-101
1	9	1	78	452	-156
4	9	1	194	285	-72
7	9	1	95	223	-190
-19	10	1	195	248	-148
-16	10	1	95	184	-189
-13	10	1	89	68	-309
-10	10	1	113	149	-113
-7	10	1	77	410	-154
-4	10	1	189	383	-92
-1	10	1	138	217	-98
2	10	1	130	198	-133
5	10	1	154	113	-133
8	10	1	145	9	-158
-18	11	1	177	10	-142
-15	11	1	141	313	-140
-12	11	1	246	181	-76
-9	11	1	253	284	73
-6	11	1	131	648	-113
-3	11	1	209	200	-73
0	11	1	192	102	-88
3	11	1	143	148	-137
6	11	1	233	182	-116
-17	12	1	272	188	-92
-14	12	1	254	29	-83
-11	12	1	273	146	68
-8	12	1	161	287	-113
-5	12	1	84	1	-168
-2	12	1	85	51	-171
1	12	1	251	40	67
4	12	1	95	108	-191
7	12	1	237	176	-131
-19	13	1	107	252	-215
-16	13	1	98	40	-197
-13	13	1	200	38	-81
-10	13	1	181	115	-124
-7	13	1	86	397	-173
-4	13	1	211	258	-62
-1	13	1	147	460	-119
2	13	1	97	176	-193
5	13	1	106	36	-213
-18	14	1	236	95	-114
-15	14	1	98	52	-195
-12	14	1	262	40	-108

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-9	14	1	166	200	-113
-6	14	1	93	51	-187
-3	14	1	192	261	-115
0	14	1	172	262	-110
3	14	1	138	238	-169
-17	15	1	104	177	-208
-14	15	1	165	129	-143
-11	15	1	170	33	-117
-8	15	1	183	320	-110
-5	15	1	115	172	-159
-2	15	1	168	52	-118
1	15	1	208	172	-122
-16	16	1	185	74	-113
-13	16	1	207	209	-127
-10	16	1	160	510	-136
-7	16	1	125	272	-154
-4	16	1	236	104	-87
-1	16	1	101	16	-202
-15	17	1	258	27	-106
-12	17	1	255	298	-100
-9	17	1	211	122	-113
-6	17	1	103	18	-206
-3	17	1	185	42	-137
-14	18	1	104	2	-209
-11	18	1	101	116	-202
-8	18	1	184	47	-138
-5	18	1	104	111	-209
-13	19	1	234	223	-136
-10	19	1	108	116	-216
-7	19	1	108	37	-217
0	1	2	77	1016	-29
-2	2	2	61	97	-77
1	2	2	112	513	-69
-4	3	2	259	479	50
-1	3	2	75	71	-87
2	3	2	65	326	-129
-6	4	2	95	149	-102
-3	4	2	397	979	-145
0	4	2	183	232	-75
3	4	2	70	18	-172
-8	5	2	157	629	-99
-5	5	2	106	19	-94
-2	5	2	109	56	-82
1	5	2	88	478	-103
4	5	2	73	111	-146
-10	6	2	76	547	-151
-7	6	2	73	664	-145
-4	6	2	134	948	-76
-1	6	2	65	391	-130
2	6	2	75	43	-150
5	6	2	82	61	-165
-12	7	2	89	714	-179
-9	7	2	77	496	-154
-6	7	2	75	1346	-183
-3	7	2	226	552	-82
0	7	2	72	425	-125
3	7	2	78	352	-157
6	7	2	87	597	-175
-14	8	2	99	147	-198
-11	8	2	92	45	-183
-8	8	2	84	124	-145
-5	8	2	131	443	-105
-2	8	2	75	954	-149
1	8	2	76	480	-152
4	8	2	86	306	-172
7	8	2	96	335	-192
-16	9	2	95	404	-190
-13	9	2	88	870	-153
-10	9	2	140	471	-118
-7	9	2	76	653	-153
-4	9	2	73	145	-147
-1	9	2	99	190	-121
2	9	2	169	164	-87
5	9	2	116	112	-159
8	9	2	220	172	-129
-18	10	2	171	313	-127
-15	10	2	96	329	-192
-12	10	2	141	415	-130
-9	10	2	85	466	-171
-6	10	2	91	281	-131
-3	10	2	78	198	-157
0	10	2	156	285	-85
3	10	2	88	133	-216
6	10	2	204	87	-118
9	10	2	238	113	-138
-17	11	2	235	109	-119
-14	11	2	120	433	-164
-11	11	2	184	213	-111
-8	11	2	92	379	-185
-5	11	2	82	340	-165
-2	11	2	165	324	-103
1	11	2	179	236	-95

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
4	11	2	215	115	-111	-13	18	2	275	217	-125
7	11	2	142	382	-161	-10	18	2	177	558	-131
-19	12	2	196	219	-130	-7	18	2	189	499	-138
-16	12	2	96	627	-192	-4	18	2	105	361	-211
-13	12	2	94	783	-187	-12	19	2	107	481	-215
-10	12	2	91	639	-182	-9	19	2	243	561	-131
-7	12	2	90	178	-180	-6	19	2	200	494	-132
-4	12	2	85	286	-170	1	1	3	76	619	-74
-1	12	2	145	2	-96	-1	2	3	49	292	-99
2	12	2	95	60	-190	2	2	3	304	350	-92
5	12	2	218	343	-111	-3	3	3	93	48	-76
-18	13	2	196	166	-138	0	3	3	118	553	-60
-15	13	2	139	251	-150	3	3	3	67	100	-135
-12	13	2	274	456	-96	-5	4	3	64	706	-128
-9	13	2	173	47	-89	-2	4	3	221	131	-87
-6	13	2	123	7	-139	1	4	3	67	245	-135
-3	13	2	150	54	-183	4	4	3	73	158	-146
0	13	2	116	310	-142	-7	5	3	89	212	-118
3	13	2	183	92	-136	-4	5	3	64	54	-129
6	13	2	162	1	-171	-1	5	3	169	50	-78
-17	14	2	265	288	-120	2	5	3	72	521	-144
-14	14	2	296	308	84	5	5	3	213	166	60
-11	14	2	122	306	-167	-9	6	3	346	152	39
-8	14	2	99	164	-197	-6	6	3	249	323	65
-5	14	2	93	60	-187	-3	6	3	118	50	-92
-2	14	2	93	258	-186	0	6	3	265	334	72
1	14	2	136	207	-156	3	6	3	173	55	-82
4	14	2	222	387	-134	6	6	3	198	275	-99
-16	15	2	183	391	-122	-11	7	3	81	122	-162
-13	15	2	271	472	-103	-8	7	3	146	232	-94
-10	15	2	96	79	-192	-5	7	3	198	131	54
-7	15	2	95	161	-191	-2	7	3	130	410	-97
-4	15	2	172	99	-121	1	7	3	199	583	-69
-1	15	2	97	40	-195	4	7	3	208	111	-99
2	15	2	237	518	-108	7	7	3	92	23	-185
-15	16	2	154	192	-154	-13	8	3	123	101	-132
-12	16	2	96	81	-192	-10	8	3	79	59	-159
-9	16	2	268	160	-92	-7	8	3	97	390	-120
-6	16	2	160	90	-136	-4	8	3	158	299	-76
-3	16	2	200	216	-131	-1	8	3	132	64	-85
0	16	2	222	93	-121	2	8	3	209	239	-91
-14	17	2	163	83	-152	5	8	3	147	152	-123
-11	17	2	287	62	-124	8	8	3	235	163	-114
-8	17	2	270	152	-102	-15	9	3	228	58	-90
-5	17	2	164	30	-148	-12	9	3	174	113	-103
-2	17	2	102	22	-205	-9	9	3	350	71	59

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-6	9	3	314	107	57
-3	9	3	156	319	-85
0	9	3	199	520	-68
3	9	3	85	150	-170
6	9	3	148	226	-134
9	9	3	177	26	-139
-17	10	3	240	297	-97
-14	10	3	92	246	-184
-11	10	3	86	133	-172
-8	10	3	80	256	-161
-5	10	3	170	350	-80
-2	10	3	150	261	-99
1	10	3	206	259	-80
4	10	3	90	119	-181
7	10	3	99	139	-199
-19	11	3	226	249	-117
-16	11	3	136	440	-149
-13	11	3	226	280	-95
-10	11	3	105	439	-151
-7	11	3	99	621	-140
-4	11	3	81	86	-162
-1	11	3	82	161	-165
2	11	3	89	230	-178
5	11	3	205	153	-91
8	11	3	184	33	-148
-18	12	3	101	80	-203
-15	12	3	95	133	-190
-12	12	3	125	148	-134
-9	12	3	182	4	-113
-6	12	3	134	239	-127
-3	12	3	85	513	-170
0	12	3	142	487	-114
3	12	3	95	99	-190
6	12	3	154	16	-159
-17	13	3	102	132	-204
-14	13	3	262	15	-115
-11	13	3	203	137	-96
-8	13	3	194	418	-96
-5	13	3	118	327	-136
-2	13	3	185	212	-95
1	13	3	239	371	-86
4	13	3	102	220	-204
-16	14	3	261	161	-119
-13	14	3	170	163	-131
-10	14	3	146	347	-134
-7	14	3	92	191	-185
-4	14	3	226	95	-108
-1	14	3	176	40	-126
2	14	3	225	174	-111
-18	15	3	219	19	-120
-15	15	3	204	134	-103
-12	15	3	97	39	-195
-9	15	3	94	234	-189
-6	15	3	176	321	-94
-3	15	3	127	359	-151
0	15	3	142	389	-142
3	15	3	180	129	-144
-17	16	3	210	11	-117
-14	16	3	245	5	-91
-11	16	3	234	160	-114
-8	16	3	94	223	-188
-5	16	3	268	181	-105
-2	16	3	99	217	-199
1	16	3	273	255	-102
-16	17	3	175	65	-151
-13	17	3	250	16	-112
-10	17	3	258	24	-106
-7	17	3	101	127	-203
-4	17	3	102	128	-205
-1	17	3	217	69	-134
-15	18	3	106	79	-212
-12	18	3	102	219	-205
-9	18	3	220	261	-105
-6	18	3	157	223	-157
-3	18	3	279	274	-89
-11	19	3	229	80	-138
-8	19	3	185	65	-133
-1	1	4	136	162	12
-3	2	4	849	1012	16
0	2	4	166	110	14
-5	3	4	6589	6128	38
-2	3	4	833	842	16
1	3	4	5392	4874	35
-7	4	4	619	469	30
-4	4	4	151	55	-47
-1	4	4	5392	4953	83
2	4	4	351	229	14
-9	5	4	2101	2160	18
-6	5	4	7753	7137	81
-3	5	4	6572	6211	33
0	5	4	158	129	42
3	5	4	398	463	19

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-11	6	4	1433	1441	15
-8	6	4	5924	5640	159
-5	6	4	7805	7108	71
-2	6	4	355	230	20
1	6	4	2408	2396	21
4	6	4	1336	1227	15
-13	7	4	205	181	40
-10	7	4	726	693	13
-7	7	4	81	43	-67
-4	7	4	618	594	32
-1	7	4	2438	2135	21
2	7	4	1188	1177	10
5	7	4	1013	1006	23
-15	8	4	1004	976	23
-12	8	4	1392	1478	24
-9	8	4	4297	4241	37
-6	8	4	5915	5677	128
-3	8	4	397	505	25
0	8	4	130	96	-43
3	8	4	445	492	21
6	8	4	855	960	47
-17	9	4	222	34	53
-14	9	4	1189	1267	28
-11	9	4	3220	3282	21
-8	9	4	4321	4284	10
-5	9	4	2094	2030	28
-2	9	4	1190	1284	14
1	9	4	123	151	-67
4	9	4	774	703	19
7	9	4	165	64	-87
-19	10	4	224	56	-69
-16	10	4	189	189	-62
-13	10	4	653	636	26
-10	10	4	127	14	-60
-7	10	4	735	696	18
-4	10	4	1330	1228	4
-1	10	4	197	111	-75
2	10	4	437	398	28
5	10	4	227	134	51
8	10	4	259	228	70
-21	11	4	244	99	-88
-18	11	4	108	4	-112
-15	11	4	927	905	34
-12	11	4	2214	2236	54
-9	11	4	3241	3269	42
-6	11	4	1435	1477	14
-3	11	4	461	534	18
0	11	4	113	2	-79
3	11	4	479	544	24
6	11	4	234	174	48
9	11	4	112	78	-138
-23	12	4	177	113	-103
-20	12	4	149	116	-122
-17	12	4	249	131	-88
-14	12	4	1508	1559	41
-11	12	4	2239	2237	50
-8	12	4	1383	1446	60
-5	12	4	1019	981	35
-2	12	4	442	435	21
1	12	4	1282	1286	17
4	12	4	603	566	24
7	12	4	306	307	52
10	12	4	156	10	-84
-25	13	4	247	198	-90
-22	13	4	170	86	-92
-19	13	4	215	21	-75
-16	13	4	83	83	-119
-13	13	4	157	17	-65
-10	13	4	658	602	26
-7	13	4	204	197	43
-4	13	4	793	689	24
-1	13	4	1270	1267	14
2	13	4	771	745	26
5	13	4	761	779	23
8	13	4	268	242	-83
11	13	4	134	51	-137
-24	14	4	121	19	-148
-21	14	4	166	161	-98
-18	14	4	219	99	-71
-15	14	4	768	797	49
-12	14	4	1496	1575	44
-9	14	4	1202	1249	44
-6	14	4	865	978	41
-3	14	4	483	547	22
0	14	4	156	24	-69
3	14	4	224	265	57
6	14	4	86	130	-173
9	14	4	158	22	-120
-23	15	4	305	282	77
-20	15	4	196	217	-109
-17	15	4	196	162	-97
-14	15	4	780	783	55

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-11	15	4	922	909	39
-8	15	4	1026	955	26
-5	15	4	204	95	45
-2	15	4	772	786	23
1	15	4	617	633	26
4	15	4	537	577	48
7	15	4	199	165	-113
10	15	4	142	131	-139
-25	16	4	223	272	-124
-22	16	4	224	182	-91
-19	16	4	135	5	-120
-16	16	4	168	13	-75
-13	16	4	84	76	-120
-10	16	4	153	178	-66
-7	16	4	160	31	-77
-4	16	4	618	559	37
-1	16	4	626	615	25
2	16	4	771	759	44
5	16	4	428	400	36
8	16	4	117	8	-150
-24	17	4	91	17	-183
-21	17	4	138	99	-127
-18	17	4	144	52	-105
-15	17	4	216	167	56
-12	17	4	210	123	-66
-9	17	4	171	22	-67
-6	17	4	217	162	50
-3	17	4	218	294	61
0	17	4	171	11	-75
3	17	4	88	48	-177
6	17	4	163	24	-124
-23	18	4	217	219	-86
-20	18	4	172	126	-71
-17	18	4	167	76	-95
-14	18	4	203	111	-61
-11	18	4	108	3	-100
-8	18	4	205	243	58
-5	18	4	767	797	31
-2	18	4	761	779	38
1	18	4	653	704	34
4	18	4	418	355	69
-22	19	4	171	119	-123
-19	19	4	146	1	-76
-16	19	4	136	3	-122
-13	19	4	91	43	-129
-10	19	4	90	89	-128
-7	19	4	318	328	40
-4	19	4	543	558	36
-1	19	4	675	693	37
2	19	4	476	420	60
5	19	4	189	88	-122
-21	20	4	217	52	-110
-18	20	4	232	141	-70
-15	20	4	192	235	-93
-12	20	4	85	133	-171
-9	20	4	119	78	-134
-6	20	4	115	125	-137
-3	20	4	216	29	-105
0	20	4	91	14	-158
3	20	4	92	33	-184
-20	21	4	90	75	-180
-17	21	4	255	141	-102
-14	21	4	110	195	-143
-11	21	4	216	124	-103
-8	21	4	265	244	-78
-5	21	4	421	393	52
-2	21	4	419	438	74
1	21	4	310	265	66
-22	22	4	111	19	-140
-19	22	4	91	91	-182
-16	22	4	184	140	-104
-13	22	4	144	55	-84
-10	22	4	186	30	-71
-7	22	4	260	167	-93
-4	22	4	371	346	59
-1	22	4	292	253	73
-18	23	4	226	219	-77
-15	23	4	302	276	75
-12	23	4	137	114	-124
-9	23	4	134	7	-134
-6	23	4	91	27	-181
-3	23	4	178	3	-121
-17	24	4	140	46	-128
-14	24	4	153	41	-128
-11	24	4	215	42	-79
-8	24	4	91	4	-182
-5	24	4	135	110	-137
-16	25	4	277	247	72
-13	25	4	276	189	-111
-10	25	4	166	105	-128
0	1	5	68	2384	-236
-2	2	5	1266	1946	172

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
1	2	5	70	1100	-141
-4	3	5	67	214	-135
-1	3	5	71	1199	-144
2	3	5	66	563	-132
-6	4	5	205	39	-80
-3	4	5	157	522	-84
0	4	5	180	136	-78
3	4	5	199	462	-63
-8	5	5	136	556	-133
-5	5	5	95	833	-96
-2	5	5	66	1	-132
1	5	5	177	102	-78
4	5	5	179	126	-90
-10	6	5	225	166	53
-7	6	5	208	215	-76
-4	6	5	150	24	-89
-1	6	5	158	135	-57
2	6	5	146	218	-98
5	6	5	108	135	-127
-12	7	5	140	68	-115
-9	7	5	158	93	-83
-6	7	5	127	12	-97
-3	7	5	132	350	-86
0	7	5	136	64	-85
3	7	5	243	112	69
6	7	5	280	111	58
-14	8	5	169	28	-104
-11	8	5	160	306	-113
-8	8	5	158	664	-77
-5	8	5	191	103	-82
-2	8	5	75	316	-150
1	8	5	104	314	-118
4	8	5	85	148	-171
7	8	5	134	48	-143
-16	9	5	94	229	-188
-13	9	5	87	64	-303
-10	9	5	208	66	-96
-7	9	5	225	394	55
-4	9	5	105	152	-115
-1	9	5	134	483	-85
2	9	5	125	432	-120
5	9	5	152	246	-114
8	9	5	153	71	-141
-18	10	5	100	97	-200
-15	10	5	214	44	-115
-12	10	5	343	118	64
-9	10	5	83	346	-166
-6	10	5	258	47	-78
-3	10	5	234	126	65
0	10	5	83	241	-144
3	10	5	174	157	-123
6	10	5	198	10	-106
9	10	5	104	186	-209
-17	11	5	99	157	-199
-14	11	5	201	162	-118
-11	11	5	172	450	-104
-8	11	5	156	323	-114
-5	11	5	98	343	-135
-2	11	5	80	139	-160
1	11	5	87	144	-214
4	11	5	216	131	-110
7	11	5	172	118	-142
-19	12	5	342	245	-129
-16	12	5	210	25	-117
-13	12	5	94	210	-188
-10	12	5	246	6	-84
-7	12	5	84	107	-167
-4	12	5	139	54	-114
-1	12	5	88	226	-305
2	12	5	94	109	-189
5	12	5	163	66	-143
-18	13	5	103	22	-207
-15	13	5	97	4	-195
-12	13	5	95	81	-191
-9	13	5	261	225	-112
-6	13	5	225	182	-71
-3	13	5	209	49	-90
0	13	5	292	110	81
3	13	5	300	37	-98
-17	14	5	214	61	-130
-14	14	5	244	155	-106
-11	14	5	95	38	-191
-8	14	5	90	77	-181
-5	14	5	88	82	-177
-2	14	5	191	4	-103
1	14	5	146	99	-148
4	14	5	107	144	-214
-16	15	5	276	134	-125
-13	15	5	98	106	-197
-10	15	5	249	170	-111
-7	15	5	231	139	-97
-4	15	5	91	130	-183

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-1	15	5	207	111	-107
2	15	5	104	92	-208
-15	16	5	143	147	-169
-12	16	5	163	351	-136
-9	16	5	133	298	-140
-6	16	5	95	63	-190
-3	16	5	101	34	-203
0	16	5	160	3	-130
-14	17	5	162	265	-155
-11	17	5	169	221	-141
-8	17	5	96	88	-193
-5	17	5	99	222	-198
-2	17	5	206	145	-136
-13	18	5	103	56	-206
-10	18	5	100	15	-199
-7	18	5	210	221	-131
-4	18	5	175	252	-150
-12	19	5	217	164	-130
-9	19	5	105	120	-210
0	0	6	90	1418	-100
1	1	6	197	462	56
-1	2	6	180	1157	-61
2	2	6	162	243	-81
-3	3	6	184	466	46
0	3	6	147	179	-60
3	3	6	90	418	-102
-5	4	6	142	324	-67
-2	4	6	193	899	-80
1	4	6	126	950	-83
4	4	6	260	230	-95
-7	5	6	72	660	-145
-4	5	6	65	304	-130
-1	5	6	146	499	-65
2	5	6	119	884	-104
5	5	6	79	465	-158
-9	6	6	77	753	-155
-6	6	6	121	567	-102
-3	6	6	65	456	-130
0	6	6	123	618	-91
3	6	6	73	694	-147
6	6	6	87	700	-174
-11	7	6	82	14	-164
-8	7	6	103	499	-121
-5	7	6	73	701	-146
-2	7	6	109	70	-113
1	7	6	78	428	-157
4	7	6	83	478	-166
7	7	6	157	235	-126
-13	8	6	88	267	-176
-10	8	6	122	651	-117
-7	8	6	77	580	-155
-4	8	6	75	244	-150
-1	8	6	261	979	-91
2	8	6	90	415	-180
5	8	6	95	192	-190
8	8	6	145	231	-141
-15	9	6	95	443	-191
-12	9	6	93	435	-187
-9	9	6	348	150	-109
-6	9	6	77	186	-155
-3	9	6	73	584	-147
0	9	6	128	748	-92
3	9	6	134	930	-131
6	9	6	93	639	-186
9	9	6	100	173	-201
-17	10	6	117	25	-168
-14	10	6	208	16	-112
-11	10	6	132	540	-137
-8	10	6	79	648	-159
-5	10	6	79	343	-159
-2	10	6	89	173	-178
1	10	6	90	537	-181
4	10	6	127	590	-145
7	10	6	188	134	-107
-19	11	6	160	70	-153
-16	11	6	224	159	-118
-13	11	6	89	312	-178
-10	11	6	92	524	-185
-7	11	6	101	438	-141
-4	11	6	83	478	-166
-1	11	6	234	134	-101
2	11	6	97	24	-195
5	11	6	134	44	-154
8	11	6	215	62	-135
-18	12	6	102	10	-204
-15	12	6	97	41	-195
-12	12	6	283	301	-89
-9	12	6	144	425	-137
-6	12	6	87	52	-175
-3	12	6	185	18	-101
0	12	6	193	453	-82
3	12	6	96	446	-192

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
6	12	6	245	41	-131
-17	13	6	215	62	-131
-14	13	6	265	369	-116
-11	13	6	169	781	-109
-8	13	6	88	714	-175
-5	13	6	95	682	-191
-2	13	6	96	62	-192
1	13	6	99	342	-199
4	13	6	102	224	-204
-16	14	6	204	45	-131
-13	14	6	200	236	-105
-10	14	6	175	527	-122
-7	14	6	90	752	-180
-4	14	6	91	294	-181
-1	14	6	98	107	-196
2	14	6	154	28	-155
-18	15	6	106	187	-212
-15	15	6	140	259	-146
-12	15	6	98	307	-196
-9	15	6	228	5	-118
-6	15	6	184	73	-108
-3	15	6	95	233	-190
0	15	6	175	233	-116
3	15	6	244	5	-134
-17	16	6	285	111	-118
-14	16	6	234	269	-99
-11	16	6	95	271	-190
-8	16	6	172	302	-128
-5	16	6	181	41	-115
-2	16	6	167	255	-142
1	16	6	107	221	-214
-16	17	6	238	230	-140
-13	17	6	209	136	-108
-10	17	6	97	159	-194
-7	17	6	273	34	-119
-4	17	6	149	113	-157
-1	17	6	228	187	-108
-15	18	6	107	394	-213
-12	18	6	103	220	-206
-9	18	6	167	146	-146
-6	18	6	169	13	-151
-3	18	6	256	5	-132
-11	19	6	105	179	-211
-8	19	6	106	14	-212
-1	1	7	124	204	-48
-3	2	7	59	247	-119
0	2	7	54	293	-94
-5	3	7	68	200	-135
-2	3	7	121	346	-86
1	3	7	67	265	-133
-4	4	7	95	881	-85
-1	4	7	146	7	-67
2	4	7	145	416	-81
-9	5	7	72	81	-145
-6	5	7	100	2	-127
-3	5	7	67	191	-165
0	5	7	140	333	-64
3	5	7	273	213	-97
-11	6	7	204	379	-74
-8	6	7	104	502	-114
-5	6	7	149	357	-88
-2	6	7	103	716	-95
1	6	7	256	211	-94
4	6	7	177	230	-85
-13	7	7	108	41	-148
-10	7	7	247	306	63
-7	7	7	73	386	-127
-4	7	7	280	159	-83
-1	7	7	368	138	100
2	7	7	96	305	-125
5	7	7	152	264	-105
-15	8	7	293	88	76
-12	8	7	263	72	58
-9	8	7	195	84	-65
-6	8	7	137	2	-97
-3	8	7	257	187	61
0	8	7	89	122	-113
3	8	7	165	14	-85
6	8	7	147	192	-116
-17	9	7	194	21	-126
-14	9	7	159	72	-107
-11	9	7	131	72	-124
-8	9	7	275	408	-98
-5	9	7	160	490	-87
-2	9	7	194	580	-93
1	9	7	170	444	-99
4	9	7	92	33	-225
7	9	7	125	56	-157
-19	10	7	173	7	-150
-16	10	7	179	26	-110
-13	10	7	87	217	-175
-10	10	7	121	374	-101

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-7	10	7	217	52	-92
-4	10	7	119	167	-115
-1	10	7	208	335	-69
2	10	7	201	45	-109
5	10	7	137	306	-139
8	10	7	129	121	-171
-18	11	7	103	3	-206
-15	11	7	204	17	-98
-12	11	7	90	72	-313
-9	11	7	188	122	-106
-6	11	7	149	29	-90
-3	11	7	152	30	-108
0	11	7	108	85	-129
3	11	7	138	99	-130
6	11	7	97	208	-195
-17	12	7	186	119	-136
-14	12	7	194	338	-107
-11	12	7	194	416	-125
-8	12	7	307	220	51
-5	12	7	110	194	-142
-2	12	7	138	400	-128
1	12	7	199	240	-123
4	12	7	130	39	-161
7	12	7	163	57	-154
-16	13	7	138	188	-158
-13	13	7	93	396	-161
-10	13	7	117	191	-142
-7	13	7	147	153	-124
-4	13	7	149	248	-191
-1	13	7	189	34	-110
2	13	7	98	170	-196
5	13	7	136	231	-172
-18	14	7	105	79	-211
-15	14	7	101	59	-203
-12	14	7	131	19	-155
-9	14	7	242	42	-91
-6	14	7	88	48	-176
-3	14	7	187	149	-100
0	14	7	147	201	-119
3	14	7	101	166	-203
-17	15	7	108	7	-217
-14	15	7	173	142	-141
-11	15	7	95	97	-189
-8	15	7	128	126	-152
-5	15	7	91	85	-183
-2	15	7	97	119	-194
1	15	7	238	17	-92
-16	16	7	108	8	-187
-13	16	7	193	38	-130
-10	16	7	95	108	-190
-7	16	7	198	40	-103
-4	16	7	98	14	-197
-1	16	7	102	136	-204
-15	17	7	108	179	-217
-12	17	7	186	9	-114
-9	17	7	97	92	-194
-6	17	7	128	9	-165
-3	17	7	102	88	-204
-14	18	7	106	66	-212
-11	18	7	102	268	-204
-8	18	7	186	182	-136
-5	18	7	138	121	-174
-10	19	7	106	175	-212
-7	19	7	223	173	-115
0	1	8	762	576	9
-2	2	8	3533	3586	73
1	2	8	1233	1104	10
-4	3	8	717	733	8
-1	3	8	1241	1031	22
2	3	8	2571	2708	38
-6	4	8	426	348	17
-3	4	8	720	724	13
0	4	8	5407	4673	70
3	4	8	4872	4578	126
-8	5	8	2260	2188	24
-5	5	8	568	591	13
-2	5	8	2587	2753	48
1	5	8	3080	3030	33
4	5	8	1291	1212	18
-10	6	8	1916	2028	16
-7	6	8	295	316	28
-4	6	8	427	368	19
-1	6	8	3086	3147	40
2	6	8	3626	3597	34
5	6	8	1308	1256	17
-12	7	8	735	741	17
-9	7	8	386	414	25
-6	7	8	312	368	32
-3	7	8	4513	4363	482
0	7	8	6702	6161	109
3	7	8	4104	4119	40
6	7	8	1815	1912	16

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-14	8	8	269	183	69
-11	8	8	276	247	28
-8	8	8	545	621	31
-5	8	8	2277	2346	23
1	8	8	2187	2118	30
4	8	8	1901	1962	72
7	8	8	724	732	20
-16	9	8	114	93	-89
-13	9	8	321	304	66
-10	9	8	328	359	25
-7	9	8	375	346	19
-4	9	8	1295	1357	14
-1	9	8	2180	2188	19
2	9	8	1105	1160	17
5	9	8	393	383	25
8	9	8	203	205	56
-18	10	8	108	28	-107
-15	10	8	140	47	-82
-12	10	8	318	253	30
-9	10	8	368	403	29
-6	10	8	1899	1949	12
-3	10	8	4133	4066	38
0	10	8	2891	2867	14
3	10	8	2009	2074	41
6	10	8	435	442	32
9	10	8	286	352	48
-20	11	8	156	180	-100
-17	11	8	182	241	-63
-14	11	8	444	359	23
-11	11	8	1008	920	22
-8	11	8	245	328	37
-5	11	8	1310	1310	12
-2	11	8	1115	1103	12
1	11	8	1088	1064	42
4	11	8	560	506	33
7	11	8	183	68	-86
10	11	8	189	169	-107
-22	12	8	99	86	-113
-19	12	8	216	152	-65
-16	12	8	295	336	49
-13	12	8	484	581	23
-10	12	8	334	231	30
-7	12	8	743	795	29
-4	12	8	1944	1941	16
-1	12	8	1084	1079	53
2	12	8	932	947	24
5	12	8	323	237	35
8	12	8	142	146	-118
11	12	8	278	121	-107
-24	13	8	187	146	-102
-21	13	8	87	114	-175
-18	13	8	322	270	52
-15	13	8	243	279	47
-12	13	8	499	586	21
-9	13	8	327	268	58
-6	13	8	1810	1918	27
-3	13	8	1992	2093	49
0	13	8	1585	1668	47
3	13	8	706	745	37
6	13	8	146	153	-115
9	13	8	199	180	-109
12	13	8	270	110	-110
-23	14	8	88	47	-176
-20	14	8	372	400	47
-17	14	8	862	895	32
-14	14	8	1249	1239	18
-11	14	8	433	353	28
-8	14	8	232	233	-71
-5	14	8	415	404	30
-2	14	8	930	920	24
1	14	8	401	344	31
4	14	8	148	37	-107
7	14	8	139	110	-127
10	14	8	348	303	55
-25	15	8	93	67	-186
-22	15	8	147	103	-127
-19	15	8	333	352	67
-16	15	8	693	733	25
-13	15	8	312	299	51
-10	15	8	155	64	-75
-7	15	8	734	735	22
-4	15	8	556	503	28
-1	15	8	406	367	37
2	15	8	326	240	38
5	15	8	129	113	-127
8	15	8	90	77	-180
-24	16	8	140	2	-137
-21	16	8	255	193	62
-18	16	8	543	460	34
-15	16	8	699	665	22
-12	16	8	332	327	35
-9	16	8	200	90	55

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-6	16	8	424	429	55
-3	16	8	725	759	59
0	16	8	280	295	38
3	16	8	139	132	-124
6	16	8	235	140	-74
-23	17	8	198	203	-96
-20	17	8	578	633	43
-17	17	8	1075	1181	28
-14	17	8	845	875	27
-11	17	8	235	220	55
-8	17	8	192	160	-60
-5	17	8	286	269	40
-2	17	8	276	234	47
1	17	8	202	81	-81
4	17	8	139	57	-130
7	17	8	336	262	81
-22	18	8	287	254	-99
-19	18	8	413	460	78
-16	18	8	563	507	34
-13	18	8	361	267	65
-10	18	8	201	25	-75
-7	18	8	119	75	-100
-4	18	8	184	23	-104
-1	18	8	203	82	-103
2	18	8	148	142	-95
5	18	8	196	48	-116
-21	19	8	92	121	-183
-18	19	8	353	414	70
-15	19	8	337	323	75
-12	19	8	185	157	-80
-9	19	8	309	342	42
-6	19	8	130	142	-121
-3	19	8	191	124	-87
0	19	8	328	277	45
3	19	8	156	120	-129
-23	20	8	187	184	-125
-20	20	8	486	458	41
-17	20	8	528	631	42
-14	20	8	356	384	72
-11	20	8	145	169	-118
-8	20	8	150	101	-102
-5	20	8	200	95	-93
-2	20	8	182	125	-82
1	20	8	91	80	-182
-22	21	8	122	153	-152
-19	21	8	267	153	-88
-16	21	8	221	203	56
-13	21	8	185	83	-109
-10	21	8	259	187	71
-7	21	8	87	118	-174
-4	21	8	127	67	-138
-1	21	8	92	98	-184
-21	22	8	214	142	-93
-18	22	8	173	246	-113
-15	22	8	287	116	-109
-12	22	8	173	108	-82
-9	22	8	89	176	-178
-6	22	8	127	141	-141
-3	22	8	115	118	-153
-20	23	8	207	198	-91
-17	23	8	248	219	-76
-14	23	8	89	59	-178
-11	23	8	90	113	-179
-8	23	8	156	85	-124
-5	23	8	203	60	-115
-16	24	8	91	6	-182
-13	24	8	215	146	-96
-10	24	8	249	286	-97
-7	24	8	315	262	66
-15	25	8	130	58	-146
-12	25	8	154	100	-132
0	0	9	76	631	-97
1	1	9	56	89	-113
-1	2	9	56	128	-113
2	2	9	145	39	-81
-3	3	9	69	148	-119
0	3	9	102	176	-87
3	3	9	136	111	-82
-5	4	9	193	109	-78
-2	4	9	175	45	-74
1	4	9	208	260	-63
4	4	9	73	79	-147
-7	5	9	183	13	-108
-4	5	9	243	371	-82
-1	5	9	68	555	-168
2	5	9	190	648	-62
5	5	9	118	368	-118
-9	6	9	185	183	-68
-6	6	9	225	507	57
-3	6	9	150	8	-80
0	6	9	72	284	-125
3	6	9	216	151	62

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
6	6	9	109	213	-141
-11	7	9	110	235	-129
-8	7	9	181	367	-72
-5	7	9	340	112	63
-2	7	9	98	136	-143
1	7	9	279	221	47
4	7	9	312	199	48
7	7	9	276	292	-107
-13	8	9	88	60	-306
-10	8	9	109	240	-123
-7	8	9	163	45	-85
-4	8	9	116	11	-105
-1	8	9	269	322	46
2	8	9	206	326	-83
5	8	9	89	112	-307
8	8	9	124	67	-162
-15	9	9	94	207	-189
-12	9	9	182	162	-106
-9	9	9	91	312	-121
-6	9	9	204	36	57
-3	9	9	200	126	-78
0	9	9	203	246	-72
3	9	9	87	94	-175
6	9	9	170	144	-112
9	9	9	165	34	-154
-17	10	9	97	306	-194
-14	10	9	161	399	-123
-11	10	9	84	639	-168
-8	10	9	156	315	-92
-5	10	9	192	75	-91
-2	10	9	154	190	-100
1	10	9	194	7	-102
4	10	9	179	178	-106
7	10	9	97	137	-194
-19	11	9	135	253	-186
-16	11	9	204	334	-109
-13	11	9	87	494	-175
-10	11	9	176	215	-97
-7	11	9	256	90	-89
-4	11	9	281	17	-91
-1	11	9	240	169	-81
2	11	9	93	16	-187
5	11	9	196	7	-116
8	11	9	108	165	-217
-18	12	9	107	54	-214
-15	12	9	197	67	-114
-12	12	9	89	153	-154
-9	12	9	113	20	-146
-6	12	9	85	16	-170
-3	12	9	114	12	-142
0	12	9	89	53	-155
3	12	9	96	26	-191
6	12	9	127	121	-180
-17	13	9	104	242	-209
-14	13	9	179	430	-129
-11	13	9	88	270	-177
-8	13	9	87	6	-304
-5	13	9	90	203	-314
-2	13	9	92	320	-185
1	13	9	243	84	-113
4	13	9	144	101	-156
-16	14	9	103	355	-206
-13	14	9	193	139	-125
-10	14	9	263	59	-107
-7	14	9	213	138	-107
-4	14	9	214	224	-78
-1	14	9	95	286	-190
2	14	9	169	151	-145
-15	15	9	187	161	-125
-12	15	9	160	253	-128
-9	15	9	96	250	-193
-6	15	9	148	338	-139
-3	15	9	95	254	-191
0	15	9	120	213	-150
-17	16	9	262	366	-107
-14	16	9	157	295	-156
-11	16	9	213	154	-127
-8	16	9	155	168	-148
-5	16	9	200	123	-105
-2	16	9	151	56	-149
1	16	9	106	55	-212
-16	17	9	302	132	-91
-13	17	9	214	15	-115
-10	17	9	164	19	-140
-7	17	9	158	43	-131
-4	17	9	123	30	-175
-1	17	9	104	22	-208
-12	18	9	278	148	-109
-9	18	9	105	207	-210
-6	18	9	170	159	-152
-11	19	9	152	69	-173
-8	19	9	110	64	-220

Table 54. (cont).
F(obs), F(calc), and σ_F

($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-1	1	10	247	290	61
-3	2	10	69	854	-138
0	2	10	398	558	102
-5	3	10	69	270	-168
-2	3	10	217	106	-77
1	3	10	101	96	-96
-7	4	10	76	276	-152
-4	4	10	171	266	-55
-1	4	10	133	491	-76
2	4	10	72	703	-143
-9	5	10	73	478	-147
-6	5	10	218	452	-69
-3	5	10	69	514	-139
0	5	10	199	71	-59
3	5	10	75	674	-150
-11	6	10	109	181	-135
-8	6	10	71	240	-142
-5	6	10	169	29	-71
-2	6	10	112	506	-102
1	6	10	79	248	-158
4	6	10	86	75	-173
-13	7	10	91	262	-315
-10	7	10	78	232	-156
-7	7	10	157	245	-70
-4	7	10	76	358	-152
-1	7	10	191	223	-96
2	7	10	79	409	-159
5	7	10	90	106	-181
-15	8	10	205	328	-126
-12	8	10	86	118	-171
-9	8	10	109	397	-120
-6	8	10	71	338	-143
-3	8	10	147	204	-94
0	8	10	74	540	-128
3	8	10	82	567	-165
6	8	10	140	20	-130
-17	9	10	226	527	-104
-14	9	10	157	518	-102
-11	9	10	178	271	-85
-8	9	10	161	47	-97
-5	9	10	72	428	-145
-2	9	10	231	646	-90
1	9	10	316	293	-105
4	9	10	201	20	-119
7	9	10	359	104	-132
-19	10	10	221	251	-146
-16	10	10	156	307	-152
-13	10	10	88	342	-176
-10	10	10	126	59	-107
-7	10	10	78	217	-157
-4	10	10	158	208	-113
-1	10	10	219	374	-99
2	10	10	92	182	-184
5	10	10	205	107	-111
8	10	10	108	325	-216
-18	11	10	141	256	-182
-15	11	10	152	204	-143
-12	11	10	142	120	-115
-9	11	10	142	98	-120
-6	11	10	82	539	-165
-3	11	10	82	748	-165
0	11	10	127	685	-108
3	11	10	127	393	-146
6	11	10	240	136	-121
-17	12	10	202	434	-135
-14	12	10	93	355	-186
-11	12	10	134	44	-132
-8	12	10	86	337	-173
-5	12	10	90	674	-181
-2	12	10	90	801	-181
1	12	10	139	482	-149
4	12	10	102	108	-145
-16	13	10	100	65	-201
-13	13	10	181	10	-109
-10	13	10	129	41	-136
-7	13	10	191	43	-149
-4	13	10	226	186	-113
-1	13	10	196	49	-122
2	13	10	217	38	-122
5	13	10	220	132	-137
-18	14	10	270	230	-127
-15	14	10	101	190	-201
-12	14	10	147	43	-138
-9	14	10	169	367	-123
-6	14	10	88	625	-176
-3	14	10	91	645	-183
0	14	10	95	500	-165
3	14	10	199	95	-135
-17	15	10	190	65	-154
-14	15	10	174	134	-139
-11	15	10	263	70	-118
-8	15	10	237	211	-96

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-5	15	10	141	493	-135
-2	15	10	206	623	-122
1	15	10	104	270	-208
-16	16	10	237	324	-122
-13	16	10	239	249	-120
-10	16	10	101	299	-203
-7	16	10	326	165	-117
-4	16	10	123	32	-128
-1	16	10	102	50	-205
-15	17	10	251	146	-110
-12	17	10	146	203	-157
-9	17	10	195	365	-117
-6	17	10	199	332	-125
-3	17	10	178	326	-139
-14	18	10	270	211	-126
-11	18	10	110	183	-220
-8	18	10	222	3	-139
-5	18	10	168	197	-155
-10	19	10	111	435	-222
-2	2	11	1348	1192	40
1	2	11	87	999	-303
-4	3	11	188	230	-82
-1	3	11	932	290	112
2	3	11	120	163	-91
-6	4	11	228	338	-76
-3	4	11	209	589	-75
0	4	11	158	263	-74
3	4	11	114	240	-111
-8	5	11	70	35	-141
-5	5	11	220	307	62
-2	5	11	88	31	-109
1	5	11	70	204	-139
4	5	11	156	159	-77
-10	6	11	238	25	-73
-7	6	11	130	157	-105
-4	6	11	136	517	-107
-1	6	11	193	587	-65
2	6	11	217	75	-76
5	6	11	128	286	-120
-12	7	11	84	285	-169
-9	7	11	134	39	-89
-6	7	11	213	28	-86
-3	7	11	216	206	59
0	7	11	105	221	-102
3	7	11	264	188	61
6	7	11	89	229	-310
-14	8	11	90	208	-180
-11	8	11	101	255	-137
-8	8	11	213	129	50
-5	8	11	106	272	-106
-2	8	11	222	248	-86
1	8	11	162	300	-86
4	8	11	87	414	-174
7	8	11	202	330	-103
-16	9	11	171	78	-147
-13	9	11	163	125	-107
-10	9	11	210	510	-79
-7	9	11	160	54	-78
-4	9	11	186	295	-58
-1	9	11	79	215	-158
2	9	11	84	211	-168
5	9	11	90	268	-180
8	9	11	156	100	-134
-18	10	11	222	59	-138
-15	10	11	195	11	-125
-12	10	11	252	197	56
-9	10	11	193	460	-94
-6	10	11	197	295	-75
-3	10	11	352	446	42
0	10	11	179	144	-89
3	10	11	325	134	-98
6	10	11	99	216	-198
9	10	11	214	32	-151
-17	11	11	166	122	-146
-14	11	11	162	141	-126
-11	11	11	185	50	-87
-8	11	11	207	237	-79
-5	11	11	81	275	-161
-2	11	11	164	254	-104
1	11	11	88	350	-177
4	11	11	313	369	-115
7	11	11	108	122	-216
-16	12	11	220	2	-111
-13	12	11	209	206	-119
-10	12	11	207	341	-74
-7	12	11	84	57	-169
-4	12	11	233	36	-87
-1	12	11	140	126	-115
2	12	11	148	231	-141
5	12	11	133	123	-162
-18	13	11	234	216	-106
-15	13	11	136	185	-155

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-12	13	11	281	211	73
-9	13	11	158	302	-123
-6	13	11	130	284	-217
-3	13	11	232	175	-86
0	13	11	237	43	-85
3	13	11	221	53	-123
-17	14	11	200	211	-137
-14	14	11	219	38	-115
-11	14	11	93	66	-186
-8	14	11	143	217	-130
-5	14	11	133	26	-126
-2	14	11	195	42	-97
1	14	11	98	198	-196
4	14	11	107	61	-214
-16	15	11	167	90	-147
-13	15	11	119	195	-172
-10	15	11	267	204	-111
-7	15	11	96	137	-193
-4	15	11	193	74	-122
-1	15	11	179	81	-133
2	15	11	193	64	-143
-15	16	11	105	118	-209
-12	16	11	131	65	-172
-9	16	11	104	258	-208
-6	16	11	141	102	-156
-3	16	11	224	72	-103
0	16	11	104	55	-181
-14	17	11	258	171	-124
-11	17	11	226	145	-125
-8	17	11	156	117	-144
-5	17	11	100	213	-201
-2	17	11	204	59	-120
-13	18	11	306	205	-93
-10	18	11	157	355	-165
-7	18	11	172	208	-159
-4	18	11	261	29	-108
-9	19	11	259	163	-137
0	0	12	228	217	21
1	1	12	8816	8666	190
-1	2	12	8810	8341	321
2	2	12	6533	6323	65
-3	3	12	121	28	-46
0	3	12	169	75	38
3	3	12	392	666	27
-5	4	12	5600	5199	112
-2	4	12	6548	6287	151
1	4	12	3456	3351	41
4	4	12	963	923	24
-7	5	12	2661	2780	20
-4	5	12	5656	5319	128
-1	5	12	3471	3447	53
2	5	12	1074	1184	30
5	5	12	322	256	28
-9	6	12	744	644	3
-6	6	12	144	121	-47
-3	6	12	411	509	29
0	6	12	126	4	-44
3	6	12	1057	1039	13
6	6	12	868	825	13
-11	7	12	905	920	20
-8	7	12	217	190	36
-5	7	12	2678	2614	36
-2	7	12	1108	1175	39
1	7	12	625	674	18
4	7	12	500	489	20
7	7	12	186	156	-66
-13	8	12	1710	1676	22
-10	8	12	421	348	24
-7	8	12	271	300	69
-4	8	12	950	984	11
-1	8	12	630	675	17
2	8	12	453	447	19
5	8	12	979	1002	28
8	8	12	1646	1653	36
-15	9	12	1697	1689	33
-12	9	12	321	297	32
-9	9	12	122	26	-71
-6	9	12	742	638	18
-3	9	12	1063	1044	23
0	9	12	139	25	-60
3	9	12	1041	1016	20
6	9	12	1195	1173	27
9	9	12	1246	1255	39
-17	10	12	87	66	-124
-14	10	12	215	226	50
-11	10	12	346	328	42
-8	10	12	425	344	23
-5	10	12	325	264	38
-2	10	12	476	505	46
1	10	12	157	136	-61
4	10	12	178	148	-57
7	10	12	192	125	56

Table 54. (cont).
F(obs), F(calc), and σ_F

($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
10	10	12	84	1	-169
-19	11	12	913	983	34
-16	11	12	1455	1484	39
-13	11	12	497	503	22
-10	11	12	335	354	32
-7	11	12	922	960	36
-4	11	12	493	482	20
-1	11	12	182	78	51
2	11	12	785	803	16
5	11	12	926	900	31
8	11	12	986	968	43
11	11	12	452	374	74
-21	12	12	577	596	114
-18	12	12	1077	1068	31
-15	12	12	913	891	17
-12	12	12	155	22	-68
-9	12	12	328	337	30
-6	12	12	880	900	19
-3	12	12	1044	965	18
0	12	12	127	23	-70
3	12	12	687	646	29
6	12	12	767	757	37
9	12	12	524	538	39
12	12	12	95	198	-190
-23	13	12	89	126	-179
-20	13	12	131	79	-125
-17	13	12	243	99	62
-14	13	12	221	264	48
-11	13	12	500	506	31
-8	13	12	1694	1608	40
-5	13	12	972	969	20
-2	13	12	799	818	16
1	13	12	405	408	28
4	13	12	124	5	-92
7	13	12	84	140	-168
10	13	12	211	27	-79
-25	14	12	187	14	-118
-22	14	12	227	194	-73
-19	14	12	471	490	52
-16	14	12	311	331	49
-13	14	12	239	248	43
-10	14	12	235	267	47
-7	14	12	216	181	-65
-4	14	12	142	145	-64
-1	14	12	403	411	42
2	14	12	533	530	27
5	14	12	548	574	40
8	14	12	394	360	57
11	14	12	140	50	-140
-24	15	12	114	117	-161
-21	15	12	251	207	52
-18	15	12	167	101	-96
-15	15	12	112	33	-85
-12	15	12	916	917	28
-9	15	12	1714	1694	30
-6	15	12	1170	1202	39
-3	15	12	678	624	46
0	15	12	121	23	-88
3	15	12	452	503	45
6	15	12	369	314	46
9	15	12	232	153	-98
-23	16	12	90	26	-181
-20	16	12	232	180	-81
-17	16	12	277	267	49
-14	16	12	319	363	43
-11	16	12	1465	1530	40
-8	16	12	1650	1634	36
-5	16	12	905	884	32
-2	16	12	518	483	35
1	16	12	158	69	-85
4	16	12	87	68	-174
7	16	12	171	17	-119
-22	17	12	196	102	-96
-19	17	12	241	169	66
-16	17	12	314	266	46
-13	17	12	211	143	-98
-10	17	12	102	95	-107
-7	17	12	182	120	-67
-4	17	12	106	15	-107
-1	17	12	144	48	-105
2	17	12	137	120	-127
5	17	12	162	58	-124
-24	18	12	176	66	-109
-21	18	12	198	3	-96
-18	18	12	113	9	-125
-15	18	12	202	119	-80
-12	18	12	1085	1039	26
-9	18	12	1244	1223	43
-6	18	12	729	754	50
-3	18	12	444	462	54
0	18	12	199	27	-98
3	18	12	232	62	-73

Table 54. (cont).
F(obs), F(calc), and σ_F

($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
6	18	12	93	16	-186
-23	19	12	122	50	-149
-20	19	12	163	13	-101
-17	19	12	200	169	-107
-14	19	12	430	522	43
-11	19	12	948	1003	49
-8	19	12	957	950	42
-5	19	12	530	535	39
-2	19	12	166	78	-99
1	19	12	158	23	-114
4	19	12	152	23	-117
-22	20	12	230	98	-88
-19	20	12	234	4	-88
-16	20	12	223	169	-79
-13	20	12	212	56	-104
-10	20	12	165	1	-110
-7	20	12	129	101	-129
-4	20	12	123	80	-137
-1	20	12	189	1	-112
2	20	12	118	35	-153
-21	21	12	170	25	-110
-18	21	12	170	23	-122
-15	21	12	271	229	-80
-12	21	12	550	595	60
-9	21	12	561	538	60
-6	21	12	319	305	50
-3	21	12	159	29	-119
0	21	12	152	16	-117
-20	22	12	135	74	-139
-17	22	12	299	116	75
-14	22	12	192	226	-88
-11	22	12	359	387	57
-8	22	12	331	339	63
-5	22	12	135	31	-135
-2	22	12	146	46	-122
-19	23	12	91	61	-183
-16	23	12	91	25	-182
-13	23	12	183	111	-115
-10	23	12	134	38	-136
-7	23	12	111	36	-152
-4	23	12	152	12	-126
-18	24	12	165	84	-117
-15	24	12	93	137	-187
-12	24	12	317	216	-117
-9	24	12	146	157	-129
-6	24	12	121	26	-151
-14	25	12	92	45	-185
-11	25	12	92	66	-185
-1	1	13	231	568	-75
-3	2	13	209	104	-66
0	2	13	116	43	-76
-5	3	13	66	467	-132
-2	3	13	195	70	-62
1	3	13	284	338	61
-4	4	13	226	353	49
-1	4	13	263	250	51
2	4	13	314	130	57
-9	5	13	218	290	-72
-6	5	13	347	107	-103
-3	5	13	91	782	-106
0	5	13	348	861	-105
3	5	13	192	277	55
-11	6	13	275	175	-104
-8	6	13	113	289	-104
-5	6	13	388	281	74
-2	6	13	374	535	47
1	6	13	205	616	-64
4	6	13	113	493	-122
-13	7	13	113	370	-150
-10	7	13	80	356	-160
-7	7	13	109	368	-90
-4	7	13	283	205	-95
-1	7	13	182	313	-71
2	7	13	154	19	-97
5	7	13	140	494	-125
-15	8	13	98	346	-196
-12	8	13	159	140	-113
-9	8	13	266	126	50
-6	8	13	72	260	-145
-3	8	13	133	730	-97
0	8	13	286	329	37
3	8	13	210	118	-65
6	8	13	179	175	-101
-17	9	13	101	71	-202
-14	9	13	149	1	-132
-11	9	13	134	74	-130
-8	9	13	252	263	67
-5	9	13	138	97	-83
-2	9	13	77	224	-155
1	9	13	144	145	-113
4	9	13	188	381	-115
7	9	13	226	244	-129

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-19	10	13	334	164	87
-16	10	13	252	320	-104
-13	10	13	179	292	-108
-10	10	13	476	351	95
-7	10	13	115	216	-124
-4	10	13	79	89	-159
-1	10	13	101	140	-136
2	10	13	87	230	-213
5	10	13	96	367	-192
8	10	13	200	200	-135
-18	11	13	109	273	-219
-15	11	13	158	144	-142
-12	11	13	167	8	-121
-9	11	13	88	33	-177
-6	11	13	148	118	-98
-3	11	13	203	108	-80
0	11	13	232	50	-70
3	11	13	127	85	-138
6	11	13	161	39	-144
-17	12	13	167	13	-136
-14	12	13	173	53	-116
-11	12	13	194	392	-114
-8	12	13	234	403	-104
-5	12	13	174	16	-96
-2	12	13	203	16	-128
1	12	13	92	284	-184
4	12	13	221	325	-108
-16	13	13	198	163	-134
-13	13	13	367	202	102
-10	13	13	160	266	-119
-7	13	13	91	166	-181
-4	13	13	88	4	-176
-1	13	13	211	199	-90
2	13	13	184	224	-130
5	13	13	299	208	-104
-18	14	13	106	160	-213
-15	14	13	100	69	-200
-12	14	13	130	89	-153
-9	14	13	163	128	-129
-6	14	13	156	35	-125
-3	14	13	179	182	-121
0	14	13	224	23	-84
3	14	13	175	20	-153
-17	15	13	186	158	-148
-14	15	13	280	24	-112
-11	15	13	159	304	-131
-8	15	13	185	266	-132
-5	15	13	189	83	-110
-2	15	13	97	104	-193
1	15	13	163	147	-157
-16	16	13	172	130	-137
-13	16	13	158	23	-149
-10	16	13	133	88	-169
-7	16	13	177	134	-144
-4	16	13	100	95	-200
-1	16	13	103	102	-207
-15	17	13	106	124	-212
-12	17	13	103	260	-206
-9	17	13	191	162	-133
-6	17	13	182	89	-136
-3	17	13	105	56	-211
-14	18	13	227	66	-112
-11	18	13	182	206	-153
-8	18	13	330	149	-130
-5	18	13	198	37	-147
-10	19	13	279	21	-132
0	1	14	134	235	-68
-2	2	14	135	52	-66
1	2	14	152	717	-72
-4	3	14	70	19	-140
-1	3	14	144	534	-72
2	3	14	166	691	-79
-6	4	14	76	1054	-152
-3	4	14	164	500	-69
0	4	14	192	730	-74
3	4	14	78	475	-157
-8	5	14	72	747	-145
-5	5	14	71	625	-122
-2	5	14	143	802	-72
1	5	14	105	1185	-113
4	5	14	77	410	-154
-10	6	14	86	266	-173
-7	6	14	250	82	-88
-4	6	14	215	555	-81
-1	6	14	264	384	54
2	6	14	139	425	-94
5	6	14	160	78	-108
-12	7	14	86	478	-172
-9	7	14	83	497	-167
-6	7	14	193	72	-92
-3	7	14	251	254	-91
0	7	14	157	470	-73

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
3	7	14	82	218	-164
6	7	14	90	78	-179
-14	8	14	134	381	-144
-11	8	14	87	539	-174
-8	8	14	122	926	-104
-5	8	14	114	612	-105
-2	8	14	129	555	-99
1	8	14	79	165	-157
4	8	14	87	174	-175
7	8	14	189	137	-109
-16	9	14	200	291	-125
-13	9	14	224	51	-101
-10	9	14	361	80	-109
-7	9	14	297	342	-102
-4	9	14	179	490	-92
-1	9	14	78	289	-156
2	9	14	112	20	-142
5	9	14	119	117	-150
8	9	14	256	498	-95
-18	10	14	109	357	-219
-15	10	14	100	457	-201
-12	10	14	94	773	-325
-9	10	14	419	688	120
-6	10	14	155	186	-118
-3	10	14	150	34	-109
0	10	14	122	121	-114
3	10	14	88	309	-177
6	10	14	100	450	-200
-17	11	14	102	645	-204
-14	11	14	177	591	-122
-11	11	14	224	883	-88
-8	11	14	88	830	-177
-5	11	14	83	340	-166
-2	11	14	125	110	-130
1	11	14	183	187	-112
4	11	14	169	336	-125
7	11	14	249	23	-133
-16	12	14	225	232	-135
-13	12	14	262	121	-88
-10	12	14	173	84	-144
-7	12	14	86	229	-173
-4	12	14	87	220	-175
-1	12	14	193	148	-113
2	12	14	214	157	-113
5	12	14	102	296	-205
-18	13	14	279	278	-127
-15	13	14	139	218	-155
-12	13	14	276	430	-83
-9	13	14	204	151	-116
-6	13	14	89	158	-178
-3	13	14	282	90	-110
0	13	14	195	149	-93
3	13	14	100	537	-200
-17	14	14	104	269	-209
-14	14	14	117	223	-149
-11	14	14	259	256	-79
-8	14	14	118	37	-153
-5	14	14	157	132	-126
-2	14	14	93	68	-186
1	14	14	101	288	-203
4	14	14	109	276	-219
-16	15	14	229	78	-104
-13	15	14	100	276	-200
-10	15	14	150	215	-153
-7	15	14	139	48	-141
-4	15	14	97	25	-194
-1	15	14	195	29	-134
2	15	14	144	192	-178
-15	16	14	194	247	-142
-12	16	14	104	233	-208
-9	16	14	261	164	-93
-6	16	14	256	315	-117
-3	16	14	100	105	-201
0	16	14	216	212	-114
-14	17	14	218	89	-134
-11	17	14	226	283	-108
-8	17	14	193	437	-134
-5	17	14	103	403	-207
-2	17	14	107	51	-215
-13	18	14	108	355	-216
-10	18	14	148	291	-178
-7	18	14	239	277	-122
-4	18	14	314	245	84
0	0	15	133	637	-98
1	1	15	96	123	-96
-1	2	15	106	294	-89
2	2	15	283	286	58
-3	3	15	66	131	-115
0	3	15	115	235	-83
3	3	15	221	550	-68
-5	4	15	72	117	-145
-2	4	15	223	293	-81

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
1	4	15	274	37	-92
4	4	15	168	502	-74
-7	5	15	420	290	30
-4	5	15	147	533	-103
-1	5	15	262	395	58
2	5	15	241	207	-87
5	5	15	239	91	62
-9	6	15	175	203	-76
-6	6	15	115	49	-97
-3	6	15	187	806	-72
0	6	15	111	175	-98
3	6	15	127	178	-114
6	6	15	85	174	-170
-11	7	15	104	414	-146
-8	7	15	76	244	-151
-5	7	15	444	536	73
-2	7	15	115	618	-97
1	7	15	201	104	-64
4	7	15	236	325	-77
7	7	15	89	73	-179
-13	8	15	91	139	-183
-10	8	15	286	129	69
-7	8	15	75	140	-151
-4	8	15	108	76	-106
-1	8	15	117	81	-106
2	8	15	163	198	-82
5	8	15	88	263	-176
8	8	15	279	82	-94
-15	9	15	232	46	-119
-12	9	15	88	324	-307
-9	9	15	84	251	-145
-6	9	15	185	454	-88
-3	9	15	180	638	-77
0	9	15	164	217	-94
3	9	15	120	386	-167
6	9	15	198	147	-106
9	9	15	107	196	-215
-17	10	15	155	236	-150
-14	10	15	198	18	-118
-11	10	15	268	322	-102
-8	10	15	150	180	-117
-5	10	15	257	324	74
-2	10	15	81	210	-163
1	10	15	124	15	-134
4	10	15	227	23	-112
7	10	15	162	308	-144
-16	11	15	249	84	-103
-13	11	15	95	225	-191
-10	11	15	232	84	-82
-7	11	15	85	351	-171
-4	11	15	251	487	-77
-1	11	15	85	167	-170
2	11	15	230	240	-92
5	11	15	269	14	-118
-18	12	15	246	170	-133
-15	12	15	180	102	-128
-12	12	15	169	460	-104
-9	12	15	89	461	-219
-6	12	15	210	334	-100
-3	12	15	88	345	-304
0	12	15	89	295	-155
3	12	15	193	97	-128
6	12	15	200	163	-124
-17	13	15	162	158	-153
-14	13	15	208	15	-123
-11	13	15	97	360	-194
-8	13	15	150	163	-134
-5	13	15	87	246	-175
-2	13	15	118	103	-147
1	13	15	189	168	-108
4	13	15	242	71	-127
-16	14	15	102	16	-205
-13	14	15	182	200	-118
-10	14	15	247	230	-113
-7	14	15	160	345	-122
-4	14	15	136	352	-139
-1	14	15	97	320	-194
2	14	15	104	105	-208
-15	15	15	102	36	-177
-12	15	15	182	322	-133
-9	15	15	266	152	-109
-6	15	15	241	8	-87
-3	15	15	96	158	-193
0	15	15	197	13	-121
-14	16	15	103	44	-207
-11	16	15	207	34	-133
-8	16	15	102	205	-205
-5	16	15	135	302	-156
-2	16	15	139	268	-164
-13	17	15	102	280	-205
-10	17	15	98	269	-197
-7	17	15	147	221	-154

Table 54. (cont).
F(obs), F(calc), and σ_F

($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-4	17	15	105	381	-211
-12	18	15	264	151	-130
-9	18	15	108	24	-217
-6	18	15	225	28	-135
-1	1	16	1258	1743	9
-3	2	16	1205	794	36
0	2	16	6076	5132	103
-5	3	16	1122	1019	28
-2	3	16	1206	886	28
1	3	16	2738	2721	41
-7	4	16	2821	2782	29
-4	4	16	1334	1636	13
-1	4	16	2752	2746	60
2	4	16	1974	1936	18
-9	5	16	2222	2222	21
-6	5	16	1764	1563	36
-3	5	16	1134	959	23
0	5	16	1602	1692	16
3	5	16	379	138	27
-11	6	16	1418	1508	22
-8	6	16	1319	1344	32
-5	6	16	1770	1556	30
-2	6	16	1985	1924	40
1	6	16	1831	1717	26
4	6	16	1980	1943	13
-13	7	16	874	985	62
-10	7	16	3850	3853	28
-7	7	16	3942	4043	31
-4	7	16	2838	2875	45
-1	7	16	1842	1728	15
2	7	16	1394	1498	16
5	7	16	416	347	27
-15	8	16	163	146	-64
-12	8	16	711	670	23
-9	8	16	2378	2354	5
-6	8	16	1334	1206	20
-3	8	16	362	250	19
0	8	16	321	426	23
3	8	16	194	244	49
6	8	16	300	179	38
-17	9	16	87	40	-124
-14	9	16	882	812	24
-11	9	16	2503	2491	24
-8	9	16	2350	2353	68
-5	9	16	2190	2126	4
-2	9	16	1399	1473	22
1	9	16	741	721	16
4	9	16	101	25	-90
7	9	16	162	13	-72
-19	10	16	226	197	64
-16	10	16	413	520	42
-13	10	16	2074	2166	49
-10	10	16	4863	4835	42
-7	10	16	3860	3899	46
-4	10	16	1994	1998	25
-1	10	16	748	696	17
2	10	16	473	433	23
5	10	16	357	272	33
8	10	16	313	218	43
-21	11	16	212	107	-83
-18	11	16	373	295	64
-15	11	16	834	787	29
-12	11	16	1529	1555	16
-9	11	16	2515	2477	29
-6	11	16	1429	1448	25
-3	11	16	219	215	44
0	11	16	193	92	52
3	11	16	603	705	24
6	11	16	450	521	32
9	11	16	193	19	-85
-23	12	16	111	4	-152
-20	12	16	85	68	-170
-17	12	16	233	250	48
-14	12	16	359	272	53
-11	12	16	1540	1521	17
-8	12	16	691	653	29
-5	12	16	428	377	27
-2	12	16	496	430	33
1	12	16	288	227	38
4	12	16	537	480	25
7	12	16	200	137	-79
10	12	16	204	118	-86
-22	13	16	173	211	-119
-19	13	16	84	19	-168
-16	13	16	237	268	-70
-13	13	16	1308	1348	31
-10	13	16	2103	2121	43
-7	13	16	896	987	61
-4	13	16	139	8	-75
-1	13	16	343	235	37
2	13	16	639	514	23
5	13	16	353	299	47

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
8	13	16	171	32	-114
11	13	16	202	127	-92
-24	14	16	228	248	-91
-21	14	16	343	342	38
-18	14	16	166	154	-93
-15	14	16	437	416	37
-12	14	16	338	310	30
-9	14	16	886	791	19
-6	14	16	278	167	35
-3	14	16	615	676	19
0	14	16	833	927	15
3	14	16	868	948	25
6	14	16	351	324	67
9	14	16	223	23	-101
-23	15	16	195	87	-113
-20	15	16	155	71	-117
-17	15	16	171	156	-86
-14	15	16	440	433	28
-11	15	16	818	785	21
-8	15	16	239	175	44
-5	15	16	390	279	36
-2	15	16	614	507	27
1	15	16	523	468	36
4	15	16	291	319	65
7	15	16	170	127	-105
-22	16	16	92	274	-184
-19	16	16	141	42	-125
-16	16	16	185	118	-70
-13	16	16	256	256	54
-10	16	16	468	492	27
-7	16	16	177	35	-71
-4	16	16	530	484	33
-1	16	16	560	492	26
2	16	16	458	451	56
5	16	16	202	129	-87
8	16	16	158	44	-126
-24	17	16	284	296	69
-21	17	16	332	308	68
-18	17	16	85	40	-171
-15	17	16	245	164	64
-12	17	16	196	249	-61
-9	17	16	148	11	-75
-6	17	16	453	522	57
-3	17	16	843	932	29
0	17	16	888	915	26
3	17	16	574	551	33
6	17	16	236	116	-113
-23	18	16	114	74	-159
-20	18	16	202	111	-89
-17	18	16	138	80	-114
-14	18	16	204	200	-69
-11	18	16	359	310	48
-8	18	16	307	239	49
-5	18	16	354	311	40
-2	18	16	430	429	56
1	18	16	315	306	40
4	18	16	234	137	-94
-22	19	16	225	132	-86
-19	19	16	220	88	-69
-16	19	16	150	43	-119
-13	19	16	143	23	-120
-10	19	16	240	178	-86
-7	19	16	133	135	-114
-4	19	16	247	325	70
-1	19	16	355	351	43
2	19	16	269	242	-79
-21	20	16	135	63	-137
-18	20	16	223	86	-108
-15	20	16	164	46	-113
-12	20	16	83	66	-167
-9	20	16	194	21	-104
-6	20	16	352	330	52
-3	20	16	565	559	35
0	20	16	482	486	40
-20	21	16	162	61	-121
-17	21	16	354	290	58
-14	21	16	341	335	38
-11	21	16	153	117	-121
-8	21	16	87	26	-175
-5	21	16	154	144	-129
-2	21	16	245	215	-106
1	21	16	224	121	-96
-19	22	16	163	166	-112
-16	22	16	336	320	92
-13	22	16	267	242	-103
-10	22	16	135	137	-134
-7	22	16	175	139	-103
-4	22	16	121	155	-149
-1	22	16	200	144	-89
-18	23	16	242	17	-112
-15	23	16	91	32	-181
-12	23	16	166	28	-105

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-9	23	16	91	52	-182
-6	23	16	250	155	-84
-17	24	16	314	280	77
-14	24	16	261	222	-81
-11	24	16	159	92	-130
-8	24	16	91	1	-183
0	1	17	134	574	-57
-2	2	17	120	117	-65
1	2	17	98	495	-93
-4	3	17	69	106	-139
-1	3	17	164	621	-62
2	3	17	166	213	-66
-6	4	17	74	408	-148
-3	4	17	83	12	-116
0	4	17	222	142	-72
3	4	17	235	269	66
-8	5	17	124	334	-95
-5	5	17	84	283	-107
-2	5	17	233	160	-72
1	5	17	73	13	-146
4	5	17	100	499	-135
-10	6	17	274	389	-96
-7	6	17	187	61	-90
-4	6	17	116	466	-107
-1	6	17	170	933	-86
2	6	17	203	31	-81
5	6	17	156	40	-103
-12	7	17	270	234	66
-9	7	17	83	514	-166
-6	7	17	76	372	-152
-3	7	17	163	58	-65
0	7	17	72	25	-125
3	7	17	111	243	-133
6	7	17	147	174	-114
-14	8	17	219	59	-109
-11	8	17	199	186	-94
-8	8	17	209	113	-82
-5	8	17	186	302	-86
-2	8	17	219	72	63
1	8	17	82	11	-164
4	8	17	88	92	-306
7	8	17	148	62	-129
-16	9	17	98	87	-197
-13	9	17	245	223	-74
-10	9	17	173	243	-126
-7	9	17	186	174	-75
-4	9	17	135	603	-112
-1	9	17	196	434	-97
2	9	17	180	131	-97
5	9	17	121	136	-151
8	9	17	101	36	-202
-18	10	17	182	217	-146
-15	10	17	130	180	-158
-12	10	17	204	27	-103
-9	10	17	239	287	-113
-6	10	17	223	234	-74
-3	10	17	176	80	-104
0	10	17	85	152	-147
3	10	17	203	5	-109
6	10	17	172	66	-136
-17	11	17	173	158	-122
-14	11	17	94	290	-188
-11	11	17	318	120	60
-8	11	17	130	268	-132
-5	11	17	126	44	-130
-2	11	17	153	89	-122
1	11	17	137	47	-146
4	11	17	204	54	-99
7	11	17	106	96	-212
-16	12	17	241	0	-124
-13	12	17	245	213	-113
-10	12	17	160	241	-131
-7	12	17	264	207	75
-4	12	17	91	24	-316
-1	12	17	205	154	-114
2	12	17	193	157	-109
5	12	17	292	58	-89
-18	13	17	107	154	-213
-15	13	17	206	171	-128
-12	13	17	195	5	-109
-9	13	17	211	230	-105
-6	13	17	121	129	-145
-3	13	17	90	73	-180
0	13	17	218	111	-107
3	13	17	217	4	-108
-17	14	17	146	46	-166
-14	14	17	97	89	-169
-11	14	17	170	51	-129
-8	14	17	198	1	-114
-5	14	17	169	93	-125
-2	14	17	172	191	-135
1	14	17	263	157	-86

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-16	15	17	144	103	-177
-13	15	17	101	32	-203
-10	15	17	177	215	-121
-7	15	17	236	11	-97
-4	15	17	96	84	-193
-1	15	17	101	229	-203
2	15	17	283	56	-102
-15	16	17	110	84	-220
-12	16	17	136	127	-166
-9	16	17	144	113	-144
-6	16	17	98	6	-195
-3	16	17	142	15	-149
0	16	17	109	40	-188
-14	17	17	152	232	-162
-11	17	17	241	181	-123
-8	17	17	100	194	-201
-5	17	17	105	25	-211
-2	17	17	233	232	-139
-13	18	17	161	230	-161
-10	18	17	105	149	-211
-7	18	17	170	57	-141
0	0	18	141	195	-76
1	1	18	168	401	-62
-1	2	18	196	1035	-78
2	2	18	294	621	-101
-3	3	18	66	24	-114
0	3	18	96	418	-90
3	3	18	76	22	-152
-5	4	18	134	215	-86
-2	4	18	178	173	-82
1	4	18	153	84	-77
4	4	18	78	631	-157
-7	5	18	190	520	-89
-4	5	18	153	181	-90
-1	5	18	72	634	-144
2	5	18	147	1140	-94
5	5	18	140	987	-123
-9	6	18	153	101	-106
-6	6	18	152	19	-83
-3	6	18	182	317	-90
0	6	18	177	161	-63
3	6	18	87	103	-173
6	6	18	89	162	-154
-11	7	18	93	685	-186
-8	7	18	179	139	-85
-5	7	18	176	222	-90
-2	7	18	72	199	-144
1	7	18	149	387	-97
4	7	18	161	908	-125
7	7	18	90	205	-180
-13	8	18	192	52	-109
-10	8	18	184	101	-116
-7	8	18	262	464	-98
-4	8	18	220	415	-95
-1	8	18	140	616	-96
2	8	18	142	965	-124
5	8	18	89	475	-179
8	8	18	168	242	-99
-15	9	18	95	201	-191
-12	9	18	145	910	-120
-9	9	18	156	815	-93
-6	9	18	134	893	-112
-3	9	18	291	607	-96
0	9	18	319	277	84
3	9	18	217	157	-128
6	9	18	131	223	-145
9	9	18	104	104	-209
-17	10	18	101	251	-203
-14	10	18	126	364	-151
-11	10	18	99	594	-345
-8	10	18	323	426	88
-5	10	18	207	351	-94
-2	10	18	128	322	-119
1	10	18	217	633	-92
4	10	18	184	276	-109
7	10	18	154	144	-154
-16	11	18	103	164	-206
-13	11	18	223	126	-106
-10	11	18	299	118	79
-7	11	18	265	583	-112
-4	11	18	223	20	-96
-1	11	18	90	536	-313
2	11	18	97	382	-194
5	11	18	101	470	-203
-18	12	18	171	29	-154
-15	12	18	135	222	-158
-12	12	18	92	687	-160
-9	12	18	298	594	-109
-6	12	18	89	608	-154
-3	12	18	294	422	-115
0	12	18	214	233	-116
3	12	18	187	235	-117

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
6	12	18	154	112	-163
-17	13	18	104	4	-209
-14	13	18	271	62	-85
-11	13	18	133	164	-161
-8	13	18	92	131	-184
-5	13	18	185	325	-94
-2	13	18	155	418	-136
1	13	18	197	142	-129
4	13	18	109	158	-218
-16	14	18	251	183	-127
-13	14	18	168	414	-137
-10	14	18	248	327	-96
-7	14	18	111	284	-157
-4	14	18	95	180	-190
-1	14	18	130	242	-165
2	14	18	107	401	-214
-15	15	18	248	37	-101
-12	15	18	285	276	-118
-9	15	18	215	182	-108
-6	15	18	94	179	-189
-3	15	18	125	1	-167
0	15	18	180	378	-117
-14	16	18	346	454	-132
-11	16	18	102	227	-205
-8	16	18	178	207	-91
-5	16	18	151	44	-155
-2	16	18	132	178	-175
-13	17	18	251	577	-92
-10	17	18	151	411	-155
-7	17	18	101	290	-203
-4	17	18	197	118	-145
-12	18	18	287	310	-91
-9	18	18	176	203	-136
-6	18	18	135	105	-172
-1	1	19	185	216	-58
-3	2	19	99	130	-105
0	2	19	116	31	-66
-5	3	19	140	156	-84
-2	3	19	149	286	-64
1	3	19	215	16	-76
-7	4	19	134	74	-95
-4	4	19	73	109	-126
-1	4	19	136	194	-89
2	4	19	195	465	-84
-9	5	19	128	308	-123
-6	5	19	192	466	-77
-3	5	19	226	292	61
0	5	19	179	228	-71
3	5	19	118	259	-114
-11	6	19	242	329	-80
-8	6	19	131	96	-110
-5	6	19	135	383	-93
-2	6	19	146	112	-88
1	6	19	275	287	42
4	6	19	83	525	-166
-13	7	19	141	213	-129
-10	7	19	215	230	-78
-7	7	19	280	201	53
-4	7	19	165	95	-76
-1	7	19	199	74	-59
2	7	19	225	135	-75
5	7	19	93	115	-323
-15	8	19	95	147	-191
-12	8	19	87	414	-303
-9	8	19	82	262	-164
-6	8	19	98	462	-130
-3	8	19	76	465	-153
0	8	19	180	443	-90
3	8	19	150	87	-130
6	8	19	211	146	-94
-17	9	19	164	40	-138
-14	9	19	193	375	-119
-11	9	19	240	340	-72
-8	9	19	160	7	-110
-5	9	19	170	120	-84
-2	9	19	208	14	-72
1	9	19	238	414	-77
4	9	19	117	242	-151
7	9	19	164	53	-132
-16	10	19	161	14	-134
-13	10	19	174	25	-123
-10	10	19	456	71	52
-7	10	19	172	253	-97
-4	10	19	154	223	-112
-1	10	19	310	272	51
2	10	19	180	252	-107
5	10	19	136	69	-149
8	10	19	178	187	-147
-18	11	19	106	151	-212
-15	11	19	172	268	-139
-12	11	19	206	373	-81
-9	11	19	143	275	-120

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-6	11	19	245	528	69
-3	11	19	139	592	-137
0	11	19	201	168	-112
3	11	19	136	65	-153
6	11	19	168	91	-137
-17	12	19	267	35	-126
-14	12	19	138	151	-144
-11	12	19	231	128	-113
-8	12	19	182	66	-145
-5	12	19	93	78	-323
-2	12	19	130	28	-150
1	12	19	96	180	-192
4	12	19	102	81	-205
-16	13	19	105	191	-210
-13	13	19	243	80	-90
-10	13	19	115	40	-157
-7	13	19	148	109	-124
-4	13	19	217	172	-93
-1	13	19	205	87	-101
2	13	19	231	109	-111
-15	14	19	154	290	-156
-12	14	19	124	201	-156
-9	14	19	174	27	-111
-6	14	19	93	236	-186
-3	14	19	180	148	-116
0	14	19	196	96	-93
3	14	19	240	2	-112
-14	15	19	200	32	-138
-11	15	19	241	9	-97
-8	15	19	209	73	-102
-5	15	19	215	69	-99
-2	15	19	158	101	-144
1	15	19	167	200	-159
-16	16	19	254	150	-131
-13	16	19	179	3	-151
-10	16	19	152	157	-139
-7	16	19	99	11	-199
-4	16	19	267	48	-92
-1	16	19	228	8	-112
-12	17	19	155	130	-156
-9	17	19	102	200	-204
-6	17	19	150	94	-161
-3	17	19	175	96	-154
-11	18	19	105	41	-210
-8	18	19	215	169	-135
0	1	20	161	182	34
-2	2	20	155	127	35
1	2	20	3203	2914	38
-4	3	20	3234	3213	42
-1	3	20	3221	3079	73
2	3	20	1415	1732	31
-6	4	20	1920	1647	20
-3	4	20	3227	2930	42
0	4	20	123	7	-51
3	4	20	946	707	11
-8	5	20	3487	3629	6
-5	5	20	97	107	-49
-2	5	20	1412	1659	30
1	5	20	1291	1308	15
4	5	20	2995	2894	21
-10	6	20	849	776	16
-7	6	20	1422	1199	23
-4	6	20	1921	1787	31
-1	6	20	1291	1293	17
2	6	20	3165	3234	23
5	6	20	2209	2232	16
-12	7	20	890	920	34
-9	7	20	707	685	19
-6	7	20	1444	1271	29
-3	7	20	952	794	13
0	7	20	132	7	-50
3	7	20	528	542	18
6	7	20	241	233	48
-14	8	20	265	214	36
-11	8	20	533	596	24
-8	8	20	84	34	-75
-5	8	20	3592	3520	53
-2	8	20	3173	3246	47
1	8	20	3973	3969	40
4	8	20	2744	2731	48
7	8	20	140	24	-83
-16	9	20	341	326	36
-13	9	20	337	302	27
-10	9	20	221	214	60
-7	9	20	683	714	18
-4	9	20	2995	2833	30
-1	9	20	3987	3851	47
2	9	20	2829	2810	23
5	9	20	853	865	27
8	9	20	234	224	56
-18	10	20	239	67	-90
-15	10	20	530	539	27

Table 54. (cont).
F(obs), F(calc), and σ_F

($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-12	10	20	198	204	48
-9	10	20	258	201	33
-6	10	20	858	777	23
-3	10	20	535	600	19
0	10	20	118	7	-82
3	10	20	285	344	44
6	10	20	410	412	30
9	10	20	149	21	-99
-20	11	20	86	65	-172
-17	11	20	165	97	-93
-14	11	20	444	459	28
-11	11	20	133	18	-60
-8	11	20	532	549	33
-5	11	20	2235	2266	26
-2	11	20	2842	2927	31
1	11	20	2335	2363	39
4	11	20	632	595	39
7	11	20	183	17	-76
10	11	20	142	36	-83
-22	12	20	89	103	-179
-19	12	20	156	180	-101
-16	12	20	620	632	27
-13	12	20	144	100	-77
-10	12	20	236	246	47
-7	12	20	900	924	21
-4	12	20	2746	2648	27
-1	12	20	2318	2298	34
2	12	20	969	970	28
5	12	20	417	420	34
8	12	20	266	163	68
11	12	20	264	261	-87
-24	13	20	93	110	-186
-21	13	20	197	118	-65
-18	13	20	289	352	53
-15	13	20	897	894	33
-12	13	20	156	130	-85
-9	13	20	290	277	49
-6	13	20	238	286	49
-3	13	20	315	367	32
0	13	20	160	26	-72
3	13	20	308	284	68
6	13	20	139	4	-118
9	13	20	294	246	-110
-23	14	20	160	146	-109
-20	14	20	146	12	-111
-17	14	20	111	136	-116
-14	14	20	100	3	-98
-11	14	20	421	484	30
-8	14	20	273	244	43
-5	14	20	876	887	33
-2	14	20	957	976	41
1	14	20	294	301	40
4	14	20	176	39	-86
7	14	20	182	66	-106
10	14	20	92	83	-185
-22	15	20	265	105	-77
-19	15	20	534	542	44
-16	15	20	1165	1196	34
-13	15	20	890	894	18
-10	15	20	508	527	23
-7	15	20	155	33	-78
-4	15	20	616	584	36
-1	15	20	331	302	37
2	15	20	155	188	-101
5	15	20	190	139	-98
8	15	20	346	321	77
-24	16	20	168	148	-118
-21	16	20	280	339	65
-18	16	20	775	828	40
-15	16	20	1185	1233	46
-12	16	20	606	677	29
-9	16	20	343	333	33
-6	16	20	399	398	29
-3	16	20	250	295	56
0	16	20	111	11	-117
3	16	20	183	29	-99
6	16	20	203	196	-90
-23	17	20	219	116	-94
-20	17	20	89	123	-178
-17	17	20	87	44	-151
-14	17	20	170	171	-83
-11	17	20	183	104	-80
-8	17	20	272	240	62
-5	17	20	424	428	37
-2	17	20	225	155	-77
1	17	20	148	30	-107
4	17	20	212	63	-109
-22	18	20	191	166	-102
-19	18	20	594	541	38
-16	18	20	781	794	56
-13	18	20	312	344	48
-10	18	20	159	50	-81

Table 54. (cont).
F(obs), F(calc), and σ_F

($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-7	18	20	91	45	-130
-4	18	20	83	50	-166
-1	18	20	199	34	-93
2	18	20	90	77	-180
5	18	20	286	256	-86
-21	19	20	367	379	83
-18	19	20	557	587	39
-15	19	20	565	562	36
-12	19	20	183	175	-82
-9	19	20	83	34	-167
-6	19	20	82	13	-165
-3	19	20	86	50	-171
0	19	20	160	3	-110
3	19	20	122	113	-154
-20	20	20	127	36	-127
-17	20	20	89	66	-178
-14	20	20	87	23	-173
-11	20	20	159	68	-101
-8	20	20	163	165	-97
-5	20	20	148	160	-112
-2	20	20	251	91	-104
1	20	20	156	17	-129
-19	21	20	347	350	60
-16	21	20	363	321	49
-13	21	20	167	115	-72
-10	21	20	200	45	-74
-7	21	20	122	65	-140
-4	21	20	185	54	-115
-1	21	20	111	30	-158
-18	22	20	217	174	-94
-15	22	20	260	96	-107
-12	22	20	121	109	-138
-9	22	20	302	234	-95
-6	22	20	247	201	-84
-3	22	20	93	113	-186
-17	23	20	160	121	-130
-14	23	20	197	154	-118
-11	23	20	298	274	76
-8	23	20	342	320	68
-5	23	20	260	242	-86
-16	24	20	248	162	-102
-13	24	20	222	126	-96
-10	24	20	91	98	-183
0	0	21	1001	1109	33
1	1	21	786	508	18
-1	2	21	821	929	22
2	2	21	335	691	78
-3	3	21	512	480	22
0	3	21	208	493	53
3	3	21	112	45	-105
-5	4	21	292	274	49
-2	4	21	354	299	40
1	4	21	139	238	-82
4	4	21	213	130	-86
-7	5	21	164	376	-79
-4	5	21	307	211	63
-1	5	21	240	333	58
2	5	21	138	360	-89
5	5	21	187	271	-83
-9	6	21	81	69	-163
-6	6	21	182	65	-60
-3	6	21	172	159	-72
0	6	21	229	132	49
3	6	21	151	33	-113
6	6	21	153	3	-109
-11	7	21	178	169	-94
-8	7	21	195	254	-68
-5	7	21	115	112	-111
-2	7	21	174	286	-83
1	7	21	134	225	-116
4	7	21	173	28	-102
7	7	21	117	118	-156
-13	8	21	153	212	-128
-10	8	21	156	522	-112
-7	8	21	263	83	-96
-4	8	21	239	206	67
-1	8	21	106	110	-134
2	8	21	132	168	-134
5	8	21	196	165	-115
8	8	21	234	36	-104
-15	9	21	185	318	-129
-12	9	21	169	235	-117
-9	9	21	121	102	-117
-6	9	21	82	229	-164
-3	9	21	113	424	-137
0	9	21	234	445	-71
3	9	21	135	242	-148
6	9	21	265	55	-92
9	9	21	108	140	-217
-17	10	21	107	247	-215
-14	10	21	167	175	-130
-11	10	21	201	161	-90

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-8	10	21	163	26	-97
-5	10	21	179	144	-80
-2	10	21	150	411	-123
1	10	21	272	274	-83
4	10	21	97	94	-194
7	10	21	232	76	-133
-16	11	21	103	203	-206
-13	11	21	112	369	-155
-10	11	21	210	418	-102
-7	11	21	169	468	-96
-4	11	21	144	182	-130
-1	11	21	192	47	-119
2	11	21	204	15	-121
5	11	21	162	68	-131
-15	12	21	100	514	-200
-12	12	21	93	334	-185
-9	12	21	90	539	-180
-6	12	21	87	265	-175
-3	12	21	176	260	-126
0	12	21	240	104	-110
3	12	21	223	84	-124
-17	13	21	108	231	-217
-14	13	21	182	207	-93
-11	13	21	92	207	-184
-8	13	21	191	97	-116
-5	13	21	223	46	-78
-2	13	21	232	16	-90
1	13	21	186	68	-81
4	13	21	226	26	-114
-16	14	21	182	253	-134
-13	14	21	151	131	-109
-10	14	21	226	337	-113
-7	14	21	93	252	-186
-4	14	21	96	49	-192
-1	14	21	189	53	-96
2	14	21	147	27	-169
-15	15	21	171	354	-145
-12	15	21	296	285	-126
-9	15	21	98	181	-196
-6	15	21	167	8	-135
-3	15	21	160	23	-143
0	15	21	242	10	-95
-14	16	21	109	126	-218
-11	16	21	266	59	-95
-8	16	21	245	79	-97
-5	16	21	103	99	-207
-2	16	21	169	9	-147
-13	17	21	268	170	-126
-10	17	21	166	185	-161
-7	17	21	147	26	-175
-4	17	21	106	24	-212
-9	18	21	107	158	-215
-1	1	22	413	717	37
-3	2	22	210	638	-68
0	2	22	270	425	50
-5	3	22	73	611	-146
-2	3	22	247	119	-91
1	3	22	145	502	-98
-7	4	22	75	395	-150
-4	4	22	186	710	-85
-1	4	22	119	423	-108
2	4	22	151	445	-98
-9	5	22	210	225	-77
-6	5	22	120	288	-110
-3	5	22	203	10	-85
0	5	22	92	166	-102
3	5	22	146	261	-119
-11	6	22	171	300	-107
-8	6	22	166	259	-104
-5	6	22	136	342	-94
-2	6	22	206	349	-64
1	6	22	79	284	-158
4	6	22	150	638	-100
-13	7	22	175	54	-107
-10	7	22	201	87	-102
-7	7	22	147	205	-87
-4	7	22	105	38	-120
-1	7	22	109	201	-115
2	7	22	238	441	-77
5	7	22	248	20	-89
-15	8	22	96	582	-193
-12	8	22	193	349	-94
-9	8	22	228	272	-77
-6	8	22	82	468	-164
-3	8	22	241	102	-72
0	8	22	363	283	94
3	8	22	242	298	-112
6	8	22	173	174	-116
-17	9	22	112	157	-224
-14	9	22	152	219	-144
-11	9	22	87	257	-175
-8	9	22	183	122	-99

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
-5	9	22	156	29	-98	-11	15	22	100	405	-200
-2	9	22	87	360	-174	-8	15	22	135	453	-156
1	9	22	118	789	-145	-5	15	22	160	537	-132
4	9	22	93	442	-186	-2	15	22	180	412	-140
7	9	22	192	378	-136	1	15	22	171	36	-158
-16	10	22	186	652	-141	-13	16	22	107	34	-215
-13	10	22	93	231	-185	-10	16	22	284	218	-118
-10	10	22	156	221	-122	-7	16	22	139	590	-166
-7	10	22	140	479	-109	-4	16	22	132	491	-173
-4	10	22	83	555	-167	-1	16	22	248	264	-111
-1	10	22	212	1165	-86	-12	17	22	192	273	-151
2	10	22	96	481	-193	-9	17	22	176	44	-166
5	10	22	98	74	-197	-6	17	22	112	24	-225
8	10	22	135	130	-191	-3	17	22	165	4	-159
-18	11	22	110	390	-220	-11	18	22	196	369	-145
-15	11	22	100	694	-200	-8	18	22	223	479	-143
-12	11	22	91	429	-182	0	1	23	149	96	-74
-9	11	22	87	467	-175	-2	2	23	226	226	55
-6	11	22	255	668	-75	1	2	23	154	382	-93
-3	11	22	241	638	-104	-4	3	23	182	182	-91
0	11	22	375	257	99	-1	3	23	145	190	-88
3	11	22	188	69	-117	2	3	23	118	420	-105
6	11	22	111	294	-223	-6	4	23	125	102	-94
-17	12	22	343	77	-131	-3	4	23	94	61	-131
-14	12	22	96	299	-192	0	4	23	122	352	-83
-11	12	22	163	271	-127	3	4	23	148	226	-98
-8	12	22	88	98	-177	-8	5	23	79	121	-159
-5	12	22	117	108	-150	-5	5	23	158	318	-75
-2	12	22	125	468	-155	-2	5	23	124	169	-92
1	12	22	185	302	-128	1	5	23	150	154	-79
4	12	22	226	153	-127	4	5	23	206	123	-75
-16	13	22	284	304	-126	-10	6	23	195	24	-103
-13	13	22	149	168	-130	-7	6	23	159	40	-80
-10	13	22	166	108	-129	-4	6	23	74	146	-149
-7	13	22	90	157	-180	-1	6	23	99	320	-117
-4	13	22	223	662	-94	2	6	23	173	359	-101
-1	13	22	179	564	-116	5	6	23	129	63	-124
2	13	22	101	117	-203	-12	7	23	88	97	-176
-15	14	22	167	27	-151	-9	7	23	151	104	-111
-12	14	22	181	278	-116	-6	7	23	217	256	-68
-9	14	22	231	175	-102	-3	7	23	112	299	-106
-6	14	22	200	221	-121	0	7	23	146	275	-82
-3	14	22	304	19	-94	3	7	23	134	324	-114
0	14	22	209	69	-103	6	7	23	236	237	-91
3	14	22	265	214	-129	-14	8	23	247	185	-108
-14	15	22	106	196	-212	-11	8	23	227	19	-120

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-8	8	23	231	31	-87
-5	8	23	151	34	-103
-2	8	23	110	96	-129
1	8	23	212	12	-107
4	8	23	91	94	-182
7	8	23	99	207	-198
-16	9	23	104	14	-209
-13	9	23	244	52	-100
-10	9	23	173	131	-108
-7	9	23	80	155	-161
-4	9	23	179	163	-92
-1	9	23	184	423	-95
2	9	23	92	416	-184
5	9	23	98	331	-196
8	9	23	112	168	-225
-18	10	23	153	47	-172
-15	10	23	100	16	-142
-12	10	23	235	280	-93
-9	10	23	212	31	-102
-6	10	23	102	318	-143
-3	10	23	176	196	-100
0	10	23	185	312	-89
3	10	23	93	548	-186
6	10	23	140	160	-168
-17	11	23	255	85	-114
-14	11	23	191	82	-116
-11	11	23	180	222	-105
-8	11	23	123	255	-211
-5	11	23	158	70	-118
-2	11	23	152	16	-116
1	11	23	156	87	-143
4	11	23	145	22	-154
-16	12	23	104	113	-209
-13	12	23	143	39	-143
-10	12	23	92	179	-184
-7	12	23	122	259	-139
-4	12	23	202	175	-112
-1	12	23	179	244	-116
2	12	23	173	339	-140
5	12	23	174	69	-145
-15	13	23	102	159	-204
-12	13	23	95	214	-191
-9	13	23	115	1	-155
-6	13	23	283	132	-106
-3	13	23	113	83	-163
0	13	23	202	263	-97
3	13	23	105	199	-211
-14	14	23	162	270	-131
-11	14	23	98	346	-197
-8	14	23	213	227	-122
-5	14	23	137	42	-154
-2	14	23	208	108	-124
1	14	23	297	28	-87
-16	15	23	249	199	-124
-13	15	23	286	103	-114
-10	15	23	172	131	-95
-7	15	23	98	87	-197
-4	15	23	230	94	-120
-1	15	23	102	3	-205
-15	16	23	111	61	-223
-12	16	23	290	161	-124
-9	16	23	168	177	-148
-6	16	23	105	118	-210
-3	16	23	104	80	-209
-11	17	23	171	220	-169
-8	17	23	165	186	-175
-5	17	23	246	3	-137
-10	18	23	110	1	-220
0	0	24	3657	4157	32
1	1	24	2021	1983	26
-1	2	24	2020	2032	31
2	2	24	5493	5232	151
-3	3	24	6380	6112	81
0	3	24	6895	6513	152
3	3	24	4177	3993	47
-5	4	24	1203	1249	13
-2	4	24	5466	5056	153
1	4	24	1436	1499	20
4	4	24	531	429	16
-7	5	24	1810	1728	41
-4	5	24	1212	1242	26
-1	5	24	1434	1514	21
2	5	24	1619	1609	17
5	5	24	438	548	21
-9	6	24	163	37	-81
-6	6	24	1039	1094	15
-3	6	24	4189	4108	78
0	6	24	1648	1691	14
3	6	24	189	53	51
6	6	24	341	223	27
-11	7	24	107	80	-92
-8	7	24	497	514	19

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-5	7	24	1832	1708	3
-2	7	24	1612	1550	20
1	7	24	293	240	29
4	7	24	132	85	-88
7	7	24	1443	1524	16
-13	8	24	651	593	23
-10	8	24	282	331	42
-7	8	24	506	516	23
-4	8	24	545	460	17
-1	8	24	314	248	33
2	8	24	591	648	25
5	8	24	539	459	22
8	8	24	731	733	28
-15	9	24	868	836	18
-12	9	24	329	266	29
-9	9	24	1313	1247	19
-6	9	24	150	14	-60
-3	9	24	156	24	-66
0	9	24	1145	1166	12
3	9	24	338	311	30
6	9	24	937	919	20
9	9	24	844	868	53
-17	10	24	1483	1492	31
-14	10	24	1320	1320	20
-11	10	24	589	610	22
-8	10	24	305	325	44
-5	10	24	436	514	27
-2	10	24	602	622	24
1	10	24	430	403	27
4	10	24	1361	1359	23
7	10	24	1569	1605	43
10	10	24	727	717	47
-19	11	24	333	325	75
-16	11	24	619	660	38
-13	11	24	597	625	26
-10	11	24	584	617	20
-7	11	24	175	82	-100
-4	11	24	160	84	-76
-1	11	24	449	405	31
2	11	24	686	684	22
5	11	24	765	740	21
8	11	24	393	382	56
11	11	24	259	321	-88
-21	12	24	236	180	-74
-18	12	24	601	617	41
-15	12	24	360	341	35
-12	12	24	165	83	-60
-9	12	24	301	243	37
-6	12	24	358	249	26
-3	12	24	352	330	29
0	12	24	247	240	36
3	12	24	207	189	58
6	12	24	585	607	31
9	12	24	215	128	-80
12	12	24	92	36	-185
-23	13	24	253	290	-78
-20	13	24	489	498	52
-17	13	24	787	781	42
-14	13	24	423	427	31
-11	13	24	626	588	39
-8	13	24	625	590	34
-5	13	24	558	487	23
-2	13	24	704	691	31
1	13	24	176	256	-61
4	13	24	776	792	25
7	13	24	505	500	48
10	13	24	339	274	67
-22	14	24	238	216	-101
-19	14	24	116	100	-137
-16	14	24	233	146	-78
-13	14	24	441	421	29
-10	14	24	1318	1316	26
-7	14	24	1451	1522	20
-4	14	24	1352	1356	24
-1	14	24	260	221	52
2	14	24	255	254	50
5	14	24	218	94	-100
8	14	24	287	254	64
-24	15	24	124	40	-149
-21	15	24	220	119	-100
-18	15	24	363	331	44
-15	15	24	277	311	42
-12	15	24	395	341	33
-9	15	24	867	860	21
-6	15	24	951	929	22
-3	15	24	234	187	53
0	15	24	184	59	-72
3	15	24	372	278	76
6	15	24	89	65	-179
9	15	24	163	1	-125
-23	16	24	173	163	-111
-20	16	24	239	164	-94

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-17	16	24	273	210	-100
-14	16	24	145	138	-96
-11	16	24	538	633	129
-8	16	24	748	728	31
-5	16	24	780	765	21
-2	16	24	267	221	54
1	16	24	194	163	-105
4	16	24	129	89	-137
7	16	24	175	145	-115
-22	17	24	169	76	-121
-19	17	24	182	57	-88
-16	17	24	247	254	-86
-13	17	24	762	796	29
-10	17	24	1494	1495	52
-7	17	24	1563	1591	26
-4	17	24	762	765	25
-1	17	24	200	127	-86
2	17	24	157	85	-110
5	17	24	91	70	-183
-21	18	24	138	3	-135
-18	18	24	139	158	-76
-15	18	24	304	366	54
-12	18	24	643	658	39
-9	18	24	849	893	36
-6	18	24	559	588	32
-3	18	24	321	278	64
0	18	24	220	152	53
3	18	24	90	22	-180
-20	19	24	89	15	-178
-17	19	24	136	40	-130
-14	19	24	84	58	-168
-11	19	24	278	290	75
-8	19	24	308	378	60
-5	19	24	87	92	-174
-2	19	24	164	119	-120
1	19	24	194	17	-98
-19	20	24	89	10	-179
-16	20	24	229	179	-74
-13	20	24	505	501	39
-10	20	24	760	715	30
-7	20	24	494	460	41
-4	20	24	208	72	-96
-1	20	24	139	42	-134
-21	21	24	211	91	-88
-18	21	24	135	0	-136
-15	21	24	229	146	-71
-12	21	24	221	198	-101
-9	21	24	235	120	-93
-6	21	24	164	42	-123
-3	21	24	137	20	-134
0	21	24	191	137	-98
-17	22	24	123	78	-146
-14	22	24	221	202	-84
-11	22	24	293	329	61
-8	22	24	303	258	-117
-5	22	24	257	78	-106
-16	23	24	218	170	-108
-13	23	24	299	298	66
-10	23	24	300	280	66
-7	23	24	250	145	-99
-15	24	24	92	47	-184
-12	24	24	93	43	-186
-9	24	24	92	16	-184
-1	1	25	145	36	-72
-3	2	25	261	84	72
0	2	25	210	79	-63
-5	3	25	147	324	-96
-2	3	25	138	50	-100
1	3	25	162	376	-74
-7	4	25	126	740	-114
-4	4	25	94	260	-106
-1	4	25	128	402	-89
2	4	25	155	220	-96
-9	5	25	179	5	-95
-6	5	25	75	87	-151
-3	5	25	105	38	-116
0	5	25	154	24	-85
3	5	25	79	388	-159
-11	6	25	89	412	-309
-8	6	25	229	729	-69
-5	6	25	169	324	-84
-2	6	25	75	29	-150
1	6	25	148	128	-94
4	6	25	84	261	-169
-13	7	25	174	174	-123
-10	7	25	108	468	-140
-7	7	25	135	440	-85
-4	7	25	111	116	-120
-1	7	25	213	17	-94
2	7	25	84	215	-167
5	7	25	89	245	-177
-15	8	25	139	187	-112

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-12	8	25	196	106	-96
-9	8	25	173	338	-109
-6	8	25	132	36	-106
-3	8	25	128	245	-108
0	8	25	180	316	-97
3	8	25	88	498	-176
6	8	25	255	427	-118
-17	9	25	261	412	-119
-14	9	25	127	329	-166
-11	9	25	122	514	-146
-8	9	25	87	342	-174
-5	9	25	230	97	-97
-2	9	25	146	212	-116
1	9	25	89	255	-217
4	9	25	118	234	-155
7	9	25	194	212	-139
-16	10	25	105	213	-211
-13	10	25	173	266	-129
-10	10	25	88	27	-152
-7	10	25	155	28	-114
-4	10	25	176	12	-93
-1	10	25	88	28	-304
2	10	25	162	161	-129
5	10	25	101	136	-202
-15	11	25	166	12	-148
-12	11	25	220	306	-87
-9	11	25	134	399	-141
-6	11	25	171	98	-164
-3	11	25	176	22	-98
0	11	25	159	263	-116
3	11	25	273	385	-94
6	11	25	112	354	-225
-17	12	25	304	202	-110
-14	12	25	169	255	-129
-11	12	25	328	141	93
-8	12	25	155	17	-115
-5	12	25	89	113	-178
-2	12	25	92	294	-184
1	12	25	149	307	-142
4	12	25	107	261	-214
-16	13	25	147	166	-165
-13	13	25	120	105	-106
-10	13	25	205	361	-119
-7	13	25	92	229	-185
-4	13	25	92	323	-184
-1	13	25	94	189	-189
2	13	25	139	100	-167
-15	14	25	190	120	-142
-12	14	25	241	318	-126
-9	14	25	269	416	-123
-6	14	25	197	461	-108
-3	14	25	221	271	-102
0	14	25	188	17	-100
-14	15	25	254	46	-100
-11	15	25	103	34	-205
-8	15	25	204	270	-86
-5	15	25	101	140	-203
-2	15	25	219	74	-110
-13	16	25	106	98	-212
-10	16	25	190	46	-142
-7	16	25	218	41	-138
-4	16	25	234	19	-120
-12	17	25	234	51	-119
-9	17	25	253	109	-138
-6	17	25	331	2	-100
0	1	26	109	134	-97
-2	2	26	162	177	-67
1	2	26	185	193	-72
-4	3	26	189	261	-75
-1	3	26	181	70	-89
2	3	26	153	420	-94
-6	4	26	222	294	-66
-3	4	26	159	391	-78
0	4	26	186	798	-80
3	4	26	77	262	-154
-8	5	26	147	223	-114
-5	5	26	137	378	-79
-2	5	26	186	607	-85
1	5	26	153	285	-91
4	5	26	141	129	-106
-10	6	26	198	313	-103
-7	6	26	103	148	-130
-4	6	26	111	81	-121
-1	6	26	172	327	-80
2	6	26	126	171	-123
5	6	26	88	222	-177
-12	7	26	175	42	-112
-9	7	26	89	369	-178
-6	7	26	129	382	-102
-3	7	26	106	682	-126
0	7	26	155	342	-88
3	7	26	147	30	-118

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
6	7	26	93	16	-187
-14	8	26	152	128	-142
-11	8	26	144	475	-143
-8	8	26	254	178	-93
-5	8	26	189	170	-98
-2	8	26	235	30	-79
1	8	26	191	21	-88
4	8	26	235	100	-112
7	8	26	208	437	-112
-16	9	26	104	457	-209
-13	9	26	95	542	-190
-10	9	26	217	1007	-97
-7	9	26	240	608	-108
-4	9	26	86	599	-172
-1	9	26	164	408	-97
2	9	26	89	104	-178
5	9	26	136	369	-159
8	9	26	306	142	-102
-15	10	26	103	385	-206
-12	10	26	128	369	-156
-9	10	26	134	701	-128
-6	10	26	85	902	-171
-3	10	26	184	572	-97
0	10	26	227	319	-79
3	10	26	239	381	-94
6	10	26	184	100	-151
-17	11	26	252	71	-107
-14	11	26	219	165	-119
-11	11	26	326	290	80
-8	11	26	260	252	-101
-5	11	26	131	224	-137
-2	11	26	157	193	-124
1	11	26	148	146	-140
4	11	26	101	422	-203
-16	12	26	243	387	-125
-13	12	26	216	498	-121
-10	12	26	98	535	-196
-7	12	26	361	270	-117
-4	12	26	90	9	-181
-1	12	26	92	22	-185
2	12	26	139	492	-143
5	12	26	198	382	-152
-15	13	26	102	177	-205
-12	13	26	98	92	-197
-9	13	26	137	347	-146
-6	13	26	298	133	-111
-3	13	26	95	65	-190
0	13	26	158	385	-127
3	13	26	164	95	-167
-14	14	26	145	263	-146
-11	14	26	195	192	-118
-8	14	26	190	50	-118
-5	14	26	164	195	-143
-2	14	26	188	244	-127
1	14	26	254	232	-103
-13	15	26	212	113	-131
-10	15	26	132	57	-172
-7	15	26	247	334	-115
-4	15	26	231	416	-123
-1	15	26	214	160	-114
-12	16	26	172	292	-138
-9	16	26	105	380	-210
-6	16	26	221	440	-104
-3	16	26	109	127	-218
-11	17	26	261	398	-136
-8	17	26	292	203	-117
-5	17	26	188	57	-132
0	0	27	339	219	38
1	1	27	161	377	-70
-1	2	27	232	165	44
2	2	27	92	164	-119
-3	3	27	136	277	-78
0	3	27	123	209	-86
3	3	27	78	116	-156
-5	4	27	73	153	-146
-2	4	27	111	90	-107
1	4	27	74	304	-149
4	4	27	110	194	-137
-7	5	27	147	4	-91
-4	5	27	74	171	-148
-1	5	27	94	26	-123
2	5	27	126	38	-115
5	5	27	148	90	-119
-9	6	27	89	184	-179
-6	6	27	133	209	-90
-3	6	27	78	69	-156
0	6	27	77	60	-134
3	6	27	128	2	-125
6	6	27	91	50	-182
-11	7	27	92	113	-184
-8	7	27	219	122	-101
-5	7	27	149	206	-104

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-2	7	27	78	162	-156
1	7	27	109	3	-140
4	7	27	117	146	-146
7	7	27	235	231	-86
-13	8	27	201	236	-99
-10	8	27	89	234	-308
-7	8	27	180	173	-107
-4	8	27	120	61	-121
-1	8	27	159	140	-110
2	8	27	87	98	-301
5	8	27	136	199	-143
8	8	27	188	283	-124
-15	9	27	173	131	-140
-12	9	27	190	275	-120
-9	9	27	95	252	-233
-6	9	27	119	82	-140
-3	9	27	85	336	-170
0	9	27	87	42	-214
3	9	27	184	25	-121
6	9	27	200	79	-127
-17	10	27	172	86	-147
-14	10	27	100	82	-201
-11	10	27	143	174	-147
-8	10	27	92	343	-319
-5	10	27	86	322	-173
-2	10	27	87	413	-303
1	10	27	155	254	-133
4	10	27	160	172	-142
7	10	27	109	115	-219
-16	11	27	189	83	-131
-13	11	27	195	141	-109
-10	11	27	189	181	-115
-7	11	27	172	115	-111
-4	11	27	199	19	-81
-1	11	27	256	126	-87
2	11	27	96	90	-193
5	11	27	231	196	-136
-15	12	27	174	3	-144
-12	12	27	138	22	-144
-9	12	27	172	137	-114
-6	12	27	151	278	-131
-3	12	27	193	302	-117
0	12	27	141	95	-130
3	12	27	103	24	-207
-14	13	27	154	263	-150
-11	13	27	163	408	-144
-8	13	27	170	374	-121
-5	13	27	126	322	-150
-2	13	27	119	375	-166
1	13	27	164	116	-146
-16	14	27	139	135	-175
-13	14	27	101	203	-203
-10	14	27	162	146	-146
-7	14	27	97	24	-194
-4	14	27	195	114	-109
-1	14	27	130	67	-164
2	14	27	111	3	-222
-15	15	27	199	39	-130
-12	15	27	258	147	-121
-9	15	27	101	244	-202
-6	15	27	165	319	-129
-3	15	27	214	354	-135
0	15	27	111	140	-192
-14	16	27	107	260	-215
-11	16	27	104	297	-208
-8	16	27	227	229	-108
-5	16	27	107	176	-214
-2	16	27	111	152	-222
-10	17	27	108	22	-217
-7	17	27	158	117	-168
-1	1	28	161	10	-50
-3	2	28	1714	1718	38
0	2	28	89	34	-59
-5	3	28	1338	1353	36
-2	3	28	1711	1728	37
1	3	28	1508	1471	19
-7	4	28	234	142	34
-4	4	28	155	28	-52
-1	4	28	1518	1499	30
2	4	28	1228	1302	3
-9	5	28	2773	2698	22
-6	5	28	1929	1950	30
-3	5	28	1337	1441	32
0	5	28	163	56	-54
3	5	28	2683	2620	24
-11	6	28	2232	2234	25
-8	6	28	3023	3015	29
-5	6	28	1939	1982	29
-2	6	28	1246	1205	25
1	6	28	1073	990	24
4	6	28	420	362	37
-13	7	28	173	86	-84

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-10	7	28	406	432	27
-7	7	28	139	39	-52
-4	7	28	244	151	38
-1	7	28	1071	928	19
2	7	28	341	330	35
5	7	28	751	753	17
-15	8	28	178	58	-67
-12	8	28	2179	2204	40
-9	8	28	3347	3316	30
-6	8	28	3037	3033	44
-3	8	28	2708	2707	37
0	8	28	88	12	-84
3	8	28	384	427	25
6	8	28	181	126	-74
-17	9	28	285	247	81
-14	9	28	1036	1067	39
-11	9	28	2404	2411	29
-8	9	28	3324	3365	57
-5	9	28	2779	2666	43
-2	9	28	336	289	37
1	9	28	77	13	-109
4	9	28	252	234	39
7	9	28	373	354	42
-19	10	28	160	22	-115
-16	10	28	398	413	30
-13	10	28	193	97	55
-10	10	28	135	18	-68
-7	10	28	425	364	45
-4	10	28	408	374	52
-1	10	28	106	55	-95
2	10	28	183	32	-96
5	10	28	373	386	34
8	10	28	82	66	-165
-21	11	28	155	58	-122
-18	11	28	114	20	-134
-15	11	28	623	619	24
-12	11	28	1758	1810	35
-9	11	28	2401	2413	34
-6	11	28	2241	2216	34
-3	11	28	397	438	28
0	11	28	176	4	-59
3	11	28	341	391	35
6	11	28	190	151	-67
9	11	28	165	48	-89
-23	12	28	258	217	-82
-20	12	28	238	171	62
-17	12	28	337	367	55
-14	12	28	874	897	33
-11	12	28	1796	1822	31
-8	12	28	2177	2229	50
-5	12	28	761	754	18
-2	12	28	111	25	-100
1	12	28	235	179	48
4	12	28	451	495	39
7	12	28	143	164	-124
10	12	28	142	92	-134
-22	13	28	123	204	-151
-19	13	28	156	35	-113
-16	13	28	232	91	-75
-13	13	28	174	23	-66
-10	13	28	117	82	-88
-7	13	28	139	112	-74
-4	13	28	224	245	50
-1	13	28	224	161	52
2	13	28	810	787	25
5	13	28	259	204	61
8	13	28	88	44	-177
-21	14	28	166	55	-108
-18	14	28	102	130	-146
-15	14	28	413	441	33
-12	14	28	845	883	22
-9	14	28	1011	1060	20
-6	14	28	133	118	-82
-3	14	28	344	377	58
0	14	28	126	26	-86
3	14	28	247	191	-73
6	14	28	172	111	-118
9	14	28	161	70	-114
-23	15	28	299	236	-89
-20	15	28	130	114	-135
-17	15	28	248	162	-104
-14	15	28	435	437	39
-11	15	28	642	595	28
-8	15	28	173	53	-77
-5	15	28	367	389	33
-2	15	28	791	787	31
1	15	28	1056	1101	39
4	15	28	507	498	35
7	15	28	179	115	-123
-22	16	28	281	132	-102
-19	16	28	173	55	-115
-16	16	28	155	4	-95

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-13	16	28	93	81	-109
-10	16	28	413	426	43
-7	16	28	355	343	35
-4	16	28	461	505	65
-1	16	28	1111	1090	25
2	16	28	704	704	36
5	16	28	301	245	68
-21	17	28	254	93	-109
-18	17	28	136	12	-90
-15	17	28	198	158	-86
-12	17	28	273	348	-111
-9	17	28	246	245	65
-6	17	28	231	179	57
-3	17	28	218	193	-81
0	17	28	112	13	-132
3	17	28	90	50	-180
-20	18	28	187	164	-105
-17	18	28	119	39	-98
-14	18	28	165	78	-97
-11	18	28	148	63	-100
-8	18	28	208	68	-97
-5	18	28	254	209	61
-2	18	28	679	693	34
1	18	28	500	487	46
4	18	28	191	134	-124
-19	19	28	167	40	-103
-16	19	28	120	8	-141
-13	19	28	160	4	-113
-10	19	28	218	34	-101
-7	19	28	206	167	-80
-4	19	28	524	495	41
-1	19	28	494	472	44
2	19	28	324	283	59
-21	20	28	127	89	-150
-18	20	28	149	113	-132
-15	20	28	159	105	-110
-12	20	28	282	172	-89
-9	20	28	152	35	-87
-6	20	28	153	112	-108
-3	20	28	204	61	-91
0	20	28	92	10	-159
-20	21	28	184	115	-97
-17	21	28	127	110	-142
-14	21	28	183	97	-113
-11	21	28	176	76	-100
-8	21	28	114	59	-148
-5	21	28	268	259	77
-2	21	28	254	287	-80
-16	22	28	211	112	-111
-13	22	28	207	185	-87
-10	22	28	91	66	-182
-7	22	28	177	141	-123
-4	22	28	330	146	-116
-15	23	28	95	261	-190
-12	23	28	290	209	63
-9	23	28	92	48	-184
0	1	29	70	21	-122
-2	2	29	71	127	-123
1	2	29	95	49	-118
-4	3	29	107	32	-113
-1	3	29	71	47	-142
2	3	29	206	61	-94
-6	4	29	78	188	-156
-3	4	29	150	175	-81
0	4	29	154	285	-76
3	4	29	154	373	-87
-8	5	29	278	274	-103
-5	5	29	209	375	-65
-2	5	29	124	494	-95
1	5	29	148	220	-92
4	5	29	176	83	-106
-10	6	29	162	118	-121
-7	6	29	83	49	-167
-4	6	29	153	62	-91
-1	6	29	147	140	-91
2	6	29	86	56	-173
5	6	29	132	207	-139
-12	7	29	226	279	-114
-9	7	29	91	327	-181
-6	7	29	83	116	-167
-3	7	29	191	253	-95
0	7	29	171	383	-81
3	7	29	198	423	-110
6	7	29	143	6	-142
-14	8	29	99	97	-198
-11	8	29	224	332	-92
-8	8	29	316	447	59
-5	8	29	86	699	-173
-2	8	29	106	603	-146
1	8	29	85	466	-296
4	8	29	221	253	-97
7	8	29	99	28	-199

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-16	9	29	224	148	-128
-13	9	29	96	151	-191
-10	9	29	93	11	-186
-7	9	29	123	210	-145
-4	9	29	89	284	-177
-1	9	29	90	282	-314
2	9	29	167	34	-131
5	9	29	237	165	-114
8	9	29	130	185	-181
-15	10	29	202	247	-103
-12	10	29	130	360	-160
-9	10	29	213	150	-93
-6	10	29	110	122	-151
-3	10	29	89	97	-177
0	10	29	281	163	73
3	10	29	126	83	-167
6	10	29	257	183	-109
-14	11	29	101	58	-203
-11	11	29	135	163	-143
-8	11	29	179	343	-115
-5	11	29	216	267	-90
-2	11	29	148	196	-127
1	11	29	206	62	-125
4	11	29	233	56	-129
-16	12	29	234	235	-128
-13	12	29	222	196	-107
-10	12	29	99	66	-198
-7	12	29	171	37	-119
-4	12	29	264	1	-112
-1	12	29	194	159	-114
2	12	29	171	151	-141
-15	13	29	191	103	-124
-12	13	29	100	80	-199
-9	13	29	96	219	-193
-6	13	29	94	287	-188
-3	13	29	207	311	-104
0	13	29	140	300	-145
3	13	29	150	184	-176
-14	14	29	203	132	-127
-11	14	29	165	115	-149
-8	14	29	253	181	-116
-5	14	29	97	246	-195
-2	14	29	100	202	-200
1	14	29	141	117	-180
-13	15	29	194	7	-127
-10	15	29	101	83	-202
-7	15	29	98	85	-197
-4	15	29	103	23	-206
-1	15	29	108	118	-217
-12	16	29	210	49	-139
-9	16	29	105	2	-210
-6	16	29	138	107	-176
-3	16	29	161	205	-165
-8	17	29	259	63	-116
0	0	30	71	206	-174
1	1	30	71	521	-142
-1	2	30	71	260	-143
2	2	30	250	143	-77
-3	3	30	89	451	-115
0	3	30	198	398	-63
3	3	30	147	641	-87
-5	4	30	179	102	-94
-2	4	30	140	360	-100
1	4	30	78	383	-156
4	4	30	162	406	-117
-7	5	30	149	75	-111
-4	5	30	78	113	-156
-1	5	30	98	57	-133
2	5	30	116	56	-134
5	5	30	190	379	-113
-9	6	30	303	674	-107
-6	6	30	213	246	-69
-3	6	30	138	143	-100
0	6	30	165	373	-83
3	6	30	207	859	-107
6	6	30	93	645	-186
-11	7	30	150	6	-139
-8	7	30	137	215	-129
-5	7	30	121	438	-124
-2	7	30	83	85	-166
1	7	30	141	453	-130
4	7	30	174	370	-110
7	7	30	148	68	-110
-13	8	30	181	532	-109
-10	8	30	113	509	-152
-7	8	30	245	356	-104
-4	8	30	175	365	-93
-1	8	30	89	208	-178
2	8	30	96	380	-192
5	8	30	218	388	-101
8	8	30	288	223	-109
-15	9	30	158	285	-151

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-12	9	30	273	391	-93
-9	9	30	363	232	84
-6	9	30	297	107	76
-3	9	30	262	68	-107
0	9	30	91	673	-157
3	9	30	95	626	-190
6	9	30	100	338	-200
-14	10	30	100	220	-201
-11	10	30	194	435	-111
-8	10	30	92	606	-183
-5	10	30	90	594	-179
-2	10	30	221	2	-117
1	10	30	250	203	-116
4	10	30	172	194	-141
-16	11	30	105	224	-211
-13	11	30	153	468	-98
-10	11	30	155	600	-127
-7	11	30	94	534	-189
-4	11	30	186	437	-121
-1	11	30	276	526	-118
2	11	30	103	282	-146
5	11	30	213	103	-110
-15	12	30	104	16	-208
-12	12	30	267	33	-80
-9	12	30	259	66	-93
-6	12	30	194	75	-117
-3	12	30	224	461	-94
0	12	30	149	564	-135
3	12	30	208	349	-130
-14	13	30	229	308	-127
-11	13	30	237	465	-76
-8	13	30	206	375	-120
-5	13	30	149	48	-142
-2	13	30	239	101	-87
1	13	30	270	344	-130
-13	14	30	241	99	-126
-10	14	30	101	133	-202
-7	14	30	196	24	-83
-4	14	30	101	94	-202
-1	14	30	104	61	-209
-12	15	30	105	437	-210
-9	15	30	153	449	-150
-6	15	30	101	186	-202
-3	15	30	179	72	-153
-11	16	30	105	516	-210
-8	16	30	149	316	-165
-5	16	30	107	279	-214
-1	1	31	98	79	-101
-3	2	31	94	2	-129
0	2	31	126	225	-93
-5	3	31	122	71	-107
-2	3	31	163	110	-95
1	3	31	190	179	-73
-7	4	31	83	259	-167
-4	4	31	129	328	-99
-1	4	31	106	204	-120
2	4	31	82	173	-164
-9	5	31	273	203	61
-6	5	31	110	79	-132
-3	5	31	138	140	-108
0	5	31	190	62	-87
3	5	31	165	73	-104
-11	6	31	182	102	-121
-8	6	31	171	310	-97
-5	6	31	81	243	-162
-2	6	31	199	236	-99
1	6	31	155	5	-121
4	6	31	207	45	-94
-13	7	31	96	151	-191
-10	7	31	199	440	-94
-7	7	31	141	454	-101
-4	7	31	176	410	-107
-1	7	31	152	210	-112
2	7	31	209	198	-92
5	7	31	274	112	-106
-15	8	31	204	208	-127
-12	8	31	255	203	-102
-9	8	31	267	82	-108
-6	8	31	169	183	-98
-3	8	31	88	209	-176
3	8	31	164	199	-134
6	8	31	135	169	-158
-14	9	31	162	15	-129
-11	9	31	94	332	-187
-8	9	31	190	312	-86
-5	9	31	233	283	-88
-2	9	31	174	356	-123
1	9	31	169	86	-142
4	9	31	247	88	-118
7	9	31	106	34	-212
-16	10	31	260	155	-123
-13	10	31	232	278	-100

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-10	10	31	242	328	-91
-7	10	31	89	304	-178
-4	10	31	185	282	-118
-1	10	31	99	86	-198
2	10	31	193	94	-132
5	10	31	182	140	-127
-15	11	31	224	178	-128
-12	11	31	135	23	-151
-9	11	31	179	25	-128
-6	11	31	92	185	-185
-3	11	31	117	214	-160
0	11	31	237	140	-95
3	11	31	101	270	-202
-14	12	31	102	155	-205
-11	12	31	146	216	-141
-8	12	31	94	146	-189
-5	12	31	153	291	-137
-2	12	31	100	261	-200
1	12	31	145	103	-161
4	12	31	172	41	-157
-13	13	31	101	87	-175
-10	13	31	153	76	-132
-7	13	31	153	48	-139
-4	13	31	230	35	-124
-1	13	31	102	44	-205
2	13	31	180	147	-155
-15	14	31	108	17	-217
-12	14	31	103	106	-206
-9	14	31	98	62	-196
-6	14	31	97	153	-194
-3	14	31	232	135	-100
0	14	31	105	152	-183
-14	15	31	249	88	-132
-11	15	31	180	52	-144
-8	15	31	279	34	-125
-5	15	31	219	65	-111
-2	15	31	263	79	-89
-10	16	31	103	37	-207
-7	16	31	155	132	-162
-4	16	31	107	84	-214
0	1	32	943	909	16
-2	2	32	785	885	14
1	2	32	698	786	12
-4	3	32	1116	1054	27
-1	3	32	688	807	22
2	3	32	683	799	15
-6	4	32	1144	1214	30
-3	4	32	1108	1034	26
0	4	32	2298	2190	42
3	4	32	2110	2110	25
-8	5	32	717	782	18
-5	5	32	982	1120	19
-2	5	32	690	749	24
1	5	32	1867	1850	27
4	5	32	1283	1268	14
-10	6	32	1161	1168	21
-7	6	32	909	834	23
-4	6	32	1142	1211	33
-1	6	32	1866	1882	24
2	6	32	1388	1381	26
5	6	32	1105	1059	16
-12	7	32	242	187	41
-9	7	32	474	486	22
-6	7	32	894	809	21
-3	7	32	2125	2064	36
0	7	32	3600	3589	37
3	7	32	2633	2680	27
6	7	32	813	796	18
-14	8	32	252	225	49
-11	8	32	340	308	58
-8	8	32	943	1037	16
-5	8	32	748	737	23
-2	8	32	1408	1351	31
1	8	32	2006	1915	42
4	8	32	579	571	27
7	8	32	170	39	-81
-16	9	32	158	56	-105
-13	9	32	215	200	50
-10	9	32	480	452	27
-7	9	32	489	485	38
-4	9	32	1289	1248	27
-1	9	32	2024	1963	33
2	9	32	1623	1590	21
5	9	32	611	622	22
8	9	32	239	166	-95
-18	10	32	219	42	-77
-15	10	32	262	265	46
-12	10	32	454	446	27
-9	10	32	463	431	22
-6	10	32	1146	1106	16
-3	10	32	2648	2655	34
0	10	32	3473	3536	34

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
3	10	32	1613	1626	18
6	10	32	428	436	37
9	10	32	87	79	-175
-20	11	32	115	67	-146
-17	11	32	372	372	46
-14	11	32	652	637	21
-11	11	32	251	200	44
-8	11	32	297	325	36
-5	11	32	1119	1060	14
-2	11	32	1631	1555	25
1	11	32	1207	1202	16
4	11	32	588	575	25
7	11	32	184	119	-90
10	11	32	89	68	-179
-22	12	32	276	124	75
-19	12	32	274	297	72
-16	12	32	362	423	41
-13	12	32	279	247	56
-10	12	32	454	488	50
-7	12	32	217	180	-65
-4	12	32	587	580	23
-1	12	32	1213	1197	21
2	12	32	250	230	45
5	12	32	83	112	-166
8	12	32	107	19	-150
11	12	32	197	17	-113
-21	13	32	192	71	-102
-18	13	32	195	88	-80
-15	13	32	421	393	36
-12	13	32	259	187	58
-9	13	32	218	181	63
-6	13	32	792	776	21
-3	13	32	1621	1601	17
0	13	32	1117	1130	18
3	13	32	302	236	57
6	13	32	89	72	-126
9	13	32	217	172	-114
-23	14	32	159	11	-128
-20	14	32	377	323	83
-17	14	32	656	687	41
-14	14	32	740	757	28
-11	14	32	658	626	22
-8	14	32	237	253	53
-5	14	32	638	606	22
-2	14	32	272	204	62
1	14	32	339	355	51
4	14	32	193	87	-89
7	14	32	276	243	67
-22	15	32	216	159	-94
-19	15	32	373	406	64
-16	15	32	419	395	69
-13	15	32	440	428	41
-10	15	32	268	244	48
-7	15	32	160	41	-93
-4	15	32	585	552	33
-1	15	32	357	354	50
2	15	32	86	77	-172
5	15	32	134	29	-136
-21	16	32	124	90	-152
-18	16	32	313	254	63
-15	16	32	398	378	78
-12	16	32	387	392	71
-9	16	32	143	58	-93
-6	16	32	434	420	38
-3	16	32	277	244	73
0	16	32	211	143	-78
3	16	32	136	53	-133
6	16	32	269	224	-82
-20	17	32	449	500	47
-17	17	32	623	668	34
-14	17	32	538	748	-205
-11	17	32	421	381	65
-8	17	32	192	164	-83
-5	17	32	177	107	-86
-2	17	32	86	82	-172
1	17	32	210	43	-108
4	17	32	283	227	77
-19	18	32	274	317	73
-16	18	32	353	299	92
-13	18	32	128	129	-125
-10	18	32	135	37	-124
-7	18	32	175	98	-93
-4	18	32	107	65	-147
-1	18	32	90	51	-180
2	18	32	159	91	-127
-21	19	32	264	216	73
-18	19	32	348	280	77
-15	19	32	434	404	42
-12	19	32	304	278	86
-9	19	32	87	54	-174
-6	19	32	188	87	-80
-3	19	32	89	47	-178

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
0	19	32	194	86	-99
-20	20	32	493	482	39
-17	20	32	520	531	60
-14	20	32	337	380	54
-11	20	32	278	92	-107
-8	20	32	156	7	-122
-5	20	32	149	30	-115
-2	20	32	182	82	-104
-19	21	32	299	269	66
-16	21	32	93	136	-186
-13	21	32	150	15	-129
-10	21	32	116	53	-153
-7	21	32	244	243	-88
-4	21	32	262	219	-101
-15	22	32	245	143	-89
-12	22	32	179	99	-113
-9	22	32	231	172	-77
-6	22	32	208	217	-97
-14	23	32	156	25	-130
-11	23	32	126	10	-148
0	0	33	124	869	-127
1	1	33	117	86	-106
-1	2	33	109	591	-119
2	2	33	78	627	-157
-3	3	33	77	712	-134
0	3	33	177	569	-74
3	3	33	82	468	-165
-5	4	33	125	76	-120
-2	4	33	187	123	-92
1	4	33	83	157	-167
4	4	33	249	5	-82
-7	5	33	85	232	-171
-4	5	33	82	505	-164
-1	5	33	186	497	-85
2	5	33	165	355	-109
5	5	33	203	22	-94
-9	6	33	197	290	-92
-6	6	33	105	361	-127
-3	6	33	84	302	-168
0	6	33	117	10	-126
3	6	33	90	171	-181
6	6	33	94	28	-188
-11	7	33	190	302	-103
-5	7	33	216	269	-89
-2	7	33	194	12	-92
4	7	33	209	176	-99
7	7	33	124	5	-168
-13	8	33	181	287	-130
-10	8	33	190	245	-113
-4	8	33	174	320	-114
2	8	33	181	347	-120
5	8	33	186	149	-118
8	8	33	133	193	-183
-15	9	33	192	251	-123
-12	9	33	199	23	-118
-9	9	33	116	22	-133
-6	9	33	126	103	-137
-3	9	33	190	55	-97
0	9	33	185	1	-95
3	9	33	99	90	-199
6	9	33	105	152	-210
-14	10	33	191	248	-136
-11	10	33	235	343	-113
-8	10	33	111	301	-158
-5	10	33	191	156	-90
-2	10	33	97	25	-195
1	10	33	177	283	-144
4	10	33	265	238	-101
-16	11	33	151	261	-169
-13	11	33	99	278	-199
-10	11	33	119	316	-157
-7	11	33	201	70	-107
-4	11	33	94	12	-189
-1	11	33	207	53	-117
2	11	33	235	281	-121
5	11	33	312	23	-92
-15	12	33	143	63	-170
-12	12	33	99	97	-171
-9	12	33	177	69	-133
-6	12	33	95	41	-190
-3	12	33	96	78	-193
0	12	33	101	37	-175
3	12	33	167	93	-158
-14	13	33	105	418	-210
-11	13	33	99	439	-198
-8	13	33	164	253	-118
-5	13	33	98	164	-197
-2	13	33	131	47	-171
1	13	33	236	215	-98
-13	14	33	146	331	-166
-10	14	33	100	278	-200
-7	14	33	99	139	-199

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-4	14	33	193	73	-124
-1	14	33	150	21	-166
-12	15	33	105	158	-211
-9	15	33	235	62	-99
-6	15	33	280	47	-123
-3	15	33	166	30	-160
-11	16	33	107	342	-215
-8	16	33	213	131	-147
-5	16	33	196	1	-133
-1	1	34	108	168	-110
-3	2	34	155	316	-82
0	2	34	174	67	-72
-5	3	34	175	12	-85
-2	3	34	150	218	-102
1	3	34	137	282	-118
-7	4	34	174	293	-110
-4	4	34	119	428	-105
-1	4	34	214	22	-98
2	4	34	277	515	76
-9	5	34	195	404	-93
-6	5	34	183	362	-105
-3	5	34	102	55	-138
0	5	34	203	137	-95
-11	6	34	92	131	-184
-5	6	34	85	78	-171
-2	6	34	157	87	-118
1	6	34	249	36	-81
4	6	34	224	86	-85
-13	7	34	163	325	-142
-10	7	34	186	447	-91
-4	7	34	181	458	-108
-1	7	34	188	73	-99
2	7	34	264	421	-111
5	7	34	222	214	-101
-15	8	34	128	23	-182
-12	8	34	212	171	-99
-9	8	34	119	274	-148
0	8	34	217	584	-90
3	8	34	94	475	-189
6	8	34	190	110	-133
-14	9	34	160	383	-146
-11	9	34	93	341	-187
-8	9	34	90	311	-181
-5	9	34	169	406	-115
-2	9	34	152	455	-135
1	9	34	105	365	-210
4	9	34	157	107	-154
7	9	34	235	191	-141
-16	10	34	138	281	-179
-13	10	34	204	350	-105
-10	10	34	130	453	-123
-7	10	34	193	399	-99
-4	10	34	283	373	-109
-1	10	34	220	34	-118
2	10	34	177	209	-147
5	10	34	107	57	-214
-15	11	34	235	120	-128
-12	11	34	97	40	-195
-9	11	34	200	64	-102
-6	11	34	93	175	-186
-3	11	34	167	445	-130
0	11	34	252	575	-110
3	11	34	192	264	-137
-14	12	34	222	291	-110
-11	12	34	97	209	-194
-8	12	34	122	199	-161
-5	12	34	123	517	-160
-2	12	34	166	474	-132
1	12	34	275	234	-94
-13	13	34	237	102	-118
-10	13	34	197	60	-129
-7	13	34	165	27	-130
-4	13	34	319	25	87
-1	13	34	306	230	-117
-12	14	34	229	126	-108
-9	14	34	100	137	-200
-6	14	34	161	509	-144
-3	14	34	102	592	-205
0	14	34	106	371	-184
-11	15	34	156	27	-160
-8	15	34	105	249	-211
-5	15	34	278	453	-118
-10	16	34	198	140	-144
-7	16	34	204	202	-146
0	1	35	173	100	-77
-2	2	35	84	19	-145
1	2	35	84	227	-168
-4	3	35	136	389	-116
-1	3	35	190	200	-106
2	3	35	118	203	-135
-6	4	35	211	11	-80
-3	4	35	165	119	-98

Table 54. (cont).
F(obs), F(calc), and σ_F

($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
0	4	35	158	250	-84
3	4	35	249	316	-100
-8	5	35	205	285	-74
-5	5	35	175	136	-101
-2	5	35	111	60	-138
1	5	35	243	182	-77
4	5	35	207	341	-80
-10	6	35	168	163	-101
-4	6	35	217	402	-91
-1	6	35	267	222	66
2	6	35	171	252	-102
5	6	35	160	108	-128
-12	7	35	159	70	-137
-9	7	35	90	30	-180
-3	7	35	263	182	60
0	7	35	90	284	-157
3	7	35	183	396	-120
6	7	35	153	165	-151
-14	8	35	101	19	-202
-11	8	35	188	22	-105
-8	8	35	211	85	-78
-5	8	35	87	224	-174
-2	8	35	89	239	-178
1	8	35	246	422	-89
4	8	35	96	364	-193
7	8	35	107	161	-215
-13	9	35	99	82	-198
-10	9	35	196	56	-90
-7	9	35	208	87	-114
-4	9	35	174	274	-103
-1	9	35	200	213	-97
2	9	35	123	108	-164
5	9	35	159	111	-155
-15	10	35	187	126	-146
-12	10	35	213	181	-83
-9	10	35	153	93	-134
-6	10	35	91	228	-182
-3	10	35	111	134	-159
0	10	35	367	277	69
3	10	35	143	247	-161
-14	11	35	155	16	-155
-11	11	35	191	20	-101
-8	11	35	155	96	-136
-5	11	35	214	286	-82
-2	11	35	117	268	-167
1	11	35	99	259	-198
4	11	35	141	212	-179
-13	12	35	223	262	-104
-10	12	35	195	143	-79
-7	12	35	121	91	-164
-4	12	35	97	138	-193
-1	12	35	101	96	-202
2	12	35	128	33	-177
-12	13	35	101	196	-203
-9	13	35	172	154	-125
-6	13	35	145	147	-156
-3	13	35	146	87	-156
0	13	35	241	78	-101
-11	14	35	103	12	-206
-8	14	35	101	48	-203
-5	14	35	103	119	-205
-2	14	35	193	50	-139
-10	15	35	242	170	-110
-7	15	35	194	112	-146
-4	15	35	107	28	-215
0	0	36	171	105	-85
1	1	36	4797	4847	73
-1	2	36	4785	4812	79
2	2	36	3383	3304	62
-3	3	36	104	16	-70
0	3	36	158	26	-49
3	3	36	686	744	18
-5	4	36	1584	1563	24
-2	4	36	3369	3378	42
1	4	36	2154	2227	30
4	4	36	405	473	29
-7	5	36	956	871	21
-4	5	36	1558	1494	32
-1	5	36	2158	2107	47
2	5	36	1533	1462	33
5	5	36	456	466	39
-9	6	36	620	547	19
-6	6	36	134	27	-72
-3	6	36	697	701	16
0	6	36	139	41	-65
3	6	36	183	219	-55
6	6	36	961	964	21
-11	7	36	330	355	41
-8	7	36	789	796	19
-5	7	36	955	912	17
-2	7	36	1523	1523	23
1	7	36	572	640	18

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
4	7	36	296	315	40
7	7	36	224	163	58
-13	8	36	936	935	23
-10	8	36	187	158	-67
-7	8	36	785	787	18
-4	8	36	410	409	22
-1	8	36	560	591	28
2	8	36	171	13	-74
5	8	36	1276	1263	21
8	8	36	1090	1064	23
-15	9	36	712	772	22
-12	9	36	715	720	22
-9	9	36	144	24	-62
-6	9	36	611	564	20
-3	9	36	187	200	52
0	9	36	94	16	-86
3	9	36	426	443	26
6	9	36	1097	1115	30
9	9	36	891	902	62
-17	10	36	191	62	-87
-14	10	36	195	157	-78
-11	10	36	157	46	-71
-8	10	36	186	151	-55
-5	10	36	441	482	47
-2	10	36	103	17	-94
1	10	36	160	44	-98
4	10	36	222	175	-69
7	10	36	115	86	-140
10	10	36	149	24	-130
-19	11	36	727	729	37
-16	11	36	661	665	32
-13	11	36	714	728	30
-10	11	36	177	63	-58
-7	11	36	303	315	38
-4	11	36	319	299	35
-1	11	36	83	88	-119
2	11	36	348	310	47
5	11	36	924	909	24
8	11	36	719	669	31
11	11	36	370	332	64
-21	12	36	446	446	67
-18	12	36	557	577	40
-15	12	36	307	354	47
-12	12	36	133	18	-79
-9	12	36	710	711	23
-6	12	36	978	964	17
-3	12	36	463	420	24
0	12	36	98	10	-99
3	12	36	501	497	33
6	12	36	746	763	64
9	12	36	490	459	54
-20	13	36	150	83	-118
-17	13	36	213	51	-83
-14	13	36	513	508	31
-11	13	36	711	679	26
-8	13	36	914	960	24
-5	13	36	1277	1295	24
-2	13	36	345	334	37
1	13	36	145	102	-93
4	13	36	144	31	-122
7	13	36	91	118	-182
-22	14	36	346	313	57
-19	14	36	491	453	49
-16	14	36	434	447	69
-13	14	36	518	536	44
-10	14	36	254	176	57
-7	14	36	213	196	-64
-4	14	36	239	189	56
-1	14	36	167	89	-78
2	14	36	202	170	-84
5	14	36	348	317	58
8	14	36	241	150	-85
-21	15	36	303	265	81
-18	15	36	365	391	54
-15	15	36	108	22	-121
-12	15	36	319	291	53
-9	15	36	740	750	25
-6	15	36	1110	1092	24
-3	15	36	500	481	47
0	15	36	120	3	-111
3	15	36	226	129	-82
6	15	36	274	187	-95
-20	16	36	200	60	-114
-17	16	36	160	25	-108
-14	16	36	466	410	39
-11	16	36	652	637	36
-8	16	36	1078	1068	34
-5	16	36	921	892	51
-2	16	36	170	161	-98
1	16	36	208	60	-110
4	16	36	91	42	-183
-19	17	36	120	78	-151

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-16	17	36	122	29	-142
-13	17	36	86	51	-172
-10	17	36	224	42	-102
-7	17	36	87	76	-174
-4	17	36	117	4	-140
-1	17	36	205	68	-88
2	17	36	126	75	-137
-21	18	36	93	23	-186
-18	18	36	253	34	-102
-15	18	36	374	394	52
-12	18	36	535	570	71
-9	18	36	922	920	49
-6	18	36	760	756	30
-3	18	36	202	124	-97
0	18	36	91	12	-158
3	18	36	143	43	-129
-20	19	36	180	33	-122
-17	19	36	182	132	-121
-14	19	36	477	480	75
-11	19	36	763	746	38
-8	19	36	699	690	32
-5	19	36	337	323	71
-2	19	36	125	51	-146
1	19	36	121	44	-155
-19	20	36	148	8	-139
-16	20	36	140	22	-138
-13	20	36	243	116	-79
-10	20	36	126	18	-145
-7	20	36	125	93	-145
-4	20	36	91	44	-182
-1	20	36	93	40	-186
-18	21	36	120	67	-156
-15	21	36	186	250	-124
-12	21	36	460	427	59
-9	21	36	450	465	49
-6	21	36	283	199	-98
-3	21	36	156	28	-132
-14	22	36	336	326	61
-11	22	36	395	338	102
-8	22	36	191	183	-111
-1	1	37	104	174	-132
-3	2	37	85	456	-170
0	2	37	201	188	-81
-5	3	37	85	415	-171
-2	3	37	132	377	-126
1	3	37	154	365	-103
-7	4	37	139	248	-129
-4	4	37	107	111	-127
-1	4	37	85	229	-171
2	4	37	105	488	-148
-9	5	37	136	496	-136
-3	5	37	147	193	-118
0	5	37	130	268	-117
3	5	37	153	567	-124
-11	6	37	182	93	-125
-8	6	37	89	254	-178
-2	6	37	85	330	-171
1	6	37	115	343	-148
4	6	37	173	324	-124
-13	7	37	224	542	-128
-10	7	37	195	537	-109
-7	7	37	139	377	-124
-4	7	37	88	389	-177
-1	7	37	88	194	-176
2	7	37	145	652	-135
5	7	37	98	490	-197
-15	8	37	108	399	-216
-12	8	37	126	625	-121
-9	8	37	124	473	-153
-6	8	37	131	191	-139
-3	8	37	117	38	-144
0	8	37	124	400	-121
3	8	37	150	290	-141
6	8	37	143	34	-166
-14	9	37	199	43	-136
-11	9	37	122	45	-159
-8	9	37	161	47	-131
-5	9	37	187	219	-115
-2	9	37	151	5	-130
1	9	37	253	213	-83
4	9	37	102	193	-205
-13	10	37	292	520	-102
-10	10	37	97	443	-168
-7	10	37	170	478	-128
-4	10	37	119	343	-152
-1	10	37	125	268	-157
2	10	37	262	386	-108
5	10	37	110	245	-220
-12	11	37	101	501	-201
-9	11	37	125	396	-162
-6	11	37	148	40	-142
-3	11	37	172	63	-130

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
0	11	37	235	107	-78
3	11	37	162	166	-156
-14	12	37	194	4	-143
-11	12	37	187	61	-117
-8	12	37	213	153	-86
-5	12	37	237	313	-104
-2	12	37	146	6	-149
1	12	37	103	5	-207
-13	13	37	171	194	-131
-10	13	37	103	209	-207
-7	13	37	191	201	-133
-4	13	37	102	107	-204
-1	13	37	192	11	-138
-12	14	37	188	88	-130
-9	14	37	103	68	-207
-6	14	37	104	166	-208
-3	14	37	160	68	-156
-8	15	37	270	240	-114
-5	15	37	230	140	-139
0	1	38	157	62	-102
-2	2	38	84	120	-147
1	2	38	256	424	70
-4	3	38	169	283	-110
-1	3	38	84	405	-169
2	3	38	209	237	-73
-3	4	38	181	291	-88
0	4	38	253	22	-83
3	4	38	155	119	-122
-8	5	38	123	104	-150
-2	5	38	84	379	-169
1	5	38	220	520	-103
4	5	38	90	189	-181
-10	6	38	97	56	-194
-7	6	38	311	197	-115
-1	6	38	165	372	-112
2	6	38	234	348	-99
5	6	38	95	117	-190
-12	7	38	101	221	-203
-9	7	38	272	194	-96
-6	7	38	265	92	-81
-3	7	38	147	112	-127
0	7	38	209	27	-78
3	7	38	94	88	-188
6	7	38	215	205	-106
-14	8	38	268	443	-99
-11	8	38	119	425	-166
-8	8	38	149	535	-125
-5	8	38	93	706	-186
-2	8	38	183	486	-102
1	8	38	157	566	-132
4	8	38	150	167	-150
7	8	38	204	114	-153
-13	9	38	147	163	-165
-10	9	38	183	179	-132
-7	9	38	96	402	-192
-4	9	38	132	613	-144
-1	9	38	189	488	-103
2	9	38	136	270	-150
5	9	38	105	141	-210
-15	10	38	108	335	-216
-12	10	38	167	349	-144
-9	10	38	180	274	-133
-6	10	38	274	56	-118
-3	10	38	178	170	-126
0	10	38	95	138	-166
3	10	38	153	188	-153
-14	11	38	278	406	-104
-11	11	38	169	351	-130
-8	11	38	98	426	-196
-5	11	38	148	349	-141
-2	11	38	136	211	-149
1	11	38	223	334	-126
-13	12	38	260	46	-130
-10	12	38	102	18	-204
-7	12	38	190	151	-123
-4	12	38	265	358	-82
-1	12	38	159	167	-146
2	12	38	134	56	-181
-12	13	38	178	388	-154
-9	13	38	144	267	-168
-6	13	38	105	2	-210
-3	13	38	131	86	-167
0	13	38	230	188	-101
-11	14	38	106	193	-212
-8	14	38	158	91	-155
-5	14	38	104	4	-209
-2	14	38	131	8	-178
-10	15	38	199	133	-145
-7	15	38	242	46	-111
0	0	39	84	18	-207
1	1	39	436	240	93
-1	2	39	473	335	66

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
2	2	39	87	474	-174
-3	3	39	84	207	-146
0	3	39	156	146	-93
3	3	39	86	166	-173
-2	4	39	87	26	-174
4	4	39	92	192	-184
-7	5	39	148	183	-135
2	5	39	210	118	-106
5	5	39	169	26	-131
-9	6	39	198	11	-114
-6	6	39	167	29	-114
-3	6	39	123	55	-140
0	6	39	148	96	-113
3	6	39	199	80	-115
6	6	39	203	49	-114
-11	7	39	177	30	-134
-8	7	39	239	150	-100
-5	7	39	215	4	-112
-2	7	39	256	101	74
1	7	39	92	136	-185
4	7	39	96	141	-192
7	7	39	174	205	-149
-13	8	39	161	43	-154
-10	8	39	210	82	-123
-7	8	39	192	74	-118
-4	8	39	92	130	-185
-1	8	39	91	245	-182
2	8	39	128	127	-156
5	8	39	139	100	-167
-12	9	39	101	129	-203
-9	9	39	198	234	-103
-6	9	39	194	216	-110
-3	9	39	267	169	76
0	9	39	95	238	-165
3	9	39	99	116	-198
-14	10	39	105	99	-211
-11	10	39	135	56	-163
-8	10	39	171	80	-129
-5	10	39	143	107	-134
-2	10	39	187	164	-97
1	10	39	155	23	-131
4	10	39	125	252	-180
-13	11	39	146	99	-174
-10	11	39	100	220	-201
-7	11	39	223	282	-124
-4	11	39	215	310	-116
-1	11	39	130	346	-159
2	11	39	225	48	-129
-12	12	39	175	261	-135
-9	12	39	101	325	-202
-6	12	39	172	198	-140
-3	12	39	200	111	-126
0	12	39	249	100	-95
-11	13	39	178	56	-138
-8	13	39	225	73	-108
-5	13	39	103	210	-207
-2	13	39	248	258	-96
-10	14	39	148	297	-165
-7	14	39	156	312	-145
-4	14	39	149	294	-162
-1	1	40	264	198	30
-3	2	40	786	788	15
0	2	40	1279	1307	16
-5	3	40	906	942	22
-2	3	40	767	774	16
1	3	40	94	33	-102
-7	4	40	2367	2357	50
-4	4	40	2827	2661	73
-1	4	40	186	38	-68
2	4	40	241	266	45
-9	5	40	760	716	26
-6	5	40	1834	1801	42
-3	5	40	905	902	22
0	5	40	231	187	38
3	5	40	1186	1202	16
-11	6	40	544	533	26
-8	6	40	1696	1758	55
-5	6	40	1848	1814	40
-2	6	40	244	250	39
1	6	40	130	137	-75
4	6	40	934	886	20
-13	7	40	1171	1150	36
-10	7	40	2222	2179	52
-7	7	40	3778	3745	67
-4	7	40	2382	2390	51
-1	7	40	222	171	46
2	7	40	335	308	44
5	7	40	575	588	31
-15	8	40	408	447	43
-12	8	40	1272	1288	16
-9	8	40	1493	1472	15
-6	8	40	1693	1731	35

Table 54. (cont).
F(obs), F(calc), and σ_F

($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-3	8	40	1175	1186	25
0	8	40	211	201	41
3	8	40	154	164	-82
6	8	40	218	137	-86
-17	9	40	86	24	-172
-14	9	40	221	210	57
-11	9	40	512	507	24
-8	9	40	1469	1505	22
-5	9	40	752	720	24
-2	9	40	318	315	47
1	9	40	241	203	49
4	9	40	362	336	32
7	9	40	183	176	-94
-19	10	40	178	192	-119
-16	10	40	367	328	59
-13	10	40	1340	1315	28
-10	10	40	1914	1893	29
-7	10	40	2234	2218	50
-4	10	40	931	908	18
-1	10	40	217	194	61
2	10	40	239	240	58
5	10	40	240	235	-87
8	10	40	122	12	-104
-21	11	40	170	71	-125
-18	11	40	126	86	-96
-15	11	40	316	345	57
-12	11	40	829	839	21
-9	11	40	506	491	32
-6	11	40	532	548	31
-3	11	40	202	153	-77
0	11	40	710	694	20
3	11	40	366	334	38
6	11	40	131	156	-129
9	11	40	159	119	-125
-20	12	40	171	61	-120
-17	12	40	262	196	66
-14	12	40	520	581	34
-11	12	40	839	859	32
-8	12	40	1242	1322	24
-5	12	40	590	595	31
-2	12	40	237	242	49
1	12	40	353	368	39
4	12	40	243	139	70
7	12	40	89	125	-178
10	12	40	231	5	-112
-19	13	40	128	83	-142
-16	13	40	490	529	41
-13	13	40	1197	1228	22
-10	13	40	1324	1337	18
-7	13	40	1176	1187	24
-4	13	40	367	351	38
-1	13	40	348	368	35
2	13	40	290	263	57
5	13	40	215	177	-79
8	13	40	310	105	-100
-21	14	40	92	49	-184
-18	14	40	89	4	-179
-15	14	40	310	311	51
-12	14	40	536	588	33
-9	14	40	281	227	43
-6	14	40	105	179	-114
-3	14	40	368	336	52
0	14	40	774	783	29
3	14	40	572	529	31
6	14	40	336	303	56
-20	15	40	130	94	-142
-17	15	40	124	122	-141
-14	15	40	305	284	56
-11	15	40	323	344	70
-8	15	40	426	447	57
-5	15	40	260	227	60
-2	15	40	373	264	41
1	15	40	389	392	36
4	15	40	257	232	69
-19	16	40	206	123	-90
-16	16	40	233	187	-72
-13	16	40	449	481	41
-10	16	40	361	312	93
-7	16	40	296	201	66
-4	16	40	277	144	-104
-1	16	40	372	374	41
2	16	40	178	247	-105
5	16	40	96	168	-192
-18	17	40	90	76	-180
-15	17	40	200	107	-110
-12	17	40	135	157	-120
-9	17	40	164	30	-97
-6	17	40	161	135	-116
-3	17	40	558	514	25
0	17	40	718	641	39
3	17	40	442	397	55
-20	18	40	134	83	-147

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-17	18	40	89	54	-179
-14	18	40	122	22	-144
-11	18	40	89	91	-126
-8	18	40	138	15	-99
-5	18	40	195	140	-113
-2	18	40	288	244	67
1	18	40	259	255	-75
-19	19	40	220	222	-93
-16	19	40	196	160	-115
-13	19	40	124	154	-144
-10	19	40	264	226	-88
-7	19	40	212	143	-94
-4	19	40	309	247	75
-1	19	40	293	254	68
-18	20	40	247	150	-113
-15	20	40	136	160	-141
-12	20	40	208	143	-105
-9	20	40	202	182	-93
-6	20	40	322	311	60
-3	20	40	427	412	53
-14	21	40	93	25	-186
-11	21	40	92	23	-184
-8	21	40	143	147	-130
-5	21	40	258	183	-83
-10	22	40	230	14	-111
0	1	41	204	185	-63
-2	2	41	85	268	-147
-4	3	41	193	116	-83
2	3	41	151	418	-125
-6	4	41	142	430	-139
-3	4	41	89	604	-178
0	4	41	104	133	-133
3	4	41	205	212	-117
-8	5	41	134	139	-153
-5	5	41	93	146	-161
-2	5	41	144	153	-115
1	5	41	111	120	-157
4	5	41	221	8	-95
-10	6	41	98	110	-197
-7	6	41	153	295	-144
-4	6	41	92	458	-185
-1	6	41	90	225	-180
2	6	41	94	363	-188
5	6	41	122	117	-163
-12	7	41	200	75	-136
-9	7	41	99	75	-199
-6	7	41	156	306	-144
-3	7	41	183	229	-121
0	7	41	144	144	-116
3	7	41	134	222	-153
6	7	41	103	46	-207
-14	8	41	243	242	-131
-11	8	41	173	161	-135
-8	8	41	99	375	-173
-5	8	41	133	207	-149
-2	8	41	195	31	-100
1	8	41	276	277	-112
4	8	41	212	136	-111
-13	9	41	175	189	-152
-10	9	41	180	382	-135
-7	9	41	141	731	-145
-4	9	41	202	588	-110
-1	9	41	96	500	-193
2	9	41	161	472	-144
5	9	41	198	59	-127
-12	10	41	189	122	-142
-9	10	41	211	176	-130
-6	10	41	99	360	-197
-3	10	41	221	494	-119
0	10	41	100	210	-173
3	10	41	230	56	-128
-11	11	41	140	185	-146
-8	11	41	100	279	-201
-5	11	41	97	11	-194
-2	11	41	149	188	-156
1	11	41	135	386	-177
-13	12	41	111	180	-223
-10	12	41	106	265	-212
-7	12	41	103	440	-206
-4	12	41	206	600	-111
-1	12	41	154	518	-163
-12	13	41	289	50	-135
-9	13	41	107	134	-215
-6	13	41	104	541	-208
-3	13	41	178	429	-143
-8	14	41	244	153	-124
-5	14	41	267	80	-126
0	0	42	223	392	-81
2	2	42	149	543	-116
-3	3	42	230	470	65
0	3	42	145	508	-110
3	3	42	161	380	-125

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-5	4	42	135	63	-128
-2	4	42	212	213	-109
1	4	42	210	126	-111
4	4	42	192	354	-120
-7	5	42	342	324	-120
-4	5	42	117	12	-155
-1	5	42	144	268	-129
2	5	42	93	587	-187
5	5	42	119	281	-165
-9	6	42	127	318	-156
-6	6	42	198	138	-110
-3	6	42	117	41	-149
0	6	42	231	20	-93
3	6	42	257	23	-92
6	6	42	101	132	-203
-11	7	42	148	497	-150
-8	7	42	324	558	89
-5	7	42	179	137	-103
-2	7	42	250	235	-105
1	7	42	125	511	-165
4	7	42	198	415	-128
7	7	42	107	613	-213
-13	8	42	106	359	-212
-10	8	42	247	100	-102
-7	8	42	99	8	-199
-4	8	42	137	38	-145
-1	8	42	202	351	-103
2	8	42	98	537	-196
5	8	42	104	487	-209
-12	9	42	126	221	-176
-9	9	42	99	490	-172
-6	9	42	210	181	-123
-3	9	42	146	201	-141
0	9	42	278	83	-92
3	9	42	240	190	-129
-11	10	42	319	220	-125
-8	10	42	167	215	-142
-5	10	42	98	122	-197
-2	10	42	249	299	-105
1	10	42	282	376	-100
-13	11	42	250	63	-135
-10	11	42	163	415	-149
-7	11	42	216	251	-111
-4	11	42	98	114	-196
-1	11	42	104	229	-209
2	11	42	106	547	-213
-12	12	42	250	382	-110
-9	12	42	161	531	-152
-6	12	42	103	320	-207
-3	12	42	237	194	-133
0	12	42	164	125	-145
-11	13	42	212	60	-128
-8	13	42	177	64	-137
-5	13	42	234	7	-127
-2	13	42	154	68	-156
-7	14	42	107	330	-215
-1	1	43	315	78	70
-3	2	43	165	351	-108
0	2	43	265	132	55
-5	3	43	158	67	-125
-2	3	43	209	96	-86
1	3	43	151	136	-126
-7	4	43	177	31	-110
-4	4	43	214	166	-84
-1	4	43	90	102	-180
2	4	43	169	214	-132
-9	5	43	96	218	-191
-6	5	43	91	256	-182
-3	5	43	176	266	-109
0	5	43	95	116	-165
3	5	43	248	212	-90
-11	6	43	99	210	-199
-8	6	43	209	198	-103
-5	6	43	93	31	-185
-2	6	43	138	64	-149
1	6	43	207	43	-123
4	6	43	136	106	-116
-13	7	43	267	134	-128
-10	7	43	211	38	-122
-7	7	43	256	279	69
-4	7	43	120	370	-156
-1	7	43	96	210	-193
2	7	43	172	73	-144
5	7	43	129	2	-176
-12	8	43	102	125	-205
-9	8	43	97	282	-195
-6	8	43	230	258	-116
-3	8	43	188	275	-103
0	8	43	217	88	-119
3	8	43	104	110	-208
-11	9	43	100	88	-200
-8	9	43	176	26	-153

Table 54. (cont).
F(obs), F(calc), and σ_F

($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-5	9	43	219	90	-120
-2	9	43	102	108	-203
1	9	43	104	46	-209
4	9	43	186	192	-146
-13	10	43	199	136	-130
-10	10	43	226	290	-105
-7	10	43	211	380	-112
-4	10	43	179	402	-84
-1	10	43	149	217	-159
2	10	43	168	82	-148
-12	11	43	107	357	-215
-9	11	43	100	278	-200
-6	11	43	179	227	-137
-3	11	43	184	180	-139
0	11	43	199	144	-120
-11	12	43	106	60	-212
-8	12	43	159	66	-142
-5	12	43	104	122	-208
-2	12	43	106	82	-213
-10	13	43	182	133	-153
-7	13	43	325	179	-109
-4	13	43	242	182	-129
0	1	44	151	20	-55
-2	2	44	127	40	-77
1	2	44	300	239	36
-4	3	44	918	950	24
-1	3	44	278	241	33
2	3	44	1882	1843	56
-6	4	44	778	787	21
-3	4	44	897	926	25
0	4	44	145	5	-85
3	4	44	483	471	23
-8	5	44	265	240	39
-5	5	44	110	32	-81
-2	5	44	1879	1845	43
1	5	44	3094	3072	57
4	5	44	1532	1525	18
-10	6	44	580	604	26
-7	6	44	871	857	20
-4	6	44	784	735	23
-1	6	44	3104	3046	46
2	6	44	2470	2463	29
5	6	44	1002	1019	23
-12	7	44	691	685	28
-9	7	44	613	585	30
-6	7	44	867	889	23
-3	7	44	478	444	26
0	7	44	167	24	-78
3	7	44	292	229	40
6	7	44	197	108	-65
-14	8	44	545	567	38
-11	8	44	198	216	-61
-8	8	44	94	11	-94
-5	8	44	212	218	50
-2	8	44	2494	2452	40
1	8	44	2102	2089	45
4	8	44	928	918	23
7	8	44	534	524	32
-16	9	44	236	53	-98
-13	9	44	205	206	-64
-10	9	44	164	55	-78
-7	9	44	572	570	23
-4	9	44	1523	1477	27
-1	9	44	2098	2100	48
2	9	44	1642	1658	17
5	9	44	792	792	25
8	9	44	87	20	-123
-18	10	44	214	200	-80
-15	10	44	85	39	-169
-12	10	44	300	320	46
-9	10	44	126	63	-94
-6	10	44	552	589	23
-3	10	44	289	260	65
0	10	44	234	4	-81
3	10	44	271	280	-90
6	10	44	116	130	-151
9	10	44	175	45	-102
-20	11	44	170	115	-126
-17	11	44	197	194	-90
-14	11	44	128	81	-128
-11	11	44	194	28	-62
-8	11	44	269	228	72
-5	11	44	1013	995	22
-2	11	44	1639	1640	31
1	11	44	1169	1121	19
4	11	44	571	559	51
7	11	44	198	49	-91
10	11	44	201	113	-106
-19	12	44	243	122	-90
-16	12	44	180	167	-94
-13	12	44	581	595	31
-10	12	44	326	278	53

Table 54. (cont).
F(obs), F(calc), and σ_F

($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-7	12	44	696	677	29
-4	12	44	938	879	31
-1	12	44	1171	1136	24
2	12	44	837	822	27
5	12	44	154	19	-120
8	12	44	140	115	-140
-21	13	44	174	133	-128
-18	13	44	482	443	51
-15	13	44	471	507	37
-12	13	44	584	634	47
-9	13	44	179	214	-70
-6	13	44	234	114	62
-3	13	44	327	287	51
0	13	44	85	6	-148
3	13	44	186	101	-77
6	13	44	197	21	-85
-20	14	44	226	102	-111
-17	14	44	187	245	-102
-14	14	44	177	38	-80
-11	14	44	184	141	-81
-8	14	44	566	564	57
-5	14	44	797	771	32
-2	14	44	862	845	26
1	14	44	574	545	45
4	14	44	89	10	-178
-19	15	44	335	315	59
-16	15	44	421	401	47
-13	15	44	460	475	39
-10	15	44	136	68	-113
-7	15	44	483	517	40
-4	15	44	622	566	42
-1	15	44	590	566	51
2	15	44	236	99	-104
5	15	44	187	98	-122
-18	16	44	496	532	42
-15	16	44	470	436	38
-12	16	44	275	200	71
-9	16	44	213	72	-79
-6	16	44	186	177	-109
-3	16	44	208	110	-69
0	16	44	202	13	-101
3	16	44	120	2	-149
-17	17	44	138	18	-112
-14	17	44	144	203	-133
-11	17	44	149	181	-115
-8	17	44	151	76	-93
-5	17	44	157	23	-121
-2	17	44	208	83	-89
1	17	44	128	54	-144
-16	18	44	550	541	45
-13	18	44	468	474	41
-10	18	44	240	234	-91
-7	18	44	117	89	-145
-4	18	44	222	28	-83
-1	18	44	91	52	-183
-15	19	44	350	378	56
-12	19	44	183	191	-120
-9	19	44	119	57	-147
-6	19	44	147	8	-124
-3	19	44	159	23	-115
-14	20	44	169	74	-117
-11	20	44	193	95	-116
-8	20	44	92	119	-185
-5	20	44	94	103	-188
-13	21	44	173	173	-129
-10	21	44	212	117	-116
0	0	45	91	154	-224
1	1	45	210	804	-94
-1	2	45	117	182	-147
2	2	45	187	112	-114
-3	3	45	168	292	-102
0	3	45	158	459	-115
3	3	45	140	628	-134
-5	4	45	91	680	-182
-2	4	45	218	892	-111
1	4	45	96	729	-192
4	4	45	151	333	-140
-7	5	45	94	142	-188
-4	5	45	92	559	-185
-1	5	45	195	258	-110
2	5	45	189	39	-131
5	5	45	170	2	-139
-9	6	45	112	29	-127
-6	6	45	264	5	-77
-3	6	45	162	113	-118
0	6	45	126	420	-152
3	6	45	166	348	-102
6	6	45	106	21	-213
-11	7	45	101	120	-202
-8	7	45	196	30	-106
-5	7	45	242	486	-88
-2	7	45	245	393	-93

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
1	7	45	137	266	-169
4	7	45	260	136	-122
-13	8	45	107	16	-215
-10	8	45	202	66	-98
-7	8	45	145	348	-149
-4	8	45	120	349	-162
-1	8	45	206	16	-106
2	8	45	287	38	-98
5	8	45	106	69	-213
-12	9	45	170	340	-152
-9	9	45	144	483	-136
-6	9	45	204	193	-80
-3	9	45	253	136	-78
0	9	45	204	16	-114
3	9	45	156	81	-156
-11	10	45	104	347	-208
-8	10	45	99	124	-199
-5	10	45	136	86	-158
-2	10	45	103	241	-206
1	10	45	107	103	-215
-10	11	45	138	185	-172
-7	11	45	101	31	-202
-4	11	45	177	133	-142
-1	11	45	172	252	-143
-9	12	45	155	242	-157
-6	12	45	209	33	-134
-3	12	45	147	14	-172
-8	13	45	106	23	-212
-5	13	45	159	9	-149
-1	1	46	219	25	-87
-3	2	46	201	112	-97
0	2	46	182	354	-110
-5	3	46	171	306	-128
-2	3	46	182	290	-121
1	3	46	176	71	-126
-7	4	46	130	313	-151
-4	4	46	112	3	-141
-1	4	46	205	164	-105
2	4	46	218	111	-108
-9	5	46	162	240	-124
-6	5	46	167	181	-128
-3	5	46	123	198	-149
0	5	46	141	94	-129
3	5	46	99	386	-199
-11	6	46	130	366	-172
-8	6	46	97	560	-195
-5	6	46	225	329	-93
-2	6	46	173	205	-108
1	6	46	218	478	-107
4	6	46	193	244	-117
-10	7	46	160	49	-146
-7	7	46	97	140	-167
-4	7	46	95	131	-191
-1	7	46	134	280	-156
2	7	46	242	199	-95
5	7	46	106	65	-213
-12	8	46	182	423	-148
-9	8	46	99	458	-198
-6	8	46	212	371	-122
-3	8	46	183	456	-133
0	8	46	195	72	-115
3	8	46	294	78	-123
-11	9	46	226	418	-130
-8	9	46	100	499	-200
-5	9	46	97	246	-195
-2	9	46	243	139	-107
1	9	46	217	310	-116
-10	10	46	240	33	-116
-7	10	46	200	15	-119
-4	10	46	134	417	-160
-1	10	46	138	289	-172
2	10	46	248	272	-133
-9	11	46	191	282	-124
-6	11	46	103	278	-206
-3	11	46	260	120	-129
0	11	46	110	17	-191
-8	12	46	246	44	-129
-5	12	46	278	331	-108
-2	12	46	231	339	-135
0	1	47	232	114	-116
-2	2	47	117	197	-152
1	2	47	96	89	-193
-4	3	47	96	129	-192
-1	3	47	97	94	-195
2	3	47	249	275	-116
-6	4	47	232	232	-119
-3	4	47	95	219	-191
0	4	47	116	172	-145
3	4	47	169	127	-132
-8	5	47	138	233	-107
-5	5	47	145	257	-129
-2	5	47	96	68	-193

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
1	5	47	197	165	-113
4	5	47	229	230	-121
-10	6	47	148	157	-157
-7	6	47	118	66	-163
-4	6	47	96	82	-192
-1	6	47	215	249	-122
2	6	47	98	305	-196
5	6	47	213	299	-119
-12	7	47	209	81	-136
-9	7	47	98	46	-197
-6	7	47	173	114	-122
-3	7	47	188	159	-112
0	7	47	223	148	-69
3	7	47	159	103	-149
-11	8	47	130	90	-175
-8	8	47	226	80	-113
-5	8	47	209	38	-99
-2	8	47	236	104	-119
1	8	47	103	218	-206
4	8	47	193	223	-146
-10	9	47	102	83	-205
-7	9	47	98	202	-196
-4	9	47	129	291	-163
-1	9	47	150	372	-155
2	9	47	106	333	-212
-9	10	47	137	69	-170
-6	10	47	227	138	-114
-3	10	47	102	224	-204
0	10	47	226	168	-104
-8	11	47	161	194	-151
-5	11	47	148	85	-163
-2	11	47	105	81	-211
-7	12	47	158	222	-164
-4	12	47	106	258	-213
0	0	48	5791	5672	229
1	1	48	2215	2232	38
-1	2	48	2199	2299	52
2	2	48	438	480	30
-3	3	48	3141	3051	56
0	3	48	2971	2881	50
3	3	48	1078	1042	28
-5	4	48	1288	1306	28
-2	4	48	430	444	32
1	4	48	1121	1158	21
4	4	48	320	386	45
-7	5	48	189	21	-62
-4	5	48	1277	1314	35
-1	5	48	1120	1150	32
2	5	48	156	79	-79
5	5	48	423	463	36
-9	6	48	264	225	45
-6	6	48	1311	1253	17
-3	6	48	1091	1013	28
0	6	48	1100	1060	18
3	6	48	365	320	33
6	6	48	601	645	42
-11	7	48	810	778	30
-8	7	48	439	507	32
-5	7	48	168	31	-69
-2	7	48	184	77	-84
1	7	48	355	381	32
4	7	48	879	863	23
7	7	48	1015	984	24
-13	8	48	268	207	63
-10	8	48	183	202	-61
-7	8	48	449	484	28
-4	8	48	378	347	43
-1	8	48	331	384	37
2	8	48	510	585	32
5	8	48	339	417	47
8	8	48	423	473	32
-15	9	48	582	575	45
-12	9	48	485	526	44
-9	9	48	517	471	30
-6	9	48	238	179	53
-3	9	48	352	316	31
0	9	48	731	677	20
3	9	48	171	208	-91
6	9	48	374	331	49
9	9	48	372	311	53
-17	10	48	856	864	41
-14	10	48	707	689	40
-11	10	48	258	166	65
-8	10	48	169	172	-73
-5	10	48	435	430	39
-2	10	48	534	565	28
1	10	48	195	131	-81
4	10	48	565	508	32
7	10	48	713	670	57
10	10	48	683	605	37
-19	11	48	434	409	47
-16	11	48	267	273	64

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-13	11	48	178	126	-97
-10	11	48	191	130	-82
-7	11	48	808	809	30
-4	11	48	878	869	33
-1	11	48	165	157	-98
2	11	48	85	52	-170
5	11	48	322	280	-114
8	11	48	308	353	64
-18	12	48	340	333	65
-15	12	48	376	403	37
-12	12	48	319	349	46
-9	12	48	505	538	40
-6	12	48	617	675	46
-3	12	48	202	255	-70
0	12	48	322	327	42
3	12	48	302	249	47
6	12	48	189	182	-95
-20	13	48	506	490	48
-17	13	48	486	504	40
-14	13	48	251	217	-76
-11	13	48	204	183	-105
-8	13	48	224	171	-70
-5	13	48	398	336	40
-2	13	48	225	71	-72
1	13	48	249	216	65
4	13	48	466	393	47
7	13	48	479	428	47
-19	14	48	245	187	-81
-16	14	48	117	78	-148
-13	14	48	216	174	-74
-10	14	48	714	652	36
-7	14	48	993	964	27
-4	14	48	559	497	37
-1	14	48	302	195	54
2	14	48	293	140	57
5	14	48	318	273	66
-18	15	48	210	153	-85
-15	15	48	167	111	-92
-12	15	48	397	405	35
-9	15	48	543	561	37
-6	15	48	377	368	44
-3	15	48	272	253	60
0	15	48	119	53	-127
3	15	48	156	5	-116
-17	16	48	186	92	-106
-14	16	48	90	49	-180
-11	16	48	299	245	71
-8	16	48	471	449	38
-5	16	48	240	257	-95
-2	16	48	204	128	-91
1	16	48	212	67	-106
-16	17	48	91	75	-182
-13	17	48	508	479	50
-10	17	48	854	831	40
-7	17	48	675	688	33
-4	17	48	443	387	76
-1	17	48	90	44	-181
-15	18	48	186	141	-103
-12	18	48	348	323	61
-9	18	48	309	316	76
-6	18	48	217	210	-95
-3	18	48	250	13	-81
-14	19	48	170	196	-131
-11	19	48	418	392	62
-8	19	48	359	366	100
-5	19	48	282	285	-86
-13	20	48	467	494	48
-10	20	48	610	619	40
-7	20	48	476	480	52
-1	1	49	103	247	-178
-3	2	49	140	53	-152
0	2	49	220	309	-108
-5	3	49	266	433	-110
-2	3	49	188	80	-130
1	3	49	232	327	-117
-7	4	49	241	499	-101
-4	4	49	160	414	-115
-1	4	49	126	336	-159
2	4	49	215	75	-120
-9	5	49	100	138	-200
-6	5	49	98	26	-197
-3	5	49	96	221	-192
0	5	49	129	461	-140
3	5	49	211	642	-127
-11	6	49	208	776	-139
-8	6	49	122	544	-172
-5	6	49	180	294	-133
-2	6	49	215	74	-116
1	6	49	99	563	-198
4	6	49	236	679	-112
-10	7	49	249	480	-116
-7	7	49	237	373	-103

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-4	7	49	96	163	-193
-1	7	49	146	153	-150
2	7	49	192	204	-136
-9	8	49	167	195	-148
-6	8	49	139	215	-161
-3	8	49	197	164	-125
0	8	49	150	95	-136
3	8	49	136	362	-176
-8	9	49	295	532	-126
-5	9	49	101	418	-202
-2	9	49	247	53	-122
1	9	49	103	318	-207
-10	10	49	202	336	-105
-7	10	49	173	206	-130
-4	10	49	192	56	-121
-1	10	49	248	151	-101
-6	11	49	159	362	-161
-3	11	49	106	172	-212
0	1	50	145	248	-132
-2	2	50	167	299	-121
1	2	50	95	56	-191
-4	3	50	96	298	-193
-1	3	50	184	3	-114
2	3	50	96	195	-193
-6	4	50	189	33	-120
-3	4	50	194	345	-112
0	4	50	182	384	-93
3	4	50	120	292	-167
-8	5	50	190	12	-125
-5	5	50	299	273	-112
-2	5	50	147	287	-132
1	5	50	97	176	-194
4	5	50	124	98	-178
-10	6	50	103	32	-207
-7	6	50	173	110	-142
-4	6	50	99	244	-197
-1	6	50	143	235	-149
2	6	50	162	203	-148
5	6	50	160	164	-161
-9	7	50	175	209	-137
-6	7	50	175	550	-140
-3	7	50	191	593	-127
0	7	50	118	552	-153
3	7	50	300	437	-122
-8	8	50	106	130	-185
-5	8	50	139	337	-161
-2	8	50	100	469	-200
1	8	50	178	339	-142
-10	9	50	107	216	-215
-7	9	50	105	275	-210
-4	9	50	253	106	-121
-1	9	50	156	80	-153
-9	10	50	207	285	-128
-6	10	50	239	333	-97
-3	10	50	104	381	-209
-5	11	50	195	200	-145
0	0	51	779	600	64
1	1	51	324	199	85
-1	2	51	318	162	60
2	2	51	161	148	-137
-3	3	51	361	441	59
0	3	51	303	411	85
3	3	51	127	282	-164
-5	4	51	156	178	-148
-2	4	51	173	146	-126
1	4	51	96	137	-192
4	4	51	153	177	-154
-7	5	51	149	71	-157
-4	5	51	149	61	-155
-1	5	51	97	49	-195
2	5	51	100	85	-200
5	5	51	180	145	-148
-9	6	51	106	199	-212
-6	6	51	178	120	-124
-3	6	51	99	94	-199
0	6	51	100	13	-173
3	6	51	102	139	-205
-8	7	51	106	94	-212
-5	7	51	102	14	-204
-2	7	51	147	67	-151
1	7	51	174	86	-145
-10	8	51	198	98	-121
-7	8	51	107	38	-214
-4	8	51	204	16	-132
-1	8	51	205	8	-120
2	8	51	160	176	-155
-9	9	51	181	72	-146
-6	9	51	258	195	-131
-3	9	51	103	224	-206
0	9	51	167	142	-124
-8	10	51	109	217	-218
-5	10	51	105	291	-210

Table 54. (cont).
F(obs), F(calc), and σ_F

($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-2	10	51	105	229	-210
-1	1	52	125	16	-71
-3	2	52	507	524	25
0	2	52	163	11	-61
-5	3	52	1409	1450	58
-2	3	52	515	513	27
1	3	52	397	377	43
-7	4	52	228	162	55
-4	4	52	181	7	-87
-1	4	52	377	362	36
2	4	52	620	603	21
-9	5	52	953	924	27
-6	5	52	1909	1900	76
-3	5	52	1415	1414	43
0	5	52	130	10	-85
3	5	52	586	594	29
-11	6	52	817	794	25
-8	6	52	1931	1909	71
-5	6	52	1907	1892	61
-2	6	52	598	606	31
1	6	52	452	436	27
4	6	52	258	62	-97
-13	7	52	116	14	-139
-10	7	52	292	255	49
-7	7	52	180	9	-69
-4	7	52	239	134	59
-1	7	52	412	439	36
2	7	52	474	479	30
5	7	52	489	441	47
-15	8	52	427	389	43
-12	8	52	898	845	24
-9	8	52	1847	1829	56
-6	8	52	1931	1912	66
-3	8	52	616	602	49
0	8	52	116	7	-99
3	8	52	404	432	50
6	8	52	351	369	60
-17	9	52	130	101	-143
-14	9	52	515	543	37
-11	9	52	1552	1560	20
-8	9	52	1836	1826	38
-5	9	52	937	962	24
-2	9	52	486	479	34
1	9	52	204	114	-77
4	9	52	410	351	46
7	9	52	167	38	-122
-19	10	52	195	37	-102
-16	10	52	192	45	-114
-13	10	52	212	169	-109
-10	10	52	229	7	-95
-7	10	52	305	251	70
-4	10	52	155	68	-80
-1	10	52	169	115	-88
2	10	52	232	150	-79
5	10	52	190	62	-102
8	10	52	116	58	-154
-18	11	52	91	57	-183
-15	11	52	399	371	45
-12	11	52	1205	1199	23
-9	11	52	1542	1550	30
-6	11	52	799	838	49
-3	11	52	443	459	46
0	11	52	223	17	-70
3	11	52	168	224	-76
6	11	52	168	29	-123
-17	12	52	91	124	-183
-14	12	52	713	743	45
-11	12	52	1207	1198	40
-8	12	52	900	884	26
-5	12	52	469	487	50
-2	12	52	85	134	-171
1	12	52	516	500	32
4	12	52	304	340	60
7	12	52	203	169	-101
-16	13	52	132	155	-132
-13	13	52	192	7	-93
-10	13	52	216	157	-74
-7	13	52	130	18	-130
-4	13	52	358	323	46
-1	13	52	495	502	35
2	13	52	383	378	46
5	13	52	396	374	62
-18	14	52	223	94	-92
-15	14	52	342	276	-114
-12	14	52	710	733	37
-9	14	52	538	547	34
-6	14	52	351	393	64
-3	14	52	257	235	56
0	14	52	120	21	-125
3	14	52	150	94	-132
-17	15	52	227	60	-111
-14	15	52	317	254	82

Table 54. (cont).
F(obs), F(calc), and σ_F

($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-11	15	52	412	366	62
-8	15	52	392	388	55
-5	15	52	157	33	-110
-2	15	52	320	335	75
1	15	52	300	296	-115
-16	16	52	92	21	-159
-13	16	52	188	169	-100
-10	16	52	199	33	-111
-7	16	52	89	38	-179
-4	16	52	294	295	65
-1	16	52	300	298	62
-15	17	52	93	66	-187
-12	17	52	143	112	-124
-9	17	52	91	82	-183
-6	17	52	112	47	-156
-3	17	52	125	96	-149
-14	18	52	92	127	-185
-11	18	52	130	10	-145
-8	18	52	92	105	-184
-5	18	52	353	366	57
-10	19	52	121	73	-157
-7	19	52	226	189	-91
0	1	53	183	118	-101
-2	2	53	96	198	-118
1	2	53	96	295	-193
-4	3	53	159	304	-142
-1	3	53	97	176	-194
2	3	53	100	42	-200
-6	4	53	103	108	-206
-3	4	53	156	127	-145
0	4	53	148	308	-132
3	4	53	234	218	-126
-8	5	53	107	131	-214
-5	5	53	235	397	-86
-2	5	53	100	528	-200
1	5	53	199	453	-134
4	5	53	105	127	-209
-7	6	53	144	239	-172
-4	6	53	183	186	-130
-1	6	53	101	149	-202
2	6	53	160	106	-144
-9	7	53	172	75	-163
-6	7	53	106	240	-213
-3	7	53	264	402	-124
0	7	53	289	417	-115
-8	8	53	326	373	90
-5	8	53	258	537	-105
-2	8	53	104	614	-208
-7	9	53	215	60	-143
-4	9	53	104	78	-208
0	0	54	96	23	-236
1	1	54	178	472	-115
-1	2	54	123	429	-163
2	2	54	99	356	-198
-3	3	54	98	14	-170
0	3	54	143	5	-134
3	3	54	241	251	-123
-5	4	54	101	246	-202
-2	4	54	219	260	-106
1	4	54	217	394	-104
4	4	54	105	206	-209
-7	5	54	104	88	-208
-4	5	54	179	124	-123
-1	5	54	289	198	-118
2	5	54	184	31	-142
-9	6	54	162	364	-162
-6	6	54	169	175	-135
-3	6	54	186	41	-138
0	6	54	217	290	-120
3	6	54	107	443	-213
-8	7	54	202	86	-144
-5	7	54	214	66	-119
-2	7	54	261	179	-103
1	7	54	108	262	-216
-7	8	54	229	217	-134
-4	8	54	175	55	-149
-1	8	54	213	120	-120
-6	9	54	144	15	-170
-3	9	54	205	187	-135
-1	1	55	146	37	-133
-3	2	55	171	61	-136
0	2	55	198	52	-103
-5	3	55	124	330	-175
-2	3	55	192	155	-128
1	3	55	210	109	-124
-7	4	55	105	219	-210
-4	4	55	99	219	-172
-1	4	55	133	60	-164
2	4	55	102	114	-251
-6	5	55	105	179	-210
-3	5	55	194	89	-138
0	5	55	201	84	-112

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
3	5	55	107	166	-215
-8	6	55	241	256	-127
-5	6	55	145	344	-169
-2	6	55	228	122	-127
1	6	55	210	40	-125
-7	7	55	105	62	-183
-4	7	55	164	39	-155
-1	7	55	109	5	-217
-6	8	55	107	360	-214
-3	8	55	107	219	-215
0	1	56	272	220	37
-2	2	56	354	329	31
1	2	56	203	193	-65
-4	3	56	486	486	32
-1	3	56	210	162	52
2	3	56	756	764	25
-6	4	56	233	228	53
-3	4	56	477	441	31
0	4	56	1202	1209	24
3	4	56	1535	1486	61
-8	5	56	557	566	39
-5	5	56	290	311	44
-2	5	56	748	767	24
1	5	56	704	716	24
4	5	56	672	649	29
-10	6	56	924	878	25
-7	6	56	323	275	61
-4	6	56	194	186	-62
-1	6	56	695	701	30
2	6	56	1074	1077	24
5	6	56	691	636	29
-12	7	56	267	214	59
-9	7	56	158	180	-110
-6	7	56	276	255	47
-3	7	56	1502	1455	47
0	7	56	1966	1892	66
3	7	56	1706	1646	25
6	7	56	701	688	24
-14	8	56	88	82	-177
-11	8	56	155	189	-105
-8	8	56	216	88	-85
-5	8	56	556	559	29
-2	8	56	1108	1063	26
1	8	56	803	803	27
4	8	56	618	612	56
7	8	56	283	193	-86
-16	9	56	91	89	-182
-13	9	56	122	46	-140
-10	9	56	218	51	-100
-7	9	56	212	195	-79
-4	9	56	682	640	61
-1	9	56	796	801	46
2	9	56	708	725	30
5	9	56	304	245	82
8	9	56	247	118	-110
-18	10	56	93	19	-185
-15	10	56	197	129	-110
-12	10	56	280	201	60
-9	10	56	85	5	-171
-6	10	56	936	894	54
-3	10	56	1692	1630	50
0	10	56	1362	1355	34
3	10	56	915	903	36
6	10	56	91	144	-183
-17	11	56	93	109	-186
-14	11	56	158	96	-112
-11	11	56	206	80	-97
-8	11	56	180	198	-92
-5	11	56	633	640	36
-2	11	56	708	727	51
1	11	56	445	450	41
4	11	56	138	186	-128
7	11	56	128	14	-147
-16	12	56	166	231	-127
-13	12	56	288	255	80
-10	12	56	246	142	58
-7	12	56	228	226	-69
-4	12	56	609	577	72
-1	12	56	445	452	52
2	12	56	412	422	45
5	12	56	130	80	-144
-15	13	56	239	78	-72
-12	13	56	278	204	-83
-9	13	56	159	12	-104
-6	13	56	706	680	22
-3	13	56	920	900	53
0	13	56	696	689	29
3	13	56	281	313	-88
-17	14	56	439	455	61
-14	14	56	513	547	35
-11	14	56	89	124	-179
-8	14	56	167	72	-106

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-5	14	56	271	278	62
-2	14	56	409	424	50
1	14	56	92	150	-184
-16	15	56	338	386	60
-13	15	56	180	151	-98
-10	15	56	114	72	-150
-7	15	56	208	164	-92
-4	15	56	261	143	-86
-1	15	56	206	113	-86
-15	16	56	351	312	99
-12	16	56	237	202	-78
-9	16	56	91	98	-183
-6	16	56	234	122	-110
-3	16	56	329	257	69
-14	17	56	464	469	46
-11	17	56	228	162	-103
-8	17	56	167	129	-124
-5	17	56	92	57	-184
-10	18	56	94	8	-188
-7	18	56	93	3	-186
0	0	57	99	898	-244
1	1	57	188	150	-118
-1	2	57	180	949	-124
2	2	57	175	653	-144
-3	3	57	101	598	-176
0	3	57	101	677	-175
3	3	57	179	385	-148
-5	4	57	247	39	-126
-2	4	57	133	151	-168
1	4	57	178	33	-148
-4	5	57	104	409	-208
-1	5	57	105	582	-209
-6	6	57	105	213	-182
-3	6	57	223	271	-135
0	6	57	260	364	-97
-1	1	58	186	28	-126
-3	2	58	206	218	-132
0	2	58	184	16	-126
-5	3	58	193	39	-129
-2	3	58	104	38	-209
1	3	58	104	127	-208
-4	4	58	218	313	-124
-1	4	58	201	24	-124
2	4	58	106	276	-212
-3	5	58	105	204	-210
0	5	58	160	95	-132
-2	6	58	107	44	-213
0	1	59	107	19	-185
-2	2	59	279	67	-109
1	2	59	255	151	-105
-4	3	59	134	186	-181
-1	3	59	249	55	-96
2	3	59	226	54	-139
-3	4	59	108	27	-216
0	4	59	203	202	-116
-2	5	59	159	188	-166
0	0	60	149	4	-116
1	1	60	1930	1972	47
-1	2	60	1919	1972	70
2	2	60	1589	1635	57
-3	3	60	201	6	-69
0	3	60	155	0	-87
3	3	60	391	348	52
-5	4	60	1593	1559	74
-2	4	60	1572	1621	40
1	4	60	1390	1362	36
4	4	60	485	514	40
-7	5	60	634	632	29
-4	5	60	1614	1563	64
-1	5	60	1353	1357	55
2	5	60	443	459	68
5	5	60	137	13	-127
-9	6	60	167	113	-105
-6	6	60	222	7	-74
-3	6	60	402	365	54
0	6	60	114	5	-125
3	6	60	287	202	-84
6	6	60	215	232	-87
-11	7	60	282	255	40
-8	7	60	140	42	-122
-5	7	60	640	594	41
-2	7	60	447	413	43
1	7	60	196	155	-84
4	7	60	245	125	53
7	7	60	91	10	-182
-13	8	60	557	562	39
-10	8	60	280	278	-86
-7	8	60	84	56	-169
-4	8	60	479	473	36
-1	8	60	87	127	-175
2	8	60	204	156	-88
5	8	60	342	280	54

Table 54. (cont).
F(obs), F(calc), and σ_F

($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
8	8	60	670	721	39
-15	9	60	662	734	35
-12	9	60	201	223	-92
-9	9	60	223	22	-77
-6	9	60	157	124	-113
-3	9	60	245	200	-72
0	9	60	156	11	-106
3	9	60	355	346	97
6	9	60	560	552	38
-14	10	60	124	7	-151
-11	10	60	181	192	-97
-8	10	60	286	269	72
-5	10	60	85	28	-171
-2	10	60	242	196	-90
1	10	60	122	35	-141
4	10	60	244	179	-94
-16	11	60	601	650	53
-13	11	60	273	265	-79
-10	11	60	238	228	-71
-7	11	60	290	298	43
-4	11	60	214	50	-80
-1	11	60	218	85	-107
2	11	60	155	202	-119
5	11	60	418	377	50
-15	12	60	390	431	64
-12	12	60	185	23	-99
-9	12	60	217	167	-103
-6	12	60	244	191	-75
-3	12	60	308	308	62
0	12	60	169	42	-102
3	12	60	298	390	67
-14	13	60	137	77	-142
-11	13	60	264	247	-85
-8	13	60	525	538	52
-5	13	60	293	300	71
-2	13	60	207	191	-83
1	13	60	166	76	-120
-13	14	60	124	61	-152
-10	14	60	215	36	-115
-7	14	60	197	40	-108
-4	14	60	92	151	-184
-1	14	60	91	38	-183
-12	15	60	421	404	55
-9	15	60	689	685	35
-6	15	60	550	555	50
-3	15	60	282	376	81
-11	16	60	634	643	36
-8	16	60	686	734	78
-5	16	60	413	413	49
-1	1	61	231	25	-110
-1	1	64	338	431	42
-3	2	64	222	140	-67
0	2	64	892	837	28
-5	3	64	413	366	39
-2	3	64	85	89	-170
1	3	64	600	652	30
-7	4	64	952	946	91
-4	4	64	590	655	44
-1	4	64	609	618	43
2	4	64	486	516	36
-9	5	64	794	800	38
-6	5	64	502	517	58
-3	5	64	425	409	39
0	5	64	400	372	35
3	5	64	89	32	-178
-11	6	64	486	459	43
-8	6	64	504	492	33
-5	6	64	493	475	39
-2	6	64	488	461	35
1	6	64	365	392	58
4	6	64	746	728	38
-13	7	64	423	400	52
-10	7	64	1351	1354	50
-7	7	64	1222	1234	58
-4	7	64	985	958	31
-1	7	64	387	359	50
2	7	64	573	569	57
5	7	64	171	185	-106
-15	8	64	200	143	-108
-12	8	64	310	294	60
-9	8	64	771	762	40
-6	8	64	523	527	26
-3	8	64	124	9	-143
0	8	64	153	68	-107
3	8	64	90	20	-180
6	8	64	182	42	-109
-14	9	64	276	227	79
-11	9	64	833	846	47
-8	9	64	766	741	35
-5	9	64	794	802	45
-2	9	64	543	551	78
1	9	64	90	151	-179

Table 54. (cont).
F(obs), F(calc), and σ_F

($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
4	9	64	91	66	-183
-13	10	64	791	782	32
-10	10	64	1550	1576	55
-7	10	64	1340	1382	22
-4	10	64	766	780	39
-1	10	64	214	202	-99
2	10	64	212	46	-109
5	10	64	128	63	-152
-12	11	64	463	482	71
-9	11	64	826	870	40
-6	11	64	445	493	65
-3	11	64	89	61	-179
0	11	64	110	60	-136
3	11	64	255	247	-90
-14	12	64	137	93	-144
-11	12	64	395	472	54
-8	12	64	348	290	73
-5	12	64	128	181	-144
-2	12	64	90	47	-181
1	12	64	124	87	-151
-13	13	64	468	426	50
-10	13	64	769	780	38
-7	13	64	414	402	45
-4	13	64	92	9	-184
-1	13	64	115	70	-155
-12	14	64	139	83	-131
-9	14	64	236	213	-85
-6	14	64	228	31	-89
-3	14	64	95	209	-189
-8	15	64	119	141	-157
-5	15	64	188	82	-124
0	1	68	105	5	-130
-2	2	68	88	20	-152
1	2	68	713	696	29
-4	3	68	545	538	30
-1	3	68	669	699	38
2	3	68	483	551	32
-6	4	68	579	596	32
-3	4	68	547	565	23
0	4	68	176	24	-65
3	4	68	205	199	-114
-8	5	68	858	859	52
-5	5	68	193	20	-100
-2	5	68	495	490	26
1	5	68	565	604	72
4	5	68	814	827	50
-10	6	68	129	107	-149
-7	6	68	164	114	-108
-4	6	68	568	580	33
-1	6	68	611	608	33
2	6	68	987	967	54
5	6	68	570	559	43
-12	7	68	284	214	79
-9	7	68	330	307	55
-6	7	68	198	114	-113
-3	7	68	171	158	-107
0	7	68	182	1	-106
3	7	68	270	200	70
6	7	68	216	168	-84
-11	8	68	195	119	-98
-8	8	68	90	26	-157
-5	8	68	853	841	40
-2	8	68	948	948	36
1	8	68	1210	1247	45
4	8	68	788	815	31
-13	9	68	142	96	-128
-10	9	68	172	161	-110
-7	9	68	314	327	71
-4	9	68	800	854	33
-1	9	68	1229	1239	24
2	9	68	878	920	40
-12	10	68	173	29	-120
-9	10	68	204	115	-102
-6	10	68	176	91	-123
-3	10	68	268	225	-84
0	10	68	192	1	-89
-11	11	68	157	62	-119
-8	11	68	131	180	-137
-5	11	68	574	567	38
-2	11	68	884	895	63
1	11	68	704	776	36
-10	12	68	93	78	-186
-7	12	68	314	263	-95
-4	12	68	815	837	46
-1	12	68	774	770	84
-9	13	68	92	72	-185
-6	13	68	154	194	-138
0	0	72	1387	1476	130
1	1	72	699	732	100
-1	2	72	674	687	44
2	2	72	859	868	42
-3	3	72	1322	1416	50

Table 54. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
0	3	72	1451	1517	25
3	3	72	855	917	34
-5	4	72	365	374	53
-2	4	72	851	900	42
1	4	72	478	470	40
4	4	72	166	130	-111
-7	5	72	380	332	57
-4	5	72	349	331	59
-1	5	72	481	440	89
2	5	72	312	328	81
5	5	72	152	12	-133
-9	6	72	92	45	-184
-6	6	72	375	356	49
-3	6	72	832	876	27
0	6	72	551	563	35
3	6	72	115	94	-156
-11	7	72	175	155	-125
-8	7	72	203	93	-102
-5	7	72	330	336	55
-2	7	72	329	311	73
1	7	72	252	48	-109
4	7	72	119	47	-155
-10	8	72	93	34	-186
-7	8	72	200	102	-113
-4	8	72	175	92	-120
-1	8	72	226	42	-98
2	8	72	187	66	-117
-9	9	72	249	260	-77
-6	9	72	113	8	-157
-3	9	72	91	10	-183
0	9	72	200	153	-92
-8	10	72	133	9	-144
-5	10	72	216	72	-109
-2	10	72	272	136	-85
-7	11	72	195	137	-104
-4	11	72	159	51	-130
-1	1	76	170	18	-91
-3	2	76	248	290	69
0	2	76	235	28	-97
-5	3	76	397	478	46
-2	3	76	294	311	62
1	3	76	237	61	-90
-7	4	76	94	68	-189
-4	4	76	142	50	-115
-1	4	76	173	125	-120
2	4	76	221	292	-81
-6	5	76	709	710	34
-3	5	76	426	416	90
0	5	76	188	41	-92
3	5	76	503	534	65

APPENDIX G

TABLE 55

Table 55. Adamantane Thiourea Host/Guest Adduct
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
-1	2	0	105	389	-11	0	21	0	114	102	-37
0	3	0	3362	3239	26	-11	22	0	128	118	35
-2	4	0	938	973	8	-8	22	0	93	32	-35
-1	5	0	1748	1568	4	-5	22	0	142	58	36
-3	6	0	79	35	16	-2	22	0	89	54	-38
0	6	0	677	639	15	-10	23	0	178	182	20
-2	7	0	103	129	12	-7	23	0	159	119	24
-4	8	0	862	829	9	-4	23	0	117	55	-44
-1	8	0	813	766	8	-1	23	0	48	17	-65
-3	9	0	423	422	5	-12	24	0	85	9	-60
0	9	0	924	950	10	-9	24	0	130	49	35
-5	10	0	312	298	9	-6	24	0	107	63	-42
-2	10	0	305	279	9	-11	25	0	108	115	-35
-4	11	0	471	470	6	-8	25	0	48	47	-65
-1	11	0	32	31	-43	-13	26	0	113	92	-45
-6	12	0	63	30	-40	-2	3	1	291	277	6
-3	12	0	177	140	11	-1	4	1	1447	1380	12
0	12	0	47	5	-46	-3	5	1	1434	1345	9
-5	13	0	61	39	-34	-5	6	1	1991	1855	11
-2	13	0	150	102	13	-2	6	1	208	211	7
-7	14	0	515	476	9	-4	7	1	84	69	13
-4	14	0	280	229	8	-1	7	1	907	801	4
-1	14	0	82	52	-23	-6	8	1	1322	1313	10
-6	15	0	138	135	19	-3	8	1	108	92	13
-3	15	0	144	150	16	-8	9	1	1238	1200	1
0	15	0	148	134	16	-5	9	1	639	625	5
-8	16	0	254	270	18	-2	9	1	471	520	6
-5	16	0	143	157	14	-7	10	1	254	245	9
-2	16	0	89	72	-28	-4	10	1	519	479	6
-7	17	0	374	414	11	-1	10	1	231	233	8
-4	17	0	213	230	16	-9	11	1	961	958	12
-1	17	0	67	77	-38	-6	11	1	384	384	7
-9	18	0	290	238	14	-3	11	1	271	254	9
-6	18	0	240	224	12	-11	12	1	787	823	7
-3	18	0	164	164	26	-8	12	1	580	589	9
0	18	0	181	152	24	-5	12	1	430	451	8
-8	19	0	286	264	12	-2	12	1	96	77	26
-5	19	0	97	107	-28	-10	13	1	251	265	9
-2	19	0	85	24	-39	-7	13	1	76	48	-24
-10	20	0	411	465	21	-4	13	1	61	17	-33
-7	20	0	352	365	10	-1	13	1	162	166	15
-4	20	0	206	195	16	-12	14	1	648	635	8
-1	20	0	119	97	30	-9	14	1	523	523	10
-9	21	0	244	234	14	-6	14	1	454	457	8
-6	21	0	194	209	19	-3	14	1	282	262	11
-3	21	0	147	152	18	-14	15	1	421	430	9

Table 55. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-11	15	1	422	448	12
-8	15	1	478	477	7
-5	15	1	181	193	13
-2	15	1	97	63	20
-13	16	1	133	143	17
-10	16	1	107	10	-29
-7	16	1	100	81	20
-4	16	1	100	90	24
-1	16	1	132	126	23
-15	17	1	264	256	14
-12	17	1	275	256	10
-9	17	1	241	255	11
-6	17	1	89	82	19
-3	17	1	85	50	-28
-17	18	1	165	166	22
-14	18	1	113	100	25
-11	18	1	123	110	22
-8	18	1	101	47	-28
-5	18	1	162	163	17
-2	18	1	226	225	14
-16	19	1	85	61	-40
-13	19	1	118	129	29
-10	19	1	145	130	21
-7	19	1	177	165	16
-4	19	1	264	258	12
-1	19	1	286	306	13
-18	20	1	126	124	23
-15	20	1	125	106	23
-12	20	1	163	181	26
-9	20	1	173	191	17
-6	20	1	92	62	-36
-3	20	1	102	52	-29
-20	21	1	150	85	34
-17	21	1	107	76	-30
-14	21	1	44	26	-59
-11	21	1	91	49	-38
-8	21	1	66	4	-48
-5	21	1	106	121	-30
-2	21	1	189	200	18
-19	22	1	61	23	-52
-16	22	1	70	35	-46
-13	22	1	75	32	-40
-10	22	1	107	85	-35
-7	22	1	139	112	29
-4	22	1	183	177	26
-1	22	1	131	137	29
-21	23	1	61	20	-56
-18	23	1	61	0	-54
-15	23	1	91	25	-39
-12	23	1	86	56	-39
-9	23	1	72	71	-46
-6	23	1	76	14	-49
-3	23	1	63	19	-53
-20	24	1	112	19	-43
-17	24	1	99	24	-41
-14	24	1	105	7	-35
-11	24	1	90	13	-41
-8	24	1	80	27	-45
-5	24	1	112	105	-37
-16	25	1	124	96	28
-13	25	1	117	29	-46
-10	25	1	67	14	-53
-7	25	1	82	22	-47
-12	26	1	106	53	-33
0	1	2	1131	1030	7
-2	2	2	1874	1905	30
-1	3	2	262	386	-5
-3	4	2	336	257	9
0	4	2	1167	1190	4
-5	5	2	105	82	17
-2	5	2	886	790	7
-4	6	2	221	198	10
-1	6	2	881	784	8
-6	7	2	315	355	5
-3	7	2	1049	1003	7
0	7	2	1550	1501	10
-8	8	2	92	64	18
-5	8	2	882	882	6
-2	8	2	1087	1051	6
-7	9	2	225	226	10
-4	9	2	312	308	6
-1	9	2	537	492	5
-9	10	2	56	10	-31
-6	10	2	631	653	6
-3	10	2	1208	1223	1
0	10	2	844	850	9
-11	11	2	80	6	-36
-8	11	2	265	277	8
-5	11	2	345	357	7
-2	11	2	269	281	11
-10	12	2	298	277	8
-7	12	2	109	96	21

Table 55. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-4	12	2	558	590	6
-1	12	2	352	352	8
-12	13	2	57	61	-33
-9	13	2	308	303	8
-6	13	2	785	786	7
-3	13	2	829	813	6
0	13	2	705	723	11
-14	14	2	220	226	14
-11	14	2	115	133	17
-8	14	2	142	173	13
-5	14	2	120	153	18
-2	14	2	411	421	8
-13	15	2	107	96	21
-10	15	2	60	4	-34
-7	15	2	301	309	13
-4	15	2	297	308	9
-1	15	2	281	254	17
-15	16	2	213	208	12
-12	16	2	100	70	21
-9	16	2	198	224	15
-6	16	2	290	297	9
-3	16	2	433	454	10
0	16	2	266	281	14
-17	17	2	352	380	16
-14	17	2	207	206	12
-11	17	2	83	49	-27
-8	17	2	84	11	-30
-5	17	2	142	123	18
-2	17	2	143	141	26
-16	18	2	207	187	13
-13	18	2	205	199	20
-10	18	2	182	161	16
-7	18	2	189	178	13
-4	18	2	201	205	15
-1	18	2	77	81	-35
-18	19	2	175	154	23
-15	19	2	64	42	-43
-12	19	2	151	138	19
-9	19	2	70	56	-40
-6	19	2	120	139	21
-3	19	2	143	146	21
0	19	2	135	68	-38
-20	20	2	208	205	22
-17	20	2	229	240	15
-14	20	2	158	135	19
-11	20	2	49	29	-52
-8	20	2	88	31	-36
-5	20	2	67	39	-41
-2	20	2	73	7	-44
-19	21	2	92	45	-40
-16	21	2	110	104	-33
-13	21	2	117	163	27
-10	21	2	80	77	-37
-7	21	2	116	108	29
-4	21	2	105	88	-33
-1	21	2	67	31	-52
-21	22	2	148	90	35
-18	22	2	141	117	28
-15	22	2	101	4	26
-12	22	2	83	82	-36
-9	22	2	98	61	-30
-6	22	2	109	69	-33
-3	22	2	119	75	30
0	22	2	113	78	-41
-20	23	2	131	126	28
-17	23	2	155	128	27
-14	23	2	100	66	-37
-11	23	2	85	44	-39
-8	23	2	109	37	-39
-5	23	2	85	49	-44
-2	23	2	112	71	-34
-19	24	2	48	1	-64
-16	24	2	107	40	-33
-13	24	2	97	16	-40
-10	24	2	87	68	-42
-7	24	2	93	78	-37
-4	24	2	70	56	-53
-18	25	2	87	83	-48
-15	25	2	97	47	-40
-12	25	2	89	25	-40
-9	25	2	86	60	-44
-1	2	3	2270	2163	28
-2	4	3	1773	1642	13
-4	5	3	1646	1544	16
-1	5	3	938	945	5
-3	6	3	74	72	16
-5	7	3	898	919	8
-2	7	3	570	506	4
-7	8	3	321	315	7
-4	8	3	454	455	7
-1	8	3	426	437	8
-6	9	3	544	469	7

Table 55. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-3	9	3	308	277	6
-8	10	3	102	109	14
-5	10	3	209	204	10
-2	10	3	273	258	8
-10	11	3	210	216	11
-7	11	3	91	60	19
-4	11	3	293	284	9
-1	11	3	104	99	16
-9	12	3	67	80	-27
-6	12	3	136	139	13
-3	12	3	301	312	8
-11	13	3	83	9	-28
-8	13	3	386	383	7
-5	13	3	67	59	-31
-2	13	3	70	26	-28
-13	14	3	167	188	16
-10	14	3	101	110	24
-7	14	3	50	34	-38
-4	14	3	89	43	24
-1	14	3	113	110	19
-12	15	3	194	190	14
-9	15	3	455	476	11
-6	15	3	289	313	12
-3	15	3	204	198	12
-14	16	3	128	136	21
-11	16	3	469	474	8
-8	16	3	442	441	10
-5	16	3	182	179	13
-2	16	3	152	174	22
-16	17	3	228	216	15
-13	17	3	77	91	-30
-10	17	3	80	15	-33
-7	17	3	100	72	24
-4	17	3	54	28	-44
-1	17	3	107	42	28
-15	18	3	64	15	-45
-12	18	3	330	333	11
-9	18	3	389	416	10
-6	18	3	217	239	18
-3	18	3	154	169	20
-17	19	3	160	163	24
-14	19	3	204	227	17
-11	19	3	326	353	14
-8	19	3	406	394	9
-5	19	3	292	289	13
-2	19	3	142	159	20
-19	20	3	118	95	31
-16	20	3	191	190	18
-13	20	3	84	23	-35
-10	20	3	43	14	-57
-7	20	3	96	99	-38
-4	20	3	110	62	26
-1	20	3	114	130	27
-18	21	3	82	31	-42
-15	21	3	133	109	27
-12	21	3	252	258	18
-9	21	3	222	240	16
-6	21	3	117	120	29
-3	21	3	95	7	-37
-20	22	3	95	50	-47
-17	22	3	148	156	31
-14	22	3	140	145	17
-11	22	3	193	207	29
-8	22	3	256	232	10
-5	22	3	141	117	29
-2	22	3	109	85	-33
-19	23	3	125	41	-36
-16	23	3	47	43	-63
-13	23	3	98	44	-38
-10	23	3	64	17	-51
-7	23	3	101	33	-35
-4	23	3	83	69	-45
-18	24	3	118	96	32
-15	24	3	109	121	-32
-12	24	3	161	165	22
-9	24	3	130	138	31
-6	24	3	106	30	-36
-17	25	3	143	114	29
-14	25	3	107	81	-36
-11	25	3	95	91	-43
-8	25	3	115	68	-43
-1	1	4	53	80	-28
0	2	4	1486	1499	7
-2	3	4	441	473	5
-4	4	4	130	137	11
-1	4	4	538	506	5
-3	5	4	170	180	10
0	5	4	474	433	7
-5	6	4	458	426	6
-2	6	4	499	420	5
-7	7	4	1011	1029	13
-4	7	4	584	611	5

Table 55. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-1	7	4	521	562	6
-6	8	4	356	353	7
-3	8	4	59	6	-21
0	8	4	382	369	10
-8	9	4	677	702	9
-5	9	4	431	420	8
-2	9	4	259	263	8
-10	10	4	1451	1442	15
-7	10	4	1082	1047	12
-4	10	4	550	550	7
-1	10	4	316	302	9
-9	11	4	713	751	10
-6	11	4	521	555	8
-3	11	4	271	301	9
0	11	4	288	305	10
-11	12	4	535	562	11
-8	12	4	175	181	18
-5	12	4	64	22	-29
-2	12	4	111	96	19
-13	13	4	498	511	11
-10	13	4	702	702	10
-7	13	4	382	379	10
-4	13	4	120	119	16
-1	13	4	84	39	-30
-12	14	4	88	65	-25
-9	14	4	290	282	8
-6	14	4	229	218	18
-3	14	4	68	28	-35
0	14	4	112	119	29
-14	15	4	277	272	12
-11	15	4	424	421	8
-8	15	4	168	154	14
-5	15	4	146	127	15
-2	15	4	136	118	18
-16	16	4	265	300	19
-13	16	4	256	263	14
-10	16	4	346	378	12
-7	16	4	194	205	12
-4	16	4	80	22	-30
-1	16	4	96	75	25
-15	17	4	84	15	-37
-12	17	4	81	78	-33
-9	17	4	81	74	-31
-6	17	4	96	80	-30
-3	17	4	235	236	14
0	17	4	326	298	13
-17	18	4	151	144	20
-14	18	4	200	196	14
-11	18	4	263	274	12
-8	18	4	199	212	14
-5	18	4	137	146	21
-2	18	4	160	164	18
-19	19	4	191	223	21
-16	19	4	194	186	21
-13	19	4	183	171	22
-10	19	4	255	269	16
-7	19	4	107	96	27
-4	19	4	62	40	-47
-1	19	4	129	122	27
-18	20	4	112	97	22
-15	20	4	101	64	-38
-12	20	4	66	31	-46
-9	20	4	74	4	-41
-6	20	4	95	100	-30
-3	20	4	230	227	19
0	20	4	253	231	22
-20	21	4	61	44	-54
-17	21	4	88	21	-41
-14	21	4	107	20	-34
-11	21	4	86	96	-44
-8	21	4	104	80	-34
-5	21	4	127	102	31
-2	21	4	137	114	32
-22	22	4	74	8	-62
-19	22	4	85	33	-42
-16	22	4	95	17	-37
-13	22	4	81	8	-31
-10	22	4	90	36	-32
-7	22	4	46	7	-61
-4	22	4	121	76	32
-1	22	4	112	88	-32
-21	23	4	79	13	-45
-18	23	4	105	27	-34
-15	23	4	65	22	-56
-12	23	4	100	41	-37
-9	23	4	69	47	-51
-6	23	4	82	97	-45
-3	23	4	117	128	30
-17	24	4	48	58	-65
-14	24	4	80	21	-43
-11	24	4	60	28	-55
-8	24	4	77	36	-50

Table 55. (cont).
F(obs), F(calc), and σ_F

($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-5	24	4	118	23	-33
-16	25	4	118	34	-34
-13	25	4	93	40	-42
-10	25	4	94	27	-43
-1	3	5	630	639	5
-3	4	5	739	666	7
-2	5	5	253	255	6
-4	6	5	410	443	6
-1	6	5	241	278	6
-6	7	5	346	298	8
-3	7	5	170	169	9
-5	8	5	830	835	11
-2	8	5	813	813	9
-7	9	5	335	355	6
-4	9	5	843	828	10
-1	9	5	1040	1026	9
-9	10	5	302	288	9
-6	10	5	74	56	-22
-3	10	5	230	258	10
-8	11	5	49	40	-37
-5	11	5	609	646	6
-2	11	5	832	872	6
-10	12	5	270	294	11
-7	12	5	392	408	7
-4	12	5	780	755	7
-1	12	5	707	706	7
-12	13	5	92	99	23
-9	13	5	223	212	13
-6	13	5	115	104	22
-3	13	5	94	112	23
-11	14	5	110	102	21
-8	14	5	71	25	-29
-5	14	5	409	439	10
-2	14	5	451	473	10
-13	15	5	166	150	24
-10	15	5	73	59	-33
-7	15	5	137	126	16
-4	15	5	253	256	10
-1	15	5	253	245	11
-15	16	5	330	343	10
-12	16	5	151	158	16
-9	16	5	123	130	15
-6	16	5	186	195	13
-3	16	5	149	142	17
-14	17	5	131	143	19
-11	17	5	203	219	18
-8	17	5	267	275	13
-5	17	5	342	352	10
-2	17	5	243	254	12
-16	18	5	213	232	15
-13	18	5	86	22	-32
-10	18	5	164	149	26
-7	18	5	157	149	22
-4	18	5	148	148	25
-1	18	5	181	160	16
-18	19	5	184	177	23
-15	19	5	136	154	22
-12	19	5	102	80	-30
-9	19	5	57	54	-49
-6	19	5	99	73	-29
-3	19	5	70	36	-43
-17	20	5	80	27	-42
-14	20	5	101	104	-28
-11	20	5	133	119	-36
-8	20	5	126	98	28
-5	20	5	97	98	-39
-2	20	5	88	99	-37
-19	21	5	175	166	27
-16	21	5	130	121	24
-13	21	5	103	2	-40
-10	21	5	92	57	-34
-7	21	5	106	55	29
-4	21	5	84	61	-45
-1	21	5	114	79	29
-21	22	5	135	115	29
-18	22	5	114	83	29
-15	22	5	102	90	-32
-12	22	5	107	33	-41
-9	22	5	101	19	-34
-6	22	5	111	29	-44
-3	22	5	85	26	-41
-20	23	5	82	47	-49
-17	23	5	81	29	-44
-14	23	5	47	8	-63
-11	23	5	63	12	-51
-8	23	5	93	37	-46
-5	23	5	105	31	-43
-16	24	5	134	94	29
-13	24	5	98	52	-39
-10	24	5	57	21	-58
-7	24	5	47	14	-63
-15	25	5	122	65	-39

Table 55. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-12	25	5	115	12	-39
0	0	6	203	71	11
-1	2	6	965	1160	5
-3	3	6	1426	1277	19
0	3	6	1531	1360	7
-2	4	6	1395	1427	15
-4	5	6	328	274	8
-1	5	6	379	352	5
-6	6	6	530	573	8
-3	6	6	1226	1272	2
0	6	6	648	682	6
-5	7	6	322	281	7
-2	7	6	309	275	10
-7	8	6	66	42	-30
-4	8	6	286	237	8
-1	8	6	77	46	-23
-9	9	6	137	103	-39
-6	9	6	253	258	12
-3	9	6	240	242	10
0	9	6	70	114	-30
-8	10	6	34	35	-45
-5	10	6	143	109	17
-2	10	6	88	38	20
-10	11	6	99	68	20
-7	11	6	214	250	9
-4	11	6	267	293	11
-1	11	6	110	104	20
-12	12	6	136	124	23
-9	12	6	108	87	21
-6	12	6	85	81	23
-3	12	6	105	53	24
0	12	6	213	202	19
-11	13	6	274	281	10
-8	13	6	275	277	10
-5	13	6	245	245	10
-2	13	6	291	284	9
-13	14	6	72	70	-32
-10	14	6	244	261	14
-7	14	6	294	306	10
-4	14	6	263	285	10
-1	14	6	69	38	-31
-15	15	6	113	108	28
-12	15	6	82	68	-31
-9	15	6	211	200	12
-6	15	6	231	223	11
-3	15	6	90	30	-28
0	15	6	75	43	-43
-14	16	6	69	28	-42
-11	16	6	170	154	18
-8	16	6	211	203	15
-5	16	6	199	187	13
-2	16	6	79	5	-36
-16	17	6	118	115	23
-13	17	6	226	236	15
-10	17	6	427	424	10
-7	17	6	456	462	9
-4	17	6	241	247	14
-1	17	6	105	94	-33
-18	18	6	131	143	32
-15	18	6	171	180	19
-12	18	6	237	219	16
-9	18	6	233	258	14
-6	18	6	200	208	19
-3	18	6	154	175	20
0	18	6	147	159	31
-17	19	6	111	77	-31
-14	19	6	59	22	-47
-11	19	6	89	79	-36
-8	19	6	119	104	26
-5	19	6	104	20	-34
-2	19	6	99	98	-31
-19	20	6	85	45	-40
-16	20	6	131	106	26
-13	20	6	218	207	19
-10	20	6	261	266	15
-7	20	6	202	201	18
-4	20	6	103	80	-36
-1	20	6	86	36	-43
-21	21	6	110	53	-41
-18	21	6	110	103	-36
-15	21	6	129	121	25
-12	21	6	104	95	-34
-9	21	6	100	70	-39
-6	21	6	115	98	-32
-3	21	6	118	102	31
0	21	6	72	31	-58
-20	22	6	66	18	-51
-17	22	6	103	16	-35
-14	22	6	98	103	-32
-11	22	6	148	152	22
-8	22	6	139	114	33
-5	22	6	95	15	-43

Table 55. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-2	22	6	72	5	-50
-19	23	6	68	63	-54
-16	23	6	137	141	26
-13	23	6	200	191	18
-10	23	6	185	180	24
-7	23	6	129	133	26
-4	23	6	91	70	-47
-15	24	6	102	73	-35
-12	24	6	120	58	29
-9	24	6	89	57	-43
-2	3	7	305	330	6
-1	4	7	359	345	6
-3	5	7	231	229	8
-5	6	7	373	388	6
-2	6	7	250	281	8
-4	7	7	31	7	-42
-1	7	7	225	198	10
-6	8	7	725	694	9
-3	8	7	597	621	7
-8	9	7	837	854	11
-5	9	7	722	744	12
-2	9	7	219	203	12
-7	10	7	165	161	13
-4	10	7	34	40	-46
-1	10	7	197	223	10
-9	11	7	658	655	9
-6	11	7	539	560	10
-3	11	7	81	48	-34
-11	12	7	532	536	11
-8	12	7	609	631	9
-5	12	7	318	321	11
-2	12	7	182	165	16
-10	13	7	84	3	-32
-7	13	7	83	21	-27
-4	13	7	177	192	14
-1	13	7	55	73	-38
-12	14	7	393	394	9
-9	14	7	407	404	10
-6	14	7	93	96	-27
-3	14	7	93	71	21
-14	15	7	266	263	11
-11	15	7	251	250	13
-8	15	7	126	119	21
-5	15	7	68	63	-35
-2	15	7	128	133	20
-13	16	7	116	66	21
-10	16	7	170	185	21
-7	16	7	102	135	26
-4	16	7	117	119	22
-1	16	7	305	310	12
-15	17	7	205	235	17
-12	17	7	267	296	15
-9	17	7	224	231	13
-6	17	7	207	197	16
-3	17	7	132	124	22
-17	18	7	108	121	29
-14	18	7	127	142	24
-11	18	7	95	103	-27
-8	18	7	118	116	24
-5	18	7	89	48	-31
-2	18	7	210	200	15
-16	19	7	54	29	-54
-13	19	7	93	43	-33
-10	19	7	43	50	-58
-7	19	7	110	82	27
-4	19	7	158	153	23
-1	19	7	162	161	20
-18	20	7	73	71	-46
-15	20	7	117	102	23
-12	20	7	64	73	-49
-9	20	7	142	97	29
-6	20	7	120	110	26
-3	20	7	98	21	-41
-20	21	7	81	45	-50
-17	21	7	93	31	-38
-14	21	7	65	36	-51
-11	21	7	46	32	-62
-8	21	7	90	5	-45
-5	21	7	123	95	25
-2	21	7	157	136	28
-19	22	7	77	5	-50
-16	22	7	81	6	-42
-13	22	7	60	10	-54
-10	22	7	64	34	-53
-7	22	7	101	97	-35
-4	22	7	94	72	-37
-18	23	7	73	15	-53
-15	23	7	109	11	-41
-12	23	7	55	1	-58
-9	23	7	92	28	-40
-6	23	7	48	15	-64
-14	24	7	89	2	-43

Table 55. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-11	24	7	89	29	-45
-8	24	7	149	81	34
0	1	8	58	47	-33
-2	2	8	276	352	8
-1	3	8	193	215	9
-3	4	8	255	284	9
0	4	8	418	446	11
-5	5	8	111	123	19
-2	5	8	82	11	22
-4	6	8	148	114	11
-1	6	8	313	270	10
-6	7	8	356	373	7
-3	7	8	490	535	7
0	7	8	873	895	8
-8	8	8	322	364	10
-5	8	8	144	130	16
-2	8	8	292	262	12
-7	9	8	42	19	-39
-4	9	8	201	189	10
-1	9	8	481	491	7
-9	10	8	219	203	11
-6	10	8	317	313	11
-3	10	8	662	667	10
0	10	8	952	965	11
-11	11	8	97	137	-28
-8	11	8	232	248	10
-5	11	8	391	386	8
-2	11	8	440	456	12
-10	12	8	86	94	-27
-7	12	8	62	18	-37
-4	12	8	168	161	14
-1	12	8	376	390	12
-12	13	8	63	39	-42
-9	13	8	135	142	18
-6	13	8	273	271	13
-3	13	8	482	492	10
0	13	8	422	412	14
-14	14	8	87	97	-34
-11	14	8	106	55	26
-8	14	8	185	176	16
-5	14	8	201	198	13
-2	14	8	48	30	-48
-13	15	8	88	71	-31
-10	15	8	130	107	25
-7	15	8	122	101	23
-4	15	8	260	281	12
-1	15	8	175	189	19
-15	16	8	77	40	-37
-12	16	8	41	2	-55
-9	16	8	193	197	14
-6	16	8	299	297	12
-3	16	8	237	212	23
0	16	8	237	229	19
-17	17	8	167	173	22
-14	17	8	145	144	21
-11	17	8	84	47	-33
-8	17	8	82	92	-37
-5	17	8	90	31	-42
-2	17	8	69	20	-43
-16	18	8	111	87	-35
-13	18	8	71	59	-46
-10	18	8	123	116	23
-7	18	8	143	159	23
-4	18	8	129	122	25
-1	18	8	138	108	17
-18	19	8	117	96	28
-15	19	8	88	68	-45
-12	19	8	81	24	-39
-9	19	8	176	179	18
-6	19	8	122	106	26
-3	19	8	136	119	24
0	19	8	163	155	31
-20	20	8	198	187	26
-17	20	8	191	168	17
-14	20	8	104	86	-34
-11	20	8	110	18	-35
-8	20	8	96	13	-28
-5	20	8	90	45	-38
-2	20	8	103	75	-35
-19	21	8	92	102	-40
-16	21	8	92	76	-39
-13	21	8	85	55	-47
-10	21	8	126	83	33
-7	21	8	93	7	-46
-4	21	8	118	13	-37
-1	21	8	90	35	-49
-18	22	8	88	53	-45
-15	22	8	67	14	-50
-12	22	8	85	20	-48
-9	22	8	115	7	-45
-6	22	8	81	12	-42
-3	22	8	76	30	-46

Table 55. (cont).
F(obs), F(calc), and σ_F

($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-17	23	8	57	67	-59
-14	23	8	78	30	-47
-11	23	8	91	36	-37
-8	23	8	89	16	-43
-1	2	9	1030	1031	8
-2	4	9	809	785	7
-4	5	9	403	399	7
-1	5	9	572	578	7
-3	6	9	147	169	12
-5	7	9	376	338	7
-2	7	9	500	496	9
-7	8	9	316	327	8
-4	8	9	188	187	11
-1	8	9	237	233	12
-6	9	9	117	115	18
-3	9	9	148	154	15
-8	10	9	167	163	13
-5	10	9	105	87	22
-2	10	9	149	154	15
-10	11	9	105	98	21
-7	11	9	197	212	14
-4	11	9	72	8	-32
-1	11	9	169	162	17
-9	12	9	126	146	17
-6	12	9	143	166	17
-3	12	9	71	50	-38
-11	13	9	122	68	24
-8	13	9	108	62	23
-5	13	9	223	239	14
-2	13	9	40	14	-53
-13	14	9	131	119	26
-10	14	9	85	5	-36
-7	14	9	64	17	-38
-4	14	9	79	19	-32
-1	14	9	103	65	-30
-12	15	9	82	69	-36
-9	15	9	151	141	20
-6	15	9	280	273	11
-3	15	9	121	100	23
-14	16	9	126	114	22
-11	16	9	129	118	25
-8	16	9	248	246	15
-5	16	9	219	241	17
-2	16	9	88	68	-32
-16	17	9	88	25	-36
-13	17	9	61	37	-45
-10	17	9	117	30	29
-7	17	9	67	34	-43
-4	17	9	87	47	-40
-1	17	9	132	106	30
-15	18	9	130	122	24
-12	18	9	149	154	21
-9	18	9	262	251	16
-6	18	9	222	206	18
-3	18	9	54	6	-54
-17	19	9	132	99	29
-14	19	9	171	185	19
-11	19	9	245	242	14
-8	19	9	194	205	20
-5	19	9	139	135	22
-2	19	9	138	91	26
-19	20	9	133	88	30
-16	20	9	94	43	-40
-13	20	9	118	67	-41
-10	20	9	89	0	-37
-7	20	9	47	6	-62
-4	20	9	83	89	-42
-1	20	9	89	47	-40
-18	21	9	124	8	-42
-15	21	9	118	94	-34
-12	21	9	182	168	21
-9	21	9	166	172	24
-6	21	9	109	81	-37
-3	21	9	86	27	-42
-17	22	9	119	86	-35
-14	22	9	170	164	25
-11	22	9	160	147	25
-8	22	9	120	102	30
-5	22	9	146	102	32
-13	23	9	48	8	-65
-10	23	9	99	12	-43
-1	1	10	33	5	-55
0	2	10	313	357	12
-2	3	10	70	47	-25
-4	4	10	546	569	7
-1	4	10	54	42	-33
-3	5	10	152	138	13
0	5	10	62	99	-36
-5	6	10	281	277	10
-2	6	10	65	61	-30
-7	7	10	755	771	12
-4	7	10	502	536	10

Table 55. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-1	7	10	75	77	-26
-6	8	10	367	378	9
-3	8	10	291	292	9
0	8	10	119	100	20
-8	9	10	298	296	11
-5	9	10	134	111	18
-2	9	10	134	162	17
-10	10	10	435	431	7
-7	10	10	501	511	8
-4	10	10	242	251	14
-1	10	10	81	19	-26
-9	11	10	162	123	15
-6	11	10	167	169	13
-3	11	10	169	157	13
0	11	10	53	25	-53
-11	12	10	236	217	17
-8	12	10	327	340	14
-5	12	10	121	112	21
-2	12	10	40	39	-58
-13	13	10	424	433	11
-10	13	10	416	412	10
-7	13	10	348	358	11
-4	13	10	163	165	16
-1	13	10	41	24	-55
-12	14	10	199	195	17
-9	14	10	86	75	-33
-6	14	10	119	107	26
-3	14	10	92	28	-33
0	14	10	119	144	28
-14	15	10	149	135	19
-11	15	10	154	151	19
-8	15	10	161	164	23
-5	15	10	74	56	-41
-2	15	10	43	59	-58
-16	16	10	155	162	25
-13	16	10	262	263	13
-10	16	10	178	182	19
-7	16	10	175	154	23
-4	16	10	101	62	-30
-1	16	10	122	81	-37
-15	17	10	103	65	26
-12	17	10	88	61	-39
-9	17	10	74	9	-43
-6	17	10	76	15	-42
-3	17	10	137	110	26
0	17	10	166	175	27
-17	18	10	122	49	-46
-14	18	10	102	103	-40
-11	18	10	71	69	-43
-8	18	10	102	72	-37
-5	18	10	118	92	22
-2	18	10	104	81	-30
-19	19	10	104	30	-47
-16	19	10	92	63	-37
-13	19	10	80	69	-44
-10	19	10	73	35	-43
-7	19	10	84	54	-43
-4	19	10	46	37	-62
-1	19	10	111	81	-38
-18	20	10	106	3	-40
-15	20	10	88	30	-40
-12	20	10	60	27	-53
-9	20	10	74	35	-47
-6	20	10	106	91	-33
-3	20	10	130	130	27
-17	21	10	49	55	-65
-14	21	10	83	72	-45
-11	21	10	113	60	-38
-8	21	10	132	101	33
-5	21	10	96	73	-38
-13	22	10	70	43	-51
-10	22	10	92	54	-44
-7	22	10	83	4	-45
-1	3	11	34	17	-46
-3	4	11	195	204	12
-2	5	11	328	335	9
-4	6	11	161	164	15
-1	6	11	559	593	10
-6	7	11	245	255	11
-3	7	11	124	102	17
-5	8	11	64	3	-34
-2	8	11	474	468	8
-7	9	11	192	199	14
-4	9	11	310	323	10
-1	9	11	433	454	6
-9	10	11	96	70	-31
-6	10	11	168	179	13
-3	10	11	100	54	26
-8	11	11	102	87	27
-5	11	11	238	219	11
-2	11	11	399	396	9
-10	12	11	107	35	-32

Table 55. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-7	12	11	242	234	13
-4	12	11	263	260	14
-1	12	11	312	316	11
-12	13	11	84	49	-37
-9	13	11	41	9	-55
-6	13	11	67	2	-38
-3	13	11	107	91	24
-11	14	11	69	78	-41
-8	14	11	176	203	17
-5	14	11	272	265	15
-2	14	11	278	285	12
-13	15	11	44	30	-59
-10	15	11	134	106	34
-7	15	11	225	219	14
-4	15	11	209	204	18
-1	15	11	229	213	19
-15	16	11	115	60	-34
-12	16	11	94	8	-40
-9	16	11	69	28	-43
-6	16	11	73	1	-40
-3	16	11	67	12	-46
-14	17	11	52	24	-57
-11	17	11	58	23	-51
-8	17	11	128	97	23
-5	17	11	122	110	28
-2	17	11	147	120	22
-16	18	11	125	116	26
-13	18	11	115	65	30
-10	18	11	72	17	-49
-7	18	11	86	40	-36
-4	18	11	53	59	-58
-1	18	11	101	68	-43
-18	19	11	135	143	27
-15	19	11	128	110	25
-12	19	11	122	67	-36
-9	19	11	68	63	-51
-6	19	11	101	45	-38
-3	19	11	61	21	-55
-17	20	11	83	21	-44
-14	20	11	121	35	-37
-11	20	11	132	71	-47
-8	20	11	115	65	-39
-5	20	11	95	55	-37
-13	21	11	62	2	-56
-10	21	11	48	11	-64
-7	21	11	109	11	-36
0	0	12	1053	1141	11
-1	2	12	428	410	8
-3	3	12	598	609	12
0	3	12	572	583	10
-2	4	12	109	53	20
-4	5	12	298	297	10
-1	5	12	260	260	12
-6	6	12	340	342	13
-3	6	12	284	261	9
0	6	12	317	312	18
-5	7	12	76	33	-30
-2	7	12	52	39	-43
-7	8	12	176	182	13
-4	8	12	165	157	17
-1	8	12	141	143	22
-9	9	12	186	230	19
-6	9	12	157	160	16
-3	9	12	181	181	16
0	9	12	241	259	14
-8	10	12	115	84	22
-5	10	12	130	121	23
-2	10	12	159	152	16
-10	11	12	77	21	-37
-7	11	12	101	84	27
-4	11	12	97	106	24
-1	11	12	67	12	-44
-12	12	12	43	3	-70
-9	12	12	41	16	-55
-6	12	12	91	48	-30
-3	12	12	96	31	-30
0	12	12	116	31	-43
-11	13	12	102	25	-34
-8	13	12	63	33	-44
-5	13	12	77	70	-36
-2	13	12	87	9	-33
-13	14	12	66	23	-46
-10	14	12	127	89	23
-7	14	12	155	143	25
-4	14	12	52	58	-53
-1	14	12	82	36	-44
-15	15	12	46	29	-75
-12	15	12	90	52	-43
-9	15	12	137	75	34
-6	15	12	50	34	-54
-3	15	12	88	41	-35
0	15	12	46	42	-75

Table 55. (cont).
F(obs), F(calc), and σ_F

($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-14	16	12	101	15	-34
-11	16	12	65	63	-47
-8	16	12	89	103	-35
-5	16	12	94	55	-33
-2	16	12	78	22	-43
-16	17	12	97	37	-45
-13	17	12	145	113	25
-10	17	12	227	192	26
-7	17	12	189	152	21
-4	17	12	115	94	-34
-1	17	12	88	40	-42
-18	18	12	123	83	-43
-15	18	12	119	77	-45
-12	18	12	124	94	30
-9	18	12	130	87	29
-6	18	12	115	69	-37
-3	18	12	106	44	-33
0	18	12	74	43	-62
-17	19	12	90	31	-38
-14	19	12	97	27	-38
-11	19	12	111	100	-41
-8	19	12	108	86	-34
-5	19	12	63	49	-54
-2	19	12	61	11	-57
-13	20	12	150	144	29
-10	20	12	188	184	20
-7	20	12	148	140	28
-2	3	13	102	63	21
-1	4	13	106	90	22
-3	5	13	205	232	16
-5	6	13	324	339	12
-2	6	13	112	126	23
-4	7	13	84	8	-29
-1	7	13	134	150	26
-6	8	13	317	321	11
-3	8	13	74	55	-34
-8	9	13	350	339	11
-5	9	13	184	180	16
-2	9	13	151	157	17
-7	10	13	79	41	-41
-4	10	13	91	59	-32
-1	10	13	96	41	-31
-9	11	13	321	329	14
-6	11	13	171	152	18
-3	11	13	129	102	24
-11	12	13	281	282	15
-8	12	13	239	201	23
-5	12	13	155	150	18
-2	12	13	64	47	-48
-10	13	13	97	39	-37
-7	13	13	85	34	-36
-4	13	13	63	32	-43
-1	13	13	96	47	-33
-12	14	13	216	220	12
-9	14	13	165	170	19
-6	14	13	108	120	25
-3	14	13	98	81	-42
-14	15	13	113	114	29
-11	15	13	136	123	28
-8	15	13	157	145	20
-5	15	13	96	49	-28
-2	15	13	104	22	-37
-13	16	13	79	64	-43
-10	16	13	87	10	-39
-7	16	13	88	6	-37
-4	16	13	97	50	-36
-1	16	13	107	40	-43
-15	17	13	91	89	-49
-12	17	13	144	103	26
-9	17	13	76	91	-45
-6	17	13	92	30	-35
-3	17	13	80	3	-45
-14	18	13	63	22	-55
-11	18	13	90	46	-40
-8	18	13	95	23	-36
-5	18	13	131	65	36
-2	18	13	119	75	-36
-13	19	13	82	53	-50
-10	19	13	103	53	-41
-7	19	13	92	62	-41
0	1	14	54	13	-52
-2	2	14	82	42	-34
-1	3	14	97	48	-34
-3	4	14	102	19	-35
0	4	14	175	153	25
-5	5	14	56	80	-50
-2	5	14	145	167	19
-4	6	14	60	33	-41
-1	6	14	131	130	23
-6	7	14	76	21	-37
-3	7	14	234	224	16
0	7	14	320	292	13

Table 55. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-8	8	14	98	35	-31
-5	8	14	158	156	20
-2	8	14	198	218	14
-7	9	14	80	6	-36
-4	9	14	115	110	25
-1	9	14	149	140	18
-9	10	14	76	17	-38
-6	10	14	170	177	18
-3	10	14	303	298	15
0	10	14	253	235	17
-11	11	14	92	60	-39
-8	11	14	97	100	-32
-5	11	14	166	141	22
-2	11	14	164	135	23
-10	12	14	98	69	-33
-7	12	14	94	48	-31
-4	12	14	131	149	27
-1	12	14	118	102	31
-12	13	14	57	8	-54
-9	13	14	86	50	-45
-6	13	14	185	188	23
-3	13	14	222	222	15
0	13	14	193	194	22
-14	14	14	155	64	40
-11	14	14	82	51	-46
-8	14	14	80	58	-48
-5	14	14	111	66	29
-2	14	14	129	121	26
-13	15	14	78	20	-45
-10	15	14	65	11	-52
-7	15	14	94	77	-37
-4	15	14	99	75	-37
-1	15	14	97	61	-36
-15	16	14	48	56	-65
-12	16	14	71	15	-46
-9	16	14	87	43	-43
-6	16	14	125	83	30
-3	16	14	108	127	-33
0	16	14	134	72	-40
-14	17	14	121	70	31
-11	17	14	98	7	-43
-8	17	14	47	18	-63
-5	17	14	78	25	-45
-2	17	14	95	34	-40
-13	18	14	93	63	-42
-10	18	14	73	47	-50
-7	18	14	75	55	-51
-1	2	15	325	314	16
-2	4	15	274	276	14
-4	5	15	278	285	14
-1	5	15	224	228	14
-3	6	15	66	33	-42
-5	7	15	173	168	17
-2	7	15	126	114	28
-7	8	15	65	50	-48
-4	8	15	121	125	23
-1	8	15	118	87	28
-6	9	15	90	56	-38
-3	9	15	76	31	-41
-8	10	15	102	28	-36
-5	10	15	89	64	-38
-2	10	15	78	30	-42
-10	11	15	79	23	-44
-7	11	15	80	17	-41
-4	11	15	77	69	-43
-1	11	15	86	22	-46
-9	12	15	84	13	-43
-6	12	15	45	13	-61
-3	12	15	103	40	-37
-11	13	15	119	6	-33
-8	13	15	101	53	-37
-5	13	15	46	10	-62
-2	13	15	65	12	-52
-13	14	15	110	37	-32
-10	14	15	73	20	-47
-7	14	15	78	18	-44
-4	14	15	88	42	-40
-1	14	15	80	2	-45
-12	15	15	111	67	-40
-9	15	15	140	126	31
-6	15	15	117	76	-32
-3	15	15	88	59	-38
-14	16	15	92	43	-41
-11	16	15	113	113	-37
-8	16	15	139	117	25
-5	16	15	80	60	-46
-2	16	15	111	39	-36
-10	17	15	49	7	-65
-7	17	15	65	19	-52
-1	1	16	117	34	-32
0	2	16	96	149	-36
-2	3	16	63	39	-47

Table 55. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-4	4	16	120	51	-45
-1	4	16	71	66	-39
-3	5	16	65	69	-46
0	5	16	96	100	-48
-5	6	16	82	78	-40
-2	6	16	89	77	-37
-7	7	16	194	161	20
-4	7	16	109	104	28
-1	7	16	60	58	-50
-6	8	16	120	81	-37
-3	8	16	65	33	-45
0	8	16	101	54	-33
-8	9	16	140	123	30
-5	9	16	106	106	-33
-2	9	16	84	70	-31
-10	10	16	280	268	20
-7	10	16	220	203	16
-4	10	16	158	117	23
-1	10	16	94	53	-35
-9	11	16	160	148	22
-6	11	16	93	105	-38
-3	11	16	72	52	-48
0	11	16	135	59	-51
-11	12	16	129	99	28
-8	12	16	103	43	-41
-5	12	16	72	15	-46
-2	12	16	75	1	-50
-13	13	16	147	101	38
-10	13	16	171	146	21
-7	13	16	113	84	-34
-4	13	16	47	24	-63
-1	13	16	69	10	-53
-12	14	16	58	15	-58
-9	14	16	81	50	-43
-6	14	16	127	26	-40
-3	14	16	78	6	-49
-11	15	16	125	90	33
-8	15	16	88	43	-49
-5	15	16	48	22	-64
-1	3	17	95	85	-38
-3	4	17	99	82	-36
-2	5	17	96	51	-40
-4	6	17	77	78	-44
-1	6	17	98	63	-42
-6	7	17	64	10	-51
-3	7	17	68	18	-50
-5	8	17	161	119	-48
-2	8	17	133	124	27
-7	9	17	102	67	-36
-4	9	17	154	129	26
-1	9	17	176	175	21
-9	10	17	120	57	30
-6	10	17	94	5	-42
-3	10	17	68	35	-53
-8	11	17	89	22	-40
-5	11	17	129	93	31
-2	11	17	140	142	26
-10	12	17	106	46	-32
-7	12	17	113	65	-31
-4	12	17	150	135	28
-1	12	17	149	132	24
-9	13	17	123	36	-34
-6	13	17	130	27	-43
-3	13	17	48	13	-65
-8	14	17	101	9	-48
0	0	18	193	163	35
-1	2	18	87	73	-45
-3	3	18	198	189	22
0	3	18	196	202	22
-2	4	18	104	116	-33
-4	5	18	91	46	-46
-1	5	18	99	60	-38

APPENDIX H

TABLE 56

Table 56. 1,2,4-Trichlorobenzene Thiourea Host/Guest Adduct
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
2	0	0	392	389	2
4	0	0	220	179	3
6	0	0	191	198	4
8	0	0	71	95	10
1	1	0	86	55	2
2	1	0	341	302	2
3	1	0	605	531	2
4	1	0	196	215	3
5	1	0	191	210	4
6	1	0	137	134	5
7	1	0	163	151	5
8	1	0	62	57	11
9	1	0	23	9	-29
0	2	0	155	77	1
1	2	0	28	13	5
2	2	0	75	97	3
3	2	0	493	462	2
4	2	0	56	49	7
5	2	0	32	27	-14
6	2	0	28	32	-17
7	2	0	330	335	4
8	2	0	12	8	-49
9	2	0	49	48	14
1	3	0	63	66	3
2	3	0	358	351	2
3	3	0	779	749	2
4	3	0	44	41	9
5	3	0	96	92	5
6	3	0	22	0	-23
7	3	0	203	201	5
8	3	0	12	9	-50
9	3	0	38	37	-19
0	4	0	310	150	2
1	4	0	847	757	2
2	4	0	526	483	2
3	4	0	151	132	2
4	4	0	25	32	-16
5	4	0	11	6	-43
6	4	0	11	28	-46
7	4	0	210	207	5
8	4	0	174	178	6
9	4	0	13	13	-54
1	5	0	193	190	3
2	5	0	477	465	2
3	5	0	130	145	5
4	5	0	354	373	3
5	5	0	358	342	4
6	5	0	49	32	12
7	5	0	25	33	-25
8	5	0	71	71	10
9	5	0	55	40	14
0	6	0	229	125	3
1	6	0	143	129	3
2	6	0	240	218	3
3	6	0	66	60	6
4	6	0	219	212	4
5	6	0	238	224	4
6	6	0	29	35	-20
7	6	0	51	48	13
8	6	0	59	42	13
9	6	0	98	99	9
1	7	0	55	52	7
2	7	0	98	86	5
3	7	0	109	126	5
4	7	0	84	89	6
5	7	0	528	524	4
6	7	0	50	57	12
7	7	0	93	97	8
8	7	0	85	75	9
0	8	0	544	468	3
1	8	0	10	51	-41
2	8	0	594	561	3
3	8	0	81	86	6
4	8	0	172	183	5
5	8	0	42	20	-15
6	8	0	24	35	-25
7	8	0	82	88	9
8	8	0	130	118	7
1	9	0	89	77	6
2	9	0	444	438	3
3	9	0	11	47	-45
4	9	0	12	20	-47
5	9	0	91	96	8
6	9	0	35	22	-18
7	9	0	13	5	-51
8	9	0	14	9	-39
0	10	0	175	170	4
1	10	0	117	138	5
2	10	0	361	373	4
3	10	0	11	2	-46

Table 56. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
4	10	0	42	35	14
5	10	0	70	54	10
6	10	0	25	2	-25
7	10	0	26	18	-25
8	10	0	80	79	11
1	11	0	129	135	5
2	11	0	172	163	5
3	11	0	89	86	8
4	11	0	68	70	10
5	11	0	243	246	5
6	11	0	40	30	-17
7	11	0	13	31	-54
8	11	0	31	28	-25
0	12	0	228	231	5
1	12	0	131	133	6
2	12	0	12	24	-49
3	12	0	48	23	13
4	12	0	31	5	-20
5	12	0	22	30	-31
6	12	0	93	99	9
7	12	0	36	29	-21
8	12	0	14	13	-57
1	13	0	12	5	-49
2	13	0	12	18	-51
3	13	0	39	35	-17
4	13	0	13	32	-52
5	13	0	122	125	8
6	13	0	27	2	-23
7	13	0	14	0	-56
8	13	0	15	14	-59
0	14	0	161	159	6
1	14	0	100	90	8
2	14	0	78	76	9
3	14	0	13	9	-52
4	14	0	13	5	-53
5	14	0	44	49	13
6	14	0	14	1	-56
7	14	0	50	56	-18
8	14	0	15	30	-61
1	15	0	36	36	-19
2	15	0	62	64	12
3	15	0	131	130	8
4	15	0	31	25	-18
5	15	0	25	9	-30
6	15	0	14	22	-58
7	15	0	15	38	-61
8	15	0	15	14	-61
0	16	0	53	44	14
1	16	0	13	11	-53
2	16	0	13	9	-38
3	16	0	33	49	-24
4	16	0	24	16	-32
5	16	0	14	12	-57
6	16	0	61	54	15
7	16	0	32	39	-29
8	16	0	15	2	-61
1	17	0	13	4	-55
2	17	0	33	37	-24
3	17	0	52	55	16
4	17	0	37	37	-22
5	17	0	14	3	-58
6	17	0	15	1	-59
7	17	0	36	20	-25
0	18	0	108	104	9
1	18	0	34	14	-23
2	18	0	21	14	-38
3	18	0	68	43	13
4	18	0	27	23	-32
5	18	0	14	5	-59
6	18	0	37	26	-24
7	18	0	38	13	-24
1	19	0	14	18	-59
2	19	0	14	12	-58
3	19	0	15	23	-60
4	19	0	23	32	-40
5	19	0	15	17	-60
6	19	0	31	11	-29
0	20	0	59	51	16
1	20	0	48	12	-19
2	20	0	15	14	-60
3	20	0	24	3	-36
4	20	0	15	9	-62
1	21	0	15	2	-61
2	21	0	15	12	-60
-10	0	1	27	3	-26
-8	0	1	57	67	14
-6	0	1	97	116	6
-4	0	1	874	817	2
-2	0	1	146	137	2
0	0	1	8	28	-7
2	0	1	734	754	2
4	0	1	451	439	3

Table 56. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
6	0	1	324	311	4
8	0	1	18	14	-36
-10	1	1	50	56	15
-9	1	1	34	21	-19
-8	1	1	388	380	4
-7	1	1	11	21	-46
-6	1	1	258	242	4
-5	1	1	244	259	3
-4	1	1	152	141	3
-3	1	1	306	259	2
-2	1	1	73	63	3
-1	1	1	117	65	2
0	1	1	20	10	5
1	1	1	105	62	2
2	1	1	1221	1252	2
3	1	1	42	98	8
4	1	1	164	173	4
5	1	1	210	201	4
6	1	1	94	115	7
7	1	1	34	25	-17
8	1	1	40	39	-17
9	1	1	121	111	8
-9	2	1	30	16	-22
-8	2	1	54	54	13
-7	2	1	60	60	10
-6	2	1	18	28	-29
-5	2	1	389	418	3
-4	2	1	391	339	3
-3	2	1	378	338	2
-2	2	1	374	330	2
0	2	1	6	41	-16
1	2	1	99	121	2
2	2	1	374	363	2
3	2	1	509	491	2
4	2	1	131	128	4
5	2	1	438	443	3
6	2	1	60	63	9
7	2	1	155	137	5
8	2	1	12	14	-51
9	2	1	14	27	-56
-9	3	1	79	80	10
-8	3	1	37	43	-18
-7	3	1	100	96	7
-6	3	1	397	370	4
-5	3	1	91	109	5
-4	3	1	144	112	3
-3	3	1	374	317	2
-2	3	1	714	628	2
-1	3	1	1469	1680	2
0	3	1	157	112	2
1	3	1	175	178	2
2	3	1	132	142	3
3	3	1	218	177	3
4	3	1	132	150	4
5	3	1	52	37	10
6	3	1	11	39	-47
7	3	1	12	31	-49
8	3	1	62	48	11
9	3	1	187	183	6
-9	4	1	35	36	-20
-8	4	1	44	52	-16
-7	4	1	12	5	-49
-6	4	1	211	223	4
-5	4	1	126	111	4
-4	4	1	225	243	3
-3	4	1	258	263	2
-2	4	1	329	268	2
-1	4	1	1768	1594	2
0	4	1	420	437	5
1	4	1	119	89	3
2	4	1	282	268	3
3	4	1	152	118	2
4	4	1	301	327	3
5	4	1	317	312	4
6	4	1	253	252	4
7	4	1	40	56	-16
8	4	1	13	2	-51
9	4	1	43	35	-18
-8	5	1	180	168	6
-7	5	1	30	35	-21
-6	5	1	312	324	4
-5	5	1	46	39	10
-4	5	1	105	70	5
-3	5	1	21	5	-11
-2	5	1	102	72	4
-1	5	1	249	248	3
0	5	1	778	701	11
1	5	1	610	531	2
2	5	1	533	479	3
3	5	1	69	93	4
4	5	1	16	7	-26
5	5	1	59	32	9

Table 56. (cont).
F(obs), F(calc), and σ_F

($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
6	5	1	12	3	-48
7	5	1	184	178	5
8	5	1	38	29	-18
-9	6	1	62	55	12
-8	6	1	25	43	-27
-7	6	1	52	30	12
-6	6	1	164	152	5
-5	6	1	185	193	4
-4	6	1	123	95	5
-3	6	1	843	846	3
-2	6	1	98	139	4
-1	6	1	142	141	3
0	6	1	388	314	2
1	6	1	81	76	5
2	6	1	148	118	3
3	6	1	352	344	3
4	6	1	61	59	8
5	6	1	22	52	-23
6	6	1	151	162	5
7	6	1	183	208	6
8	6	1	13	18	-53
-9	7	1	64	72	13
-8	7	1	101	95	8
-7	7	1	12	30	-50
-6	7	1	170	186	5
-5	7	1	28	2	-19
-4	7	1	27	5	-17
-3	7	1	311	308	3
-2	7	1	202	209	3
-1	7	1	172	163	3
0	7	1	311	335	2
1	7	1	580	577	3
2	7	1	57	45	7
3	7	1	46	74	10
4	7	1	19	5	-26
5	7	1	60	64	10
6	7	1	151	142	6
7	7	1	163	175	6
8	7	1	13	13	-53
-8	8	1	63	63	12
-7	8	1	25	1	-25
-6	8	1	141	156	6
-5	8	1	59	54	10
-4	8	1	21	15	-23
-3	8	1	476	483	3
-2	8	1	292	266	3
-1	8	1	43	19	10
0	8	1	199	213	3
1	8	1	183	159	4
2	8	1	54	38	8
3	8	1	130	125	5
4	8	1	397	398	4
5	8	1	66	62	10
6	8	1	36	26	-17
7	8	1	186	183	6
8	8	1	55	48	16
-8	9	1	22	47	-32
-7	9	1	39	23	-16
-6	9	1	260	251	5
-5	9	1	145	156	6
-4	9	1	21	17	-26
-3	9	1	11	11	-46
-2	9	1	89	77	6
-1	9	1	90	73	6
0	9	1	480	445	2
1	9	1	11	12	-44
2	9	1	63	56	8
3	9	1	117	114	6
4	9	1	246	239	5
5	9	1	65	67	10
6	9	1	12	9	-50
7	9	1	23	26	-31
8	9	1	38	28	-19
-8	10	1	41	24	-19
-7	10	1	53	49	13
-6	10	1	200	201	6
-5	10	1	24	15	-25
-4	10	1	31	14	-18
-3	10	1	124	131	6
-2	10	1	57	59	10
-1	10	1	169	142	4
0	10	1	19	8	-18
1	10	1	106	116	6
2	10	1	34	22	-16
3	10	1	132	134	6
4	10	1	366	353	4
5	10	1	47	65	14
6	10	1	13	34	-51
7	10	1	13	2	-55
8	10	1	14	16	-56
-8	11	1	29	29	-25
-7	11	1	13	6	-52

Table 56. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-6	11	1	95	95	8
-5	11	1	24	2	-26
-4	11	1	88	90	8
-3	11	1	19	2	-29
-2	11	1	83	103	7
-1	11	1	162	177	5
0	11	1	100	137	6
1	11	1	234	252	4
2	11	1	47	40	12
3	11	1	28	45	-23
4	11	1	77	72	10
5	11	1	13	21	-51
6	11	1	13	8	-52
7	11	1	92	90	10
8	11	1	25	42	-33
-8	12	1	26	17	-31
-7	12	1	13	5	-55
-6	12	1	13	28	-53
-5	12	1	46	60	15
-4	12	1	50	55	13
-3	12	1	284	288	5
-2	12	1	22	3	-26
-1	12	1	53	51	11
0	12	1	55	61	9
1	12	1	29	14	-20
2	12	1	35	39	-17
3	12	1	12	7	-50
4	12	1	13	35	-53
5	12	1	46	35	15
6	12	1	22	37	-33
7	12	1	50	50	17
8	12	1	14	18	-58
-8	13	1	97	97	11
-7	13	1	65	55	12
-6	13	1	42	29	-20
-5	13	1	13	19	-52
-4	13	1	54	64	13
-3	13	1	13	11	-51
-2	13	1	86	79	8
-1	13	1	12	12	-50
0	13	1	50	52	9
1	13	1	187	180	5
2	13	1	140	150	6
3	13	1	43	41	-15
4	13	1	89	79	9
5	13	1	77	82	11
6	13	1	49	43	16
7	13	1	48	71	-18
8	13	1	15	12	-59
-8	14	1	15	14	-60
-7	14	1	53	46	16
-6	14	1	14	6	-55
-5	14	1	26	39	-29
-4	14	1	56	66	14
-3	14	1	92	85	8
-2	14	1	35	0	-19
-1	14	1	131	124	7
0	14	1	13	16	-36
1	14	1	44	38	-15
2	14	1	40	35	-17
3	14	1	21	23	-32
4	14	1	82	81	10
5	14	1	43	49	-18
6	14	1	27	31	-29
7	14	1	14	5	-58
8	14	1	22	10	-40
-8	15	1	36	23	-25
-7	15	1	15	34	-61
-6	15	1	59	57	15
-5	15	1	50	48	16
-4	15	1	30	30	-18
-3	15	1	54	48	14
-2	15	1	49	38	15
-1	15	1	120	106	7
0	15	1	75	80	7
1	15	1	24	5	-28
2	15	1	80	77	10
3	15	1	53	56	15
4	15	1	13	8	-54
6	15	1	14	7	-58
7	15	1	21	3	-41
8	15	1	45	18	-20
-8	16	1	25	15	-36
-7	16	1	14	12	-59
-6	16	1	14	10	-58
-5	16	1	74	63	12
-4	16	1	23	24	-33
-3	16	1	20	9	-37
-2	16	1	29	8	-22
-1	16	1	89	96	9
0	16	1	33	35	-20
1	16	1	31	33	-21

Table 56. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
2	16	1	56	63	11
3	16	1	32	17	-24
4	16	1	41	30	-19
5	16	1	56	63	17
6	16	1	15	25	-59
7	16	1	15	11	-60
8	16	1	15	13	-62
-8	17	1	23	20	-40
-7	17	1	15	4	-60
-6	17	1	14	2	-59
-5	17	1	14	23	-58
-4	17	1	52	50	17
-3	17	1	14	8	-56
-2	17	1	42	33	-18
-1	17	1	58	76	14
0	17	1	13	1	-39
1	17	1	14	3	-55
2	17	1	59	52	14
3	17	1	24	24	-34
4	17	1	14	9	-58
5	17	1	31	27	-29
6	17	1	15	12	-60
7	17	1	29	6	-31
-7	18	1	15	10	-61
-6	18	1	31	9	-29
-5	18	1	14	3	-59
-4	18	1	58	54	16
-3	18	1	23	8	-36
-2	18	1	14	15	-56
-1	18	1	14	12	-57
0	18	1	14	21	-40
1	18	1	28	14	-28
2	18	1	68	58	13
3	18	1	14	13	-59
4	18	1	14	2	-59
5	18	1	15	14	-61
6	18	1	46	39	-21
-6	19	1	15	4	-62
-5	19	1	15	14	-61
-4	19	1	15	2	-59
-3	19	1	14	14	-59
-2	19	1	14	26	-59
-1	19	1	14	6	-59
0	19	1	14	22	-41
1	19	1	14	10	-59
2	19	1	58	63	17
3	19	1	40	23	-22
4	19	1	15	3	-60
5	19	1	33	22	-28
-5	20	1	31	20	-30
-4	20	1	15	23	-62
-3	20	1	15	13	-61
-2	20	1	15	23	-61
-1	20	1	36	34	-26
0	20	1	25	3	-29
1	20	1	15	2	-60
2	20	1	15	15	-61
3	20	1	39	2	-23
4	20	1	15	11	-61
-3	21	1	15	0	-61
-2	21	1	15	6	-61
-1	21	1	15	29	-63
0	21	1	33	19	-21
1	21	1	40	11	-23
2	21	1	29	9	-31
-10	0	2	13	9	-53
-8	0	2	64	76	11
-6	0	2	393	367	3
-4	0	2	9	34	-37
-2	0	2	1269	1195	2
0	0	2	109	66	1
2	0	2	153	66	3
4	0	2	496	413	3
6	0	2	97	121	6
8	0	2	243	233	5
-10	1	2	13	10	-53
-9	1	2	95	95	9
-8	1	2	37	53	-18
-7	1	2	61	67	10
-6	1	2	205	210	4
-5	1	2	168	160	4
-4	1	2	133	99	3
-3	1	2	614	568	2
-2	1	2	1303	1262	2
-1	1	2	45	38	3
0	1	2	150	119	2
1	1	2	131	132	3
2	1	2	108	106	3
3	1	2	88	114	5
4	1	2	768	681	3
5	1	2	159	141	4
6	1	2	42	52	12

Table 56. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
7	1	2	59	51	11
8	1	2	140	141	7
9	1	2	20	22	-28
-10	2	2	13	30	-54
-9	2	2	202	198	6
-8	2	2	92	88	8
-7	2	2	126	117	6
-6	2	2	217	199	4
-5	2	2	174	130	4
-4	2	2	357	354	3
-3	2	2	429	359	2
-2	2	2	482	491	2
-1	2	2	200	165	2
0	2	2	500	434	14
1	2	2	109	1458	-2
2	2	2	779	739	2
3	2	2	464	457	3
4	2	2	328	336	3
5	2	2	28	29	-17
6	2	2	29	17	-18
7	2	2	12	9	-50
8	2	2	136	156	7
-10	3	2	44	38	-17
-9	3	2	177	168	6
-8	3	2	22	1	-28
-7	3	2	133	134	6
-6	3	2	222	217	4
-5	3	2	129	99	4
-4	3	2	368	376	3
-3	3	2	618	562	2
-2	3	2	1777	1531	2
-1	3	2	8	45	-31
0	3	2	251	213	3
1	3	2	242	247	2
2	3	2	393	281	2
3	3	2	140	108	4
4	3	2	130	121	5
5	3	2	161	174	4
6	3	2	221	278	4
7	3	2	68	53	10
8	3	2	28	28	-27
-9	4	2	76	74	11
-8	4	2	73	72	9
-7	4	2	66	65	10
-6	4	2	259	254	4
-5	4	2	226	243	4
-4	4	2	274	270	3
-3	4	2	437	378	5
-2	4	2	433	264	2
-1	4	2	28	40	-11
0	4	2	53	58	4
1	4	2	807	843	2
2	4	2	390	348	3
3	4	2	56	73	10
4	4	2	199	206	4
5	4	2	32	11	-15
6	4	2	34	38	-18
7	4	2	26	7	-23
8	4	2	42	42	-18
-9	5	2	98	94	9
-8	5	2	12	4	-50
-7	5	2	153	152	6
-6	5	2	146	146	5
-5	5	2	10	9	-42
-4	5	2	619	580	3
-3	5	2	266	231	3
-2	5	2	189	103	3
-1	5	2	652	517	2
0	5	2	82	60	3
1	5	2	170	141	3
2	5	2	13	20	-26
3	5	2	89	92	5
4	5	2	197	213	4
5	5	2	25	23	-21
6	5	2	268	251	5
7	5	2	23	27	-27
8	5	2	107	97	8
-9	6	2	34	40	-21
-8	6	2	24	32	-27
-7	6	2	323	325	5
-6	6	2	279	302	4
-5	6	2	24	13	-20
-4	6	2	32	8	-14
-3	6	2	70	88	6
-2	6	2	32	107	-11
-1	6	2	762	748	3
0	6	2	154	192	7
1	6	2	147	122	4
2	6	2	44	14	9
3	6	2	192	201	4
4	6	2	169	187	4
5	6	2	181	188	5

Table 56. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
6	6	2	77	70	9
7	6	2	37	19	-17
8	6	2	100	104	9
-9	7	2	26	10	-28
-8	7	2	12	28	-51
-7	7	2	13	4	-52
-6	7	2	12	14	-49
-5	7	2	37	33	-14
-4	7	2	38	32	13
-3	7	2	53	64	8
-2	7	2	469	402	3
-1	7	2	774	800	3
0	7	2	292	285	5
1	7	2	41	40	10
2	7	2	70	85	7
3	7	2	280	285	4
4	7	2	82	88	7
5	7	2	68	60	9
6	7	2	118	126	7
7	7	2	13	13	-52
8	7	2	19	15	-28
-9	8	2	14	42	-56
-8	8	2	109	111	8
-7	8	2	177	184	6
-6	8	2	28	9	-21
-5	8	2	35	37	-16
-4	8	2	202	199	4
-3	8	2	64	33	8
-2	8	2	125	102	5
-1	8	2	283	258	3
0	8	2	274	279	3
1	8	2	148	135	4
2	8	2	37	35	13
3	8	2	276	288	4
4	8	2	12	5	-47
5	8	2	38	31	-16
6	8	2	100	99	8
7	8	2	13	15	-53
8	8	2	13	8	-55
-8	9	2	13	6	-53
-7	9	2	85	82	9
-6	9	2	53	39	12
-5	9	2	17	1	-32
-4	9	2	418	435	4
-3	9	2	11	1	-45
-2	9	2	11	8	-44
-1	9	2	262	226	4
0	9	2	253	234	7
1	9	2	106	112	5
2	9	2	42	66	13
3	9	2	23	34	-26
4	9	2	54	53	11
5	9	2	40	36	-15
6	9	2	313	297	5
7	9	2	13	11	-53
8	9	2	73	68	12
-8	10	2	55	54	10
-7	10	2	48	51	14
-6	10	2	12	16	-49
-5	10	2	56	51	11
-4	10	2	205	209	5
-3	10	2	11	39	-46
-2	10	2	243	225	4
-1	10	2	218	210	4
0	10	2	214	211	5
1	10	2	76	99	8
2	10	2	298	307	4
3	10	2	183	182	5
4	10	2	85	94	8
5	10	2	40	24	-16
6	10	2	14	8	-55
7	10	2	40	33	-20
8	10	2	14	9	-57
-8	11	2	62	56	13
-7	11	2	39	30	-18
-6	11	2	12	3	-51
-5	11	2	27	12	-23
-4	11	2	147	144	6
-3	11	2	18	8	-31
-2	11	2	12	27	-47
-1	11	2	120	151	6
0	11	2	32	11	-12
1	11	2	97	95	7
2	11	2	18	35	-34
3	11	2	137	126	6
4	11	2	72	57	9
5	11	2	36	10	-18
6	11	2	144	146	7
7	11	2	13	2	-55
8	11	2	14	2	-57
-8	12	2	32	4	-25
-7	12	2	65	76	9

Table 56. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-6	12	2	75	77	10
-5	12	2	25	41	-26
-4	12	2	26	5	-24
-3	12	2	36	31	-17
-2	12	2	12	6	-49
-1	12	2	201	207	5
0	12	2	80	82	6
1	12	2	46	26	13
2	12	2	31	13	-20
3	12	2	233	233	5
4	12	2	25	38	-26
5	12	2	30	13	-23
6	12	2	31	24	-25
7	12	2	26	16	-30
8	12	2	25	35	-35
-8	13	2	44	37	-19
-7	13	2	26	29	-29
-6	13	2	47	44	16
-5	13	2	21	21	-32
-4	13	2	89	90	9
-3	13	2	46	37	14
-2	13	2	172	179	6
-1	13	2	179	163	6
0	13	2	119	120	8
1	13	2	12	20	-51
2	13	2	59	60	12
3	13	2	94	107	9
4	13	2	79	91	10
5	13	2	13	20	-38
6	13	2	42	36	-19
7	13	2	14	6	-58
8	13	2	39	31	-22
-8	14	2	53	32	17
-7	14	2	14	26	-57
-6	14	2	74	71	11
-5	14	2	100	96	9
-4	14	2	41	36	-17
-3	14	2	47	59	15
-2	14	2	13	14	-53
-1	14	2	43	43	-16
0	14	2	27	1	-21
1	14	2	122	110	7
2	14	2	60	53	12
3	14	2	13	12	-54
4	14	2	96	98	9
5	14	2	20	10	-38
6	14	2	37	18	-22
7	14	2	40	43	-23
8	14	2	27	23	-33
-8	15	2	15	20	-60
-7	15	2	14	2	-58
-6	15	2	32	27	-25
-5	15	2	13	6	-54
-4	15	2	66	58	9
-3	15	2	64	70	12
-2	15	2	13	23	-53
-1	15	2	27	23	-25
0	15	2	31	31	-16
1	15	2	13	5	-54
2	15	2	13	13	-55
3	15	2	58	53	17
4	15	2	14	11	-55
5	15	2	45	42	-18
6	15	2	27	40	-32
7	15	2	29	7	-29
8	15	2	15	11	-61
-8	16	2	39	19	-23
-7	16	2	14	11	-59
-6	16	2	37	11	-22
-5	16	2	14	44	-58
-4	16	2	38	35	-20
-3	16	2	28	1	-26
-2	16	2	39	42	-14
-1	16	2	44	32	-20
0	16	2	25	10	-16
1	16	2	150	157	6
2	16	2	48	23	16
3	16	2	14	11	-56
4	16	2	39	47	-22
5	16	2	22	28	-38
6	16	2	22	17	-38
7	16	2	15	15	-60
-8	17	2	15	16	-62
-7	17	2	15	7	-59
-6	17	2	14	18	-59
-5	17	2	33	28	-26
-4	17	2	37	6	-21
-3	17	2	32	47	-25
-2	17	2	84	80	11
-1	17	2	14	6	-55
0	17	2	30	5	-22
1	17	2	33	24	-24

Table 56. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
2	17	2	39	24	-21
3	17	2	20	2	-40
4	17	2	57	60	16
5	17	2	21	26	-41
6	17	2	15	8	-60
7	17	2	15	17	-62
-7	18	2	15	9	-61
-6	18	2	40	39	-23
-5	18	2	14	22	-59
-4	18	2	14	13	-58
-3	18	2	14	11	-58
-2	18	2	14	2	-57
-1	18	2	14	15	-57
0	18	2	14	18	-40
1	18	2	25	33	-33
2	18	2	30	42	-29
3	18	2	21	3	-41
4	18	2	32	22	-28
5	18	2	15	15	-60
6	18	2	28	5	-34
-6	19	2	30	9	-31
-5	19	2	15	13	-60
-4	19	2	14	5	-59
-3	19	2	24	6	-36
-2	19	2	63	61	15
-1	19	2	14	8	-59
0	19	2	42	24	-15
1	19	2	15	2	-60
3	19	2	14	4	-59
4	19	2	39	37	-25
5	19	2	15	2	-62
-5	20	2	15	21	-62
-4	20	2	15	7	-60
-3	20	2	15	15	-61
-2	20	2	27	23	-34
-1	20	2	15	3	-60
0	20	2	28	11	-32
1	20	2	52	37	-18
2	20	2	29	15	-31
3	20	2	15	5	-60
-3	21	2	15	23	-62
-2	21	2	15	2	-61
-1	21	2	15	0	-61
0	21	2	15	19	-61
1	21	2	15	6	-61
-10	0	3	178	172	6
-8	0	3	24	16	-27
-6	0	3	72	50	7
-4	0	3	945	857	3
-2	0	3	827	756	2
0	0	3	1145	1262	19
2	0	3	94	92	4
4	0	3	224	239	4
6	0	3	202	183	5
8	0	3	119	122	7
-10	1	3	14	25	-56
-9	1	3	66	53	11
-8	1	3	71	67	10
-7	1	3	305	288	4
-6	1	3	59	48	8
-5	1	3	382	345	3
-4	1	3	717	663	3
-3	1	3	506	590	2
-2	1	3	148	134	3
-1	1	3	333	296	2
0	1	3	1002	1018	19
1	1	3	80	22	4
2	1	3	43	39	7
3	1	3	307	340	3
4	1	3	132	136	4
5	1	3	109	65	5
6	1	3	59	65	10
7	1	3	13	26	-55
8	1	3	55	50	13
9	1	3	13	24	-54
-10	2	3	61	55	13
-9	2	3	53	49	13
-8	2	3	44	37	15
-7	2	3	113	114	7
-6	2	3	10	25	-42
-5	2	3	128	130	4
-4	2	3	239	240	3
-3	2	3	82	74	5
-2	2	3	282	744	-2
-1	2	3	51	45	5
0	2	3	492	458	14
1	2	3	9	73	-35
2	2	3	133	143	3
3	2	3	266	256	3
4	2	3	115	119	5
5	2	3	140	125	5
6	2	3	52	43	12

Table 56. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
7	2	3	247	250	5
8	2	3	13	17	-52
-10	3	3	42	43	-18
-9	3	3	69	77	10
-8	3	3	51	46	13
-7	3	3	467	473	4
-6	3	3	55	38	9
-5	3	3	50	51	9
-4	3	3	453	444	3
-3	3	3	160	188	3
-2	3	3	431	382	2
-1	3	3	14	15	-20
0	3	3	45	68	7
1	3	3	103	135	4
2	3	3	454	474	3
3	3	3	947	880	9
4	3	3	106	135	6
5	3	3	64	85	8
6	3	3	24	3	-25
7	3	3	89	101	9
8	3	3	72	68	10
-10	4	3	66	65	12
-9	4	3	56	36	12
-8	4	3	83	80	9
-7	4	3	120	109	7
-6	4	3	74	64	8
-5	4	3	317	290	3
-4	4	3	196	218	3
-3	4	3	452	427	2
-2	4	3	1234	1174	2
-1	4	3	16	12	-19
0	4	3	508	462	11
1	4	3	96	70	4
2	4	3	72	71	6
3	4	3	11	8	-31
4	4	3	71	66	8
5	4	3	105	101	6
6	4	3	147	139	6
7	4	3	152	157	6
8	4	3	118	120	8
-9	5	3	51	43	14
-8	5	3	157	160	6
-7	5	3	108	97	7
-6	5	3	31	21	-17
-5	5	3	371	384	3
-4	5	3	249	242	3
-3	5	3	285	198	2
-2	5	3	283	240	3
-1	5	3	122	115	4
0	5	3	663	593	33
1	5	3	22	67	-15
2	5	3	126	131	4
3	5	3	85	96	5
4	5	3	33	26	-15
5	5	3	80	62	8
6	5	3	23	16	-27
7	5	3	103	105	8
8	5	3	35	1	-20
-9	6	3	134	135	7
-8	6	3	67	69	10
-7	6	3	148	143	6
-6	6	3	84	101	7
-5	6	3	192	191	4
-4	6	3	158	130	4
-3	6	3	598	472	3
-2	6	3	352	303	3
-1	6	3	35	25	10
0	6	3	477	423	5
1	6	3	173	216	3
2	6	3	62	72	8
3	6	3	33	38	-15
4	6	3	52	46	10
5	6	3	352	376	4
6	6	3	103	95	7
7	6	3	13	4	-53
8	6	3	80	66	10
-9	7	3	86	88	10
-8	7	3	46	36	14
-7	7	3	103	102	7
-6	7	3	17	9	-32
-5	7	3	313	320	4
-4	7	3	95	90	6
-3	7	3	597	460	3
-2	7	3	10	34	-41
-1	7	3	148	99	4
0	7	3	164	110	4
1	7	3	503	494	3
2	7	3	28	52	-18
3	7	3	155	192	5
4	7	3	161	157	5
5	7	3	158	194	6
6	7	3	23	8	-27

Table 56. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
7	7	3	22	10	-31
8	7	3	51	51	17
-9	8	3	61	64	13
-8	8	3	97	106	8
-7	8	3	12	1	-50
-6	8	3	12	3	-48
-5	8	3	155	144	5
-4	8	3	31	10	-17
-3	8	3	36	97	-14
-2	8	3	577	544	3
-1	8	3	134	108	4
0	8	3	63	82	13
1	8	3	235	220	4
2	8	3	45	46	12
3	8	3	61	70	9
4	8	3	98	108	7
5	8	3	213	217	5
6	8	3	12	16	-51
7	8	3	13	26	-54
8	8	3	62	59	14
-8	9	3	13	26	-53
-7	9	3	12	17	-50
-6	9	3	92	95	8
-5	9	3	60	62	10
-4	9	3	54	49	11
-3	9	3	184	166	4
-2	9	3	36	13	-15
-1	9	3	140	143	5
0	9	3	11	46	-31
1	9	3	36	38	-15
2	9	3	414	416	4
3	9	3	47	52	12
4	9	3	28	24	-21
5	9	3	26	3	-26
6	9	3	20	2	-33
7	9	3	13	13	-54
8	9	3	77	80	12
-8	10	3	36	28	-20
-7	10	3	13	18	-52
-6	10	3	35	29	-19
-5	10	3	67	71	10
-4	10	3	33	18	-17
-3	10	3	19	16	-28
-2	10	3	455	475	4
-1	10	3	79	85	7
0	10	3	82	78	5
1	10	3	52	32	12
2	10	3	52	54	12
3	10	3	21	10	-28
4	10	3	25	15	-24
5	10	3	81	72	10
6	10	3	13	7	-53
7	10	3	52	35	15
8	10	3	77	76	12
-8	11	3	13	6	-55
-7	11	3	82	83	10
-6	11	3	92	85	8
-5	11	3	211	222	6
-4	11	3	12	21	-48
-3	11	3	12	24	-47
-2	11	3	93	102	7
-1	11	3	12	36	-48
0	11	3	73	62	16
1	11	3	251	245	5
2	11	3	195	194	5
3	11	3	12	5	-50
4	11	3	71	70	10
5	11	3	142	145	7
6	11	3	30	28	-21
7	11	3	35	9	-22
8	11	3	38	32	-22
-8	12	3	25	9	-31
-7	12	3	13	2	-38
-6	12	3	61	62	12
-5	12	3	61	83	12
-4	12	3	137	112	6
-3	12	3	12	4	-50
-2	12	3	77	64	9
-1	12	3	80	83	8
0	12	3	164	175	8
1	12	3	97	99	8
2	12	3	140	141	6
3	12	3	23	12	-30
4	12	3	13	8	-52
5	12	3	159	154	7
6	12	3	52	50	15
7	12	3	14	10	-57
8	12	3	41	3	-21
-8	13	3	14	5	-58
-7	13	3	41	0	-18
-6	13	3	13	25	-54
-5	13	3	111	112	8

Table 56. (cont).
F(obs), F(calc), and σ_F

($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-4	13	3	46	28	14
-3	13	3	126	97	7
-2	13	3	51	59	13
-1	13	3	31	25	-20
0	13	3	94	103	6
1	13	3	62	78	12
2	13	3	107	89	8
3	13	3	13	6	-52
4	13	3	13	16	-52
5	13	3	38	46	-21
6	13	3	27	8	-29
7	13	3	32	4	-26
8	13	3	15	21	-61
-8	14	3	25	28	-36
-7	14	3	42	37	-19
-6	14	3	13	3	-54
-5	14	3	24	15	-30
-4	14	3	76	73	10
-3	14	3	66	65	11
-2	14	3	125	135	7
-1	14	3	22	23	-29
0	14	3	96	98	12
1	14	3	68	72	12
2	14	3	50	56	15
3	14	3	59	57	13
4	14	3	13	25	-55
5	14	3	57	51	14
6	14	3	14	29	-58
7	14	3	39	34	-22
8	14	3	36	27	-25
-8	15	3	15	4	-60
-7	15	3	85	83	12
-6	15	3	21	16	-36
-5	15	3	23	4	-32
-4	15	3	48	30	-22
-3	15	3	42	69	-18
-2	15	3	13	19	-53
-1	15	3	30	43	-24
0	15	3	52	55	12
1	15	3	33	5	-22
2	15	3	21	22	-28
3	15	3	118	110	8
4	15	3	14	8	-55
5	15	3	14	8	-58
6	15	3	39	41	-23
7	15	3	15	3	-60
8	15	3	15	9	-61
-8	16	3	15	6	-60
-7	16	3	28	14	-32
-6	16	3	50	47	17
-5	16	3	14	6	-56
-4	16	3	13	2	-55
-3	16	3	64	69	13
-2	16	3	41	42	-18
-1	16	3	23	19	-25
0	16	3	39	20	12
1	16	3	44	40	-17
2	16	3	20	12	-39
3	16	3	36	19	-23
4	16	3	14	4	-57
5	16	3	14	11	-58
6	16	3	15	6	-60
7	16	3	15	36	-63
-8	17	3	15	6	-61
-7	17	3	63	42	15
-6	17	3	23	29	-37
-5	17	3	14	2	-57
-4	17	3	27	34	-31
-3	17	3	14	6	-55
-2	17	3	14	17	-56
-1	17	3	14	12	-55
0	17	3	53	45	-20
1	17	3	14	3	-57
2	17	3	14	19	-57
3	17	3	83	82	12
4	17	3	15	35	-60
5	17	3	14	3	-59
6	17	3	15	30	-62
-7	18	3	23	3	-39
-6	18	3	23	21	-39
-5	18	3	14	12	-58
-4	18	3	44	40	-20
-3	18	3	45	31	-19
-2	18	3	23	7	-35
-1	18	3	48	33	-18
0	18	3	74	74	19
1	18	3	14	3	-58
2	18	3	14	1	-59
3	18	3	15	10	-60
4	18	3	15	9	-60
5	18	3	15	5	-60
-6	19	3	15	7	-61

Table 56. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-5	19	3	15	12	-61
-4	19	3	46	32	-20
-3	19	3	42	43	-23
-2	19	3	15	4	-59
-1	19	3	30	18	-29
0	19	3	50	49	-22
1	19	3	15	3	-59
2	19	3	15	17	-60
3	19	3	15	12	-60
4	19	3	15	16	-61
-5	20	3	15	8	-61
-4	20	3	28	12	-33
-3	20	3	15	17	-61
-2	20	3	15	23	-60
-1	20	3	15	9	-60
0	20	3	26	20	-28
1	20	3	15	4	-61
2	20	3	45	7	-19
3	20	3	31	16	-29
-2	21	3	15	3	-61
-1	21	3	15	9	-61
0	21	3	28	8	-28
1	21	3	15	2	-61
-10	0	4	81	78	10
-8	0	4	273	272	5
-6	0	4	268	240	4
-4	0	4	367	333	3
-2	0	4	293	275	2
0	0	4	660	485	2
2	0	4	508	502	3
4	0	4	129	188	5
6	0	4	95	97	8
8	0	4	13	20	-38
-10	1	4	13	23	-54
-9	1	4	36	41	-19
-8	1	4	376	368	4
-7	1	4	57	83	10
-6	1	4	71	73	7
-5	1	4	284	267	3
-4	1	4	119	167	4
-3	1	4	228	203	3
-2	1	4	583	542	2
-1	1	4	741	644	2
0	1	4	439	389	7
1	1	4	83	43	5
2	1	4	174	162	3
3	1	4	23	3	-21
4	1	4	10	10	-43
5	1	4	170	161	5
6	1	4	205	178	5
7	1	4	97	107	8
8	1	4	54	51	16
9	1	4	70	57	13
-10	2	4	91	77	9
-9	2	4	33	8	-21
-8	2	4	61	45	12
-7	2	4	141	140	5
-6	2	4	155	149	4
-5	2	4	539	531	3
-4	2	4	243	217	3
-3	2	4	39	49	9
-2	2	4	308	239	2
-1	2	4	116	106	4
0	2	4	227	173	5
1	2	4	9	3	-37
2	2	4	216	263	3
3	2	4	37	8	-13
4	2	4	81	107	6
5	2	4	268	262	4
6	2	4	25	15	-26
7	2	4	27	23	-24
8	2	4	37	31	-18
-10	3	4	105	109	9
-9	3	4	51	39	14
-8	3	4	152	147	6
-7	3	4	18	12	-31
-6	3	4	105	96	6
-5	3	4	11	8	-45
-4	3	4	227	257	3
-3	3	4	336	324	3
-2	3	4	13	96	-25
-1	3	4	635	993	2
0	3	4	511	645	11
1	3	4	221	177	3
2	3	4	76	56	6
3	3	4	26	7	-16
4	3	4	82	82	7
5	3	4	243	241	4
6	3	4	13	42	-52
7	3	4	85	86	9
8	3	4	26	3	-27
-10	4	4	28	0	-28

Table 56. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-9	4	4	13	37	-52
-8	4	4	149	151	6
-7	4	4	42	30	14
-6	4	4	278	262	4
-5	4	4	591	556	3
-4	4	4	282	259	3
-3	4	4	456	441	2
-2	4	4	216	218	3
-1	4	4	146	102	4
0	4	4	181	197	2
1	4	4	384	382	3
2	4	4	663	626	3
3	4	4	192	219	4
4	4	4	243	267	4
5	4	4	132	123	6
6	4	4	81	78	9
7	4	4	97	101	9
8	4	4	13	15	-54
-10	5	4	128	125	8
-9	5	4	13	20	-52
-8	5	4	142	135	6
-7	5	4	28	39	-20
-6	5	4	86	79	7
-5	5	4	228	206	4
-4	5	4	50	24	9
-3	5	4	289	263	3
-2	5	4	157	148	3
-1	5	4	237	265	3
0	5	4	103	89	3
1	5	4	297	310	3
2	5	4	269	269	4
3	5	4	83	92	5
4	5	4	141	165	5
5	5	4	64	77	10
6	5	4	44	78	-15
7	5	4	122	133	8
8	5	4	28	35	-27
-9	6	4	33	12	-22
-8	6	4	82	88	9
-7	6	4	88	89	8
-6	6	4	20	41	-28
-5	6	4	70	58	8
-4	6	4	106	47	5
-3	6	4	461	456	3
-2	6	4	52	37	8
-1	6	4	32	18	-12
0	6	4	39	20	8
1	6	4	185	173	4
2	6	4	541	493	3
3	6	4	163	188	5
4	6	4	89	64	7
5	6	4	42	7	-15
6	6	4	41	24	-16
7	6	4	14	11	-56
8	6	4	19	16	-39
-9	7	4	20	11	-36
-8	7	4	62	60	11
-7	7	4	29	12	-21
-6	7	4	135	139	6
-5	7	4	45	78	12
-4	7	4	325	255	4
-3	7	4	559	569	3
-2	7	4	44	65	10
-1	7	4	124	133	4
0	7	4	39	10	13
1	7	4	201	192	4
2	7	4	25	31	-20
3	7	4	30	56	-18
4	7	4	38	42	-16
5	7	4	77	91	9
6	7	4	40	45	-17
7	7	4	186	188	6
8	7	4	14	29	-56
-9	8	4	23	27	-32
-8	8	4	57	54	12
-7	8	4	108	99	7
-6	8	4	173	198	5
-5	8	4	41	45	13
-4	8	4	149	105	5
-3	8	4	242	265	4
-2	8	4	24	3	-19
-1	8	4	86	63	6
0	8	4	21	52	-16
1	8	4	366	355	4
2	8	4	66	54	8
3	8	4	258	239	4
4	8	4	243	238	5
5	8	4	12	20	-50
6	8	4	13	8	-52
7	8	4	33	9	-25
8	8	4	14	23	-56
-8	9	4	13	15	-53

Table 56. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-7	9	4	37	35	-17
-6	9	4	98	81	8
-5	9	4	12	9	-47
-4	9	4	60	26	10
-3	9	4	115	92	6
-2	9	4	11	6	-45
-1	9	4	58	66	9
0	9	4	358	378	3
1	9	4	20	4	-27
2	9	4	12	1	-47
3	9	4	136	140	6
4	9	4	95	97	8
5	9	4	12	15	-51
6	9	4	32	7	-21
7	9	4	39	44	-21
8	9	4	14	18	-57
-8	10	4	49	52	16
-7	10	4	13	28	-52
-6	10	4	215	223	6
-5	10	4	87	78	8
-4	10	4	19	64	-30
-3	10	4	107	129	7
-2	10	4	24	35	-23
-1	10	4	47	59	12
0	10	4	204	200	14
1	10	4	22	13	-26
2	10	4	75	60	9
3	10	4	19	25	-31
4	10	4	226	225	5
5	10	4	33	44	-21
6	10	4	33	17	-20
7	10	4	14	8	-58
8	10	4	14	19	-58
-8	11	4	47	53	-16
-7	11	4	13	12	-53
-6	11	4	13	2	-52
-5	11	4	81	83	9
-4	11	4	92	73	8
-3	11	4	213	209	5
-2	11	4	32	33	-18
-1	11	4	61	59	10
0	11	4	291	275	6
1	11	4	175	172	5
2	11	4	18	20	-33
3	11	4	55	60	13
4	11	4	91	98	9
5	11	4	13	20	-54
6	11	4	28	23	-26
7	11	4	94	93	11
8	11	4	14	17	-58
-8	12	4	14	37	-57
-7	12	4	56	52	10
-6	12	4	13	7	-52
-5	12	4	13	42	-52
-4	12	4	100	87	8
-3	12	4	229	208	5
-2	12	4	74	63	9
-1	12	4	56	49	12
0	12	4	125	141	14
1	12	4	95	99	8
2	12	4	105	102	7
3	12	4	113	105	7
4	12	4	30	33	-25
5	12	4	64	66	13
6	12	4	54	49	15
7	12	4	15	15	-60
8	12	4	42	11	-21
-8	13	4	73	70	13
-7	13	4	68	72	12
-6	13	4	19	22	-38
-5	13	4	41	41	-18
-4	13	4	27	17	-25
-3	13	4	124	128	7
-2	13	4	36	34	-18
-1	13	4	67	61	10
0	13	4	85	60	7
1	13	4	27	28	-24
2	13	4	39	31	-18
3	13	4	26	11	-26
4	13	4	23	34	-26
5	13	4	56	54	15
6	13	4	49	13	16
7	13	4	61	57	16
8	13	4	15	8	-60
-7	14	4	14	0	-56
-6	14	4	40	45	-19
-5	14	4	32	46	-17
-4	14	4	50	38	15
-3	14	4	54	72	14
-2	14	4	13	6	-52
-1	14	4	72	75	11
0	14	4	120	107	5

Table 56. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
1	14	4	13	21	-53
2	14	4	92	114	9
3	14	4	23	35	-25
4	14	4	87	80	10
5	14	4	36	1	-22
6	14	4	34	15	-24
7	14	4	38	7	-23
8	14	4	47	0	-19
-8	15	4	25	4	-34
-7	15	4	43	48	-21
-6	15	4	14	15	-56
-5	15	4	13	1	-55
-4	15	4	26	37	-24
-3	15	4	13	27	-54
-2	15	4	20	15	-35
-1	15	4	126	132	8
0	15	4	53	44	11
1	15	4	13	21	-39
2	15	4	28	30	-28
3	15	4	33	36	-23
4	15	4	34	12	-24
5	15	4	58	54	15
6	15	4	14	3	-59
7	15	4	26	6	-34
-8	16	4	26	9	-34
-7	16	4	14	9	-59
-6	16	4	14	5	-57
-5	16	4	79	94	13
-4	16	4	61	58	14
-3	16	4	27	10	-27
-2	16	4	14	21	-55
-1	16	4	13	15	-55
0	16	4	13	14	-39
1	16	4	46	40	-17
2	16	4	14	10	-57
3	16	4	14	26	-57
4	16	4	28	22	-29
5	16	4	49	35	-18
6	16	4	26	17	-34
-8	17	4	31	32	-31
-7	17	4	15	3	-60
-6	17	4	14	5	-59
-5	17	4	25	2	-34
-4	17	4	34	28	-24
-3	17	4	14	1	-56
-2	17	4	47	37	-17
-1	17	4	70	75	13
0	17	4	20	11	-30
1	17	4	14	21	-58
2	17	4	26	28	-33
3	17	4	14	9	-59
4	17	4	14	1	-58
5	17	4	15	20	-60
6	17	4	15	12	-61
-7	18	4	29	3	-31
-6	18	4	15	1	-60
-5	18	4	15	20	-60
-4	18	4	51	48	-18
-3	18	4	14	0	-58
-2	18	4	34	1	-24
-1	18	4	15	32	-61
0	18	4	24	15	-25
1	18	4	14	2	-58
2	18	4	86	72	12
3	18	4	14	2	-59
4	18	4	15	5	-60
5	18	4	15	24	-63
-6	19	4	15	2	-61
-5	19	4	15	11	-61
-4	19	4	31	13	-29
-3	19	4	15	19	-60
-2	19	4	42	49	-22
-1	19	4	27	24	-33
0	19	4	21	10	-31
1	19	4	15	10	-59
2	19	4	15	21	-61
3	19	4	15	11	-60
4	19	4	24	4	-40
-4	20	4	15	2	-61
-3	20	4	15	5	-60
-2	20	4	15	20	-61
-1	20	4	30	19	-30
0	20	4	15	12	-42
1	20	4	15	10	-61
2	20	4	27	22	-35
-1	21	4	15	31	-63
-10	0	5	39	22	-18
-8	0	5	136	131	6
-6	0	5	192	179	4
-4	0	5	10	13	-40
-2	0	5	503	509	3
0	0	5	475	424	2

Table 56. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
2	0	5	52	43	10
4	0	5	91	77	8
6	0	5	12	5	-49
8	0	5	144	145	7
-10	1	5	38	21	-19
-9	1	5	26	18	-27
-8	1	5	128	123	6
-7	1	5	62	65	9
-6	1	5	397	387	4
-5	1	5	206	209	4
-4	1	5	383	355	3
-3	1	5	273	211	3
-2	1	5	262	251	3
-1	1	5	271	325	3
0	1	5	30	19	10
1	1	5	171	168	3
2	1	5	11	36	-45
3	1	5	130	113	5
4	1	5	526	553	1
5	1	5	97	127	7
6	1	5	12	2	-49
7	1	5	67	54	11
8	1	5	14	10	-57
9	1	5	14	12	-59
-10	2	5	13	1	-53
-9	2	5	203	197	6
-8	2	5	39	41	-17
-7	2	5	70	74	9
-6	2	5	235	234	4
-5	2	5	201	163	4
-4	2	5	142	119	4
-3	2	5	528	519	3
-2	2	5	254	204	3
-1	2	5	218	193	3
0	2	5	564	547	9
1	2	5	624	607	3
2	2	5	111	100	5
3	2	5	26	26	-17
4	2	5	50	60	14
5	2	5	47	39	14
6	2	5	134	138	6
7	2	5	95	86	8
8	2	5	62	72	14
-10	3	5	13	10	-54
-9	3	5	13	9	-54
-8	3	5	29	30	-21
-7	3	5	71	68	9
-6	3	5	11	24	-45
-5	3	5	276	252	4
-4	3	5	248	253	3
-3	3	5	569	570	3
-2	3	5	77	121	5
-1	3	5	125	110	4
0	3	5	118	108	3
1	3	5	658	582	3
2	3	5	226	222	4
3	3	5	69	81	5
4	3	5	50	65	13
5	3	5	35	7	-18
6	3	5	82	73	9
7	3	5	13	21	-53
8	3	5	55	37	15
-10	4	5	14	26	-55
-9	4	5	142	145	7
-8	4	5	139	138	6
-7	4	5	169	190	5
-6	4	5	28	11	-19
-5	4	5	264	220	4
-4	4	5	259	256	3
-3	4	5	145	158	3
-2	4	5	276	286	3
-1	4	5	86	79	5
0	4	5	159	144	6
1	4	5	368	368	3
2	4	5	72	88	7
3	4	5	28	19	-16
4	4	5	49	48	13
5	4	5	75	68	9
6	4	5	198	196	6
7	4	5	74	74	10
8	4	5	69	57	12
-10	5	5	50	26	15
-9	5	5	68	78	11
-8	5	5	51	48	13
-7	5	5	24	47	-24
-6	5	5	313	346	4
-5	5	5	194	230	4
-4	5	5	180	171	4
-3	5	5	403	383	2
-2	5	5	151	109	4
-1	5	5	136	107	4
0	5	5	42	37	8

Table 56. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
1	5	5	55	83	9
2	5	5	112	131	5
3	5	5	139	142	4
4	5	5	272	257	4
5	5	5	45	29	14
6	5	5	169	187	6
7	5	5	23	10	-22
8	5	5	14	17	-56
-9	6	5	40	28	-18
-8	6	5	12	24	-51
-7	6	5	149	144	6
-6	6	5	126	144	6
-5	6	5	26	43	-20
-4	6	5	320	313	4
-3	6	5	130	135	5
-2	6	5	174	120	4
-1	6	5	573	605	3
0	6	5	18	7	-17
1	6	5	215	212	4
2	6	5	60	42	9
3	6	5	62	74	9
4	6	5	89	94	8
5	6	5	20	19	-31
6	6	5	43	37	-18
7	6	5	57	48	13
8	6	5	56	49	14
-9	7	5	53	56	15
-8	7	5	18	11	-35
-7	7	5	136	134	6
-6	7	5	33	12	-17
-5	7	5	71	83	8
-4	7	5	257	247	4
-3	7	5	59	40	9
-2	7	5	120	139	5
-1	7	5	171	227	4
0	7	5	276	243	6
1	7	5	66	111	8
2	7	5	38	50	-14
3	7	5	244	269	4
4	7	5	109	107	7
5	7	5	41	49	-16
6	7	5	43	40	-18
7	7	5	13	1	-55
8	7	5	22	18	-37
-9	8	5	35	33	-22
-8	8	5	72	81	11
-7	8	5	18	19	-35
-6	8	5	60	49	11
-5	8	5	50	34	11
-4	8	5	24	16	-23
-3	8	5	77	76	7
-2	8	5	35	27	-15
-1	8	5	415	387	4
0	8	5	49	68	9
1	8	5	39	37	-14
2	8	5	101	112	7
3	8	5	21	22	-28
4	8	5	12	24	-50
5	8	5	30	39	-22
6	8	5	119	120	6
7	8	5	32	27	-24
8	8	5	14	16	-57
-8	9	5	74	73	11
-7	9	5	56	75	13
-6	9	5	181	150	6
-5	9	5	202	162	5
-4	9	5	382	395	4
-3	9	5	26	7	-20
-2	9	5	30	30	-18
-1	9	5	20	9	-28
0	9	5	48	66	12
1	9	5	46	59	12
2	9	5	259	259	4
3	9	5	69	59	10
4	9	5	12	5	-50
5	9	5	13	2	-53
6	9	5	111	113	9
7	9	5	28	28	-28
8	9	5	14	19	-58
-8	10	5	114	114	9
-7	10	5	82	80	10
-6	10	5	43	56	-16
-5	10	5	165	116	6
-4	10	5	53	54	13
-3	10	5	17	6	-33
-2	10	5	56	58	11
-1	10	5	260	229	5
0	10	5	129	128	6
1	10	5	12	35	-49
2	10	5	233	241	5
3	10	5	95	125	8
4	10	5	39	34	-17

Table 56. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
6	10	5	136	140	8
7	10	5	39	7	-20
8	10	5	36	1	-24
-8	11	5	13	4	-55
-7	11	5	43	25	-16
-6	11	5	13	13	-52
-5	11	5	83	54	9
-4	11	5	141	165	6
-3	11	5	71	66	9
-2	11	5	60	75	11
-1	11	5	54	65	13
0	11	5	56	52	9
1	11	5	12	3	-51
2	11	5	90	75	8
3	11	5	160	147	6
4	11	5	54	37	13
5	11	5	13	6	-54
6	11	5	14	35	-59
7	11	5	14	12	-58
8	11	5	15	4	-60
-8	12	5	30	38	-26
-7	12	5	61	69	10
-6	12	5	46	54	15
-5	12	5	67	43	11
-4	12	5	13	3	-52
-3	12	5	12	8	-50
-2	12	5	97	96	8
-1	12	5	279	301	5
0	12	5	40	38	13
1	12	5	22	17	-30
2	12	5	85	85	9
3	12	5	40	37	-18
4	12	5	46	40	-18
5	12	5	37	31	-21
6	12	5	29	19	-29
7	12	5	23	2	-35
8	12	5	34	22	-27
-8	13	5	49	41	-17
-7	13	5	20	7	-37
-6	13	5	75	69	18
-5	13	5	51	64	15
-4	13	5	64	69	12
-3	13	5	13	7	-51
-2	13	5	63	60	11
-1	13	5	35	26	-20
0	13	5	27	3	-21
1	13	5	13	5	-53
2	13	5	92	86	9
3	13	5	77	76	9
4	13	5	98	101	9
5	13	5	14	41	-57
6	13	5	14	23	-59
7	13	5	15	12	-59
8	13	5	15	9	-61
-8	14	5	15	25	-60
-7	14	5	14	7	-55
-6	14	5	46	39	-17
-5	14	5	41	55	13
-4	14	5	13	17	-54
-3	14	5	32	40	-22
-2	14	5	88	85	9
-1	14	5	74	68	10
0	14	5	13	9	-38
1	14	5	70	65	11
2	14	5	13	22	-38
3	14	5	29	25	-26
4	14	5	35	8	-22
5	14	5	14	9	-57
6	14	5	26	32	-34
7	14	5	22	17	-41
-8	15	5	37	4	-24
-7	15	5	14	3	-58
-6	15	5	30	37	-27
-5	15	5	41	39	-19
-4	15	5	42	50	-19
-3	15	5	38	55	-15
-2	15	5	68	66	8
-1	15	5	23	28	-25
0	15	5	13	6	-27
1	15	5	62	63	13
2	15	5	36	38	-21
3	15	5	14	10	-55
4	15	5	14	32	-58
5	15	5	44	33	-20
6	15	5	15	23	-61
-8	16	5	42	26	-22
-7	16	5	23	4	-38
-6	16	5	15	20	-60
-5	16	5	14	23	-57
-4	16	5	14	24	-56
-3	16	5	54	51	15
-2	16	5	36	30	-22

Table 56. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-1	16	5	13	3	-55
0	16	5	20	1	-30
1	16	5	112	108	9
2	16	5	14	15	-57
3	16	5	32	8	-25
4	16	5	32	16	-28
5	16	5	15	0	-60
6	16	5	15	11	-60
-8	17	5	15	12	-62
-7	17	5	15	13	-61
-6	17	5	53	42	18
-5	17	5	40	11	-22
-4	17	5	26	0	-31
-3	17	5	60	51	14
-2	17	5	90	84	11
-1	17	5	14	9	-57
0	17	5	41	31	-21
1	17	5	62	54	15
2	17	5	14	11	-58
3	17	5	14	7	-58
4	17	5	38	33	-24
5	17	5	38	7	-23
-7	18	5	28	2	-33
-6	18	5	33	25	-29
-5	18	5	27	28	-34
-4	18	5	15	9	-60
-3	18	5	22	4	-39
-2	18	5	45	33	-19
-1	18	5	41	7	-20
0	18	5	44	38	-19
1	18	5	31	5	-28
2	18	5	28	11	-30
3	18	5	34	3	-26
4	18	5	28	11	-33
-6	19	5	39	34	-25
-5	19	5	25	11	-36
-4	19	5	15	3	-59
-3	19	5	15	12	-60
-2	19	5	48	34	-19
-1	19	5	15	1	-59
0	19	5	15	5	-42
1	19	5	15	0	-60
2	19	5	31	9	-29
3	19	5	15	8	-61
-4	20	5	15	3	-60
-3	20	5	15	29	-62
-2	20	5	15	15	-61
-1	20	5	28	7	-33
0	20	5	31	25	-26
1	20	5	15	31	-62
-10	0	6	35	29	-21
-8	0	6	42	51	-15
-6	0	6	90	74	7
-4	0	6	909	958	3
-2	0	6	108	140	4
0	0	6	154	139	4
2	0	6	72	91	7
4	0	6	31	25	-20
6	0	6	213	219	6
8	0	6	28	24	-28
-10	1	6	76	71	11
-9	1	6	106	108	7
-8	1	6	40	9	-15
-7	1	6	119	125	6
-6	1	6	233	231	4
-5	1	6	50	59	10
-4	1	6	43	60	12
-3	1	6	10	11	-40
-2	1	6	146	130	4
-1	1	6	34	71	-12
0	1	6	891	816	2
1	1	6	160	185	4
2	1	6	114	98	5
3	1	6	190	192	5
4	1	6	12	4	-51
5	1	6	51	48	12
6	1	6	81	78	10
7	1	6	39	34	-19
8	1	6	49	30	16
9	1	6	27	14	-31
-10	2	6	34	22	-21
-9	2	6	61	53	12
-8	2	6	12	6	-49
-7	2	6	202	194	5
-6	2	6	49	27	11
-5	2	6	328	277	4
-4	2	6	497	447	3
-3	2	6	255	179	3
-2	2	6	242	267	3
-1	2	6	188	206	4
0	2	6	46	21	-21
1	2	6	150	170	4

Table 56. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
2	2	6	43	21	11
3	2	6	525	536	4
4	2	6	125	100	6
5	2	6	56	44	11
6	2	6	30	19	-23
7	2	6	63	69	13
8	2	6	14	21	-58
-10	3	6	35	12	-21
-9	3	6	87	81	9
-8	3	6	116	109	7
-7	3	6	317	325	4
-6	3	6	152	173	5
-5	3	6	21	28	-24
-4	3	6	139	136	4
-3	3	6	88	68	5
-2	3	6	395	366	3
-1	3	6	253	250	3
0	3	6	178	128	3
1	3	6	80	80	7
2	3	6	140	175	5
3	3	6	241	244	3
4	3	6	12	6	-50
5	3	6	22	16	-29
6	3	6	13	12	-54
7	3	6	93	97	9
8	3	6	74	72	12
-10	4	6	14	35	-56
-9	4	6	66	80	12
-8	4	6	12	11	-50
-7	4	6	58	67	11
-6	4	6	203	179	5
-5	4	6	19	7	-25
-4	4	6	178	171	4
-3	4	6	21	29	-13
-2	4	6	334	341	3
-1	4	6	113	99	5
0	4	6	104	123	4
1	4	6	33	42	-15
2	4	6	86	88	6
3	4	6	325	326	3
4	4	6	30	20	-20
5	4	6	62	41	11
6	4	6	79	78	10
7	4	6	13	7	-55
8	4	6	34	22	-26
-9	5	6	99	105	9
-8	5	6	33	14	-19
-7	5	6	68	85	9
-6	5	6	138	135	5
-5	5	6	92	105	7
-4	5	6	56	62	9
-3	5	6	23	7	-15
-2	5	6	139	161	4
-1	5	6	94	82	5
0	5	6	373	359	5
1	5	6	156	174	5
2	5	6	102	94	6
3	5	6	42	41	10
4	5	6	41	53	-15
5	5	6	57	53	13
6	5	6	105	111	8
7	5	6	36	40	-22
8	5	6	83	76	12
-9	6	6	72	73	12
-8	6	6	62	65	11
-7	6	6	149	147	6
-6	6	6	26	51	-21
-5	6	6	223	242	4
-4	6	6	274	262	4
-3	6	6	15	8	-30
-2	6	6	94	85	6
-1	6	6	213	238	4
0	6	6	85	76	9
1	6	6	50	56	11
2	6	6	85	101	7
3	6	6	25	38	-23
4	6	6	22	15	-29
5	6	6	271	291	5
6	6	6	52	52	11
7	6	6	14	1	-55
8	6	6	15	21	-61
-9	7	6	150	145	7
-8	7	6	55	53	13
-7	7	6	127	112	7
-6	7	6	27	22	-21
-5	7	6	12	19	-48
-4	7	6	107	123	6
-3	7	6	26	27	-20
-2	7	6	79	63	7
-1	7	6	130	133	5
0	7	6	16	32	-23
1	7	6	359	362	4

Table 56. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
2	7	6	62	70	9
3	7	6	40	30	-15
4	7	6	66	66	10
5	7	6	30	44	-26
6	7	6	38	22	-18
7	7	6	14	8	-56
8	7	6	15	24	-60
-9	8	6	52	29	15
-8	8	6	78	75	10
-7	8	6	67	77	11
-6	8	6	51	51	12
-5	8	6	152	175	6
-4	8	6	11	13	-47
-3	8	6	35	24	-16
-2	8	6	349	365	4
-1	8	6	61	79	10
0	8	6	20	26	-21
1	8	6	88	70	8
2	8	6	60	61	10
3	8	6	44	47	14
4	8	6	118	112	7
5	8	6	150	140	7
6	8	6	13	2	-54
7	8	6	14	9	-57
8	8	6	15	11	-62
-8	9	6	47	50	-16
-7	9	6	20	1	-33
-6	9	6	138	118	7
-5	9	6	83	92	8
-4	9	6	139	136	6
-3	9	6	51	59	12
-2	9	6	391	427	4
-1	9	6	12	13	-49
0	9	6	28	12	-19
1	9	6	86	76	8
2	9	6	161	160	6
3	9	6	37	37	-17
4	9	6	13	4	-52
5	9	6	44	57	13
6	9	6	13	2	-55
7	9	6	36	0	-21
8	9	6	87	87	13
-8	10	6	13	8	-38
-7	10	6	25	28	-28
-6	10	6	69	92	11
-5	10	6	78	82	9
-4	10	6	40	31	-15
-3	10	6	53	51	12
-2	10	6	287	281	5
-1	10	6	82	61	8
0	10	6	64	74	7
1	10	6	78	80	10
2	10	6	86	70	9
3	10	6	62	65	11
4	10	6	79	74	10
5	10	6	69	66	12
6	10	6	36	45	-22
7	10	6	29	30	-29
8	10	6	15	16	-63
-8	11	6	13	13	-54
-7	11	6	40	42	-18
-6	11	6	45	72	-16
-5	11	6	118	107	8
-4	11	6	56	45	11
-3	11	6	12	11	-50
-2	11	6	222	191	5
-1	11	6	45	47	15
0	11	6	118	96	5
1	11	6	222	218	5
2	11	6	13	11	-51
3	11	6	13	16	-53
4	11	6	40	34	13
5	11	6	14	11	-57
6	11	6	32	30	-25
7	11	6	14	9	-59
8	11	6	45	32	-21
-8	12	6	28	18	-28
-7	12	6	41	45	-19
-6	12	6	34	2	-21
-5	12	6	140	124	7
-4	12	6	82	77	9
-3	12	6	12	13	-50
-2	12	6	60	75	12
-1	12	6	27	1	-24
0	12	6	28	29	-17
1	12	6	80	78	10
2	12	6	19	19	-36
3	12	6	34	41	-19
4	12	6	13	30	-55
5	12	6	98	97	10
6	12	6	14	18	-58
7	12	6	28	5	-31

Table 56. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-8	13	6	38	2	-21
-7	13	6	35	26	-22
-6	13	6	71	43	11
-5	13	6	13	35	-54
-4	13	6	42	30	-17
-3	13	6	67	55	11
-2	13	6	85	69	9
-1	13	6	33	9	-20
0	13	6	103	114	6
1	13	6	127	122	7
2	13	6	46	38	-20
3	13	6	14	8	-56
4	13	6	44	48	-18
5	13	6	24	17	-35
6	13	6	27	21	-32
7	13	6	15	5	-60
-8	14	6	41	23	-21
-7	14	6	14	3	-57
-6	14	6	56	30	14
-5	14	6	13	17	-55
-4	14	6	78	78	8
-3	14	6	99	106	9
-2	14	6	79	69	10
-1	14	6	13	20	-53
0	14	6	37	31	-20
1	14	6	33	23	-23
2	14	6	13	21	-55
3	14	6	63	61	13
4	14	6	21	21	-38
5	14	6	40	32	-22
6	14	6	31	24	-29
-8	15	6	15	10	-61
-7	15	6	90	80	12
-6	15	6	57	40	15
-5	15	6	14	6	-56
-4	15	6	32	8	-24
-3	15	6	31	35	-25
-2	15	6	13	8	-54
-1	15	6	47	44	-16
0	15	6	42	44	14
1	15	6	32	29	-24
2	15	6	14	5	-55
3	15	6	62	58	14
4	15	6	14	0	-58
5	15	6	31	8	-28
6	15	6	15	2	-61
-8	16	6	44	13	-21
-7	16	6	15	33	-63
-6	16	6	37	6	-23
-5	16	6	14	2	-58
-4	16	6	27	17	-30
-3	16	6	57	49	15
-2	16	6	43	31	-19
-1	16	6	33	17	-23
0	16	6	53	55	14
1	16	6	14	18	-58
2	16	6	26	28	-31
3	16	6	55	61	17
4	16	6	15	14	-59
5	16	6	15	10	-60
-8	17	6	15	5	-62
-7	17	6	15	33	-63
-6	17	6	33	44	-29
-5	17	6	38	11	-23
-4	17	6	31	9	-27
-3	17	6	32	24	-26
-2	17	6	31	7	-26
-1	17	6	20	40	-42
0	17	6	62	68	13
1	17	6	14	4	-58
2	17	6	14	4	-58
3	17	6	15	26	-60
4	17	6	15	7	-60
-7	18	6	15	11	-63
-6	18	6	15	4	-61
-5	18	6	30	18	-29
-4	18	6	56	58	17
-3	18	6	14	9	-59
-2	18	6	23	2	-36
-1	18	6	35	33	-25
0	18	6	29	24	-25
1	18	6	14	4	-59
2	18	6	15	21	-60
3	18	6	15	14	-61
-5	19	6	15	0	-61
-4	19	6	15	7	-61
-3	19	6	15	14	-61
-2	19	6	15	3	-60
-1	19	6	15	14	-61
0	19	6	56	47	15
1	19	6	15	1	-60
2	19	6	15	9	-61

Table 56. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-3	20	6	28	21	-33
-2	20	6	28	10	-33
-1	20	6	33	11	-27
0	20	6	15	3	-43
-10	0	7	149	143	7
-8	0	7	247	244	5
-6	0	7	58	57	9
-4	0	7	129	152	5
-2	0	7	137	129	5
0	0	7	291	270	3
2	0	7	650	673	4
4	0	7	52	54	12
6	0	7	13	2	-37
8	0	7	85	79	11
-10	1	7	28	50	-28
-9	1	7	13	3	-51
-8	1	7	13	23	-52
-7	1	7	54	65	11
-6	1	7	58	67	10
-5	1	7	311	293	4
-4	1	7	74	74	7
-3	1	7	113	92	5
-2	1	7	198	212	4
-1	1	7	346	302	3
0	1	7	25	11	-17
1	1	7	10	25	-42
2	1	7	247	250	4
3	1	7	13	4	-52
4	1	7	18	7	-32
5	1	7	197	193	6
6	1	7	39	46	-13
7	1	7	49	45	16
8	1	7	15	28	-60
9	1	7	15	1	-60
-10	2	7	14	17	-55
-9	2	7	13	12	-52
-8	2	7	124	145	7
-7	2	7	149	174	6
-6	2	7	79	111	8
-5	2	7	274	246	4
-4	2	7	79	60	6
-3	2	7	213	225	4
-2	2	7	94	89	6
-1	2	7	349	328	3
0	2	7	11	40	-32
1	2	7	127	145	5
2	2	7	242	226	4
3	2	7	34	7	-19
4	2	7	12	21	-48
5	2	7	31	3	-26
6	2	7	21	31	-23
7	2	7	47	42	-17
8	2	7	58	40	15
-10	3	7	113	112	8
-9	3	7	40	24	-16
-8	3	7	12	18	-50
-7	3	7	122	130	6
-6	3	7	19	1	-27
-5	3	7	386	383	4
-4	3	7	17	18	-28
-3	3	7	111	97	5
-2	3	7	212	184	4
-1	3	7	281	299	4
0	3	7	58	50	10
1	3	7	19	34	-25
2	3	7	42	38	-16
3	3	7	21	29	-23
4	3	7	71	70	9
5	3	7	243	248	5
6	3	7	37	22	-18
7	3	7	31	46	-27
8	3	7	29	5	-30
-10	4	7	88	96	10
-9	4	7	24	31	-28
-8	4	7	134	139	7
-7	4	7	63	68	10
-6	4	7	134	141	6
-5	4	7	247	296	4
-4	4	7	124	126	5
-3	4	7	11	8	-31
-2	4	7	277	247	4
-1	4	7	281	318	4
0	4	7	228	241	7
1	4	7	158	145	5
2	4	7	195	203	5
3	4	7	59	94	8
4	4	7	12	38	-51
5	4	7	32	43	-23
6	4	7	13	6	-53
7	4	7	27	14	-30
8	4	7	15	20	-59
-9	5	7	49	57	15

Table 56. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-8	5	7	13	5	-53
-7	5	7	97	94	8
-6	5	7	71	77	9
-5	5	7	12	8	-48
-4	5	7	105	125	6
-3	5	7	429	429	3
-2	5	7	221	234	4
-1	5	7	169	149	4
0	5	7	73	66	6
1	5	7	108	90	6
2	5	7	70	61	9
3	5	7	121	113	5
4	5	7	154	160	6
5	5	7	66	62	11
6	5	7	13	9	-53
7	5	7	57	52	15
8	5	7	14	19	-59
-9	6	7	23	23	-31
-8	6	7	143	142	7
-7	6	7	141	143	6
-6	6	7	58	71	10
-5	6	7	109	101	6
-4	6	7	11	27	-47
-3	6	7	57	28	11
-2	6	7	58	75	10
-1	6	7	52	31	10
0	6	7	87	95	5
1	6	7	108	113	6
2	6	7	148	126	6
3	6	7	126	161	7
4	6	7	40	27	-17
5	6	7	13	9	-53
6	6	7	26	30	-28
7	6	7	66	72	15
8	6	7	23	20	-37
-9	7	7	13	6	-54
-8	7	7	51	57	15
-7	7	7	69	49	11
-6	7	7	12	14	-49
-5	7	7	139	141	6
-4	7	7	41	7	14
-3	7	7	568	570	4
-2	7	7	202	196	5
-1	7	7	87	86	7
0	7	7	72	66	6
1	7	7	29	71	-20
2	7	7	20	19	-30
3	7	7	120	145	7
4	7	7	26	67	-29
5	7	7	36	41	-16
6	7	7	14	22	-55
7	7	7	95	86	11
8	7	7	33	4	-26
-8	8	7	39	40	-19
-7	8	7	138	123	7
-6	8	7	177	163	6
-5	8	7	55	58	12
-4	8	7	25	21	-23
-3	8	7	188	164	5
-2	8	7	119	129	6
-1	8	7	105	86	7
0	8	7	321	333	6
1	8	7	60	67	11
2	8	7	12	18	-50
3	8	7	116	127	7
4	8	7	133	146	7
5	8	7	40	16	-18
6	8	7	14	23	-56
7	8	7	57	51	17
8	8	7	15	5	-61
-8	9	7	58	44	13
-7	9	7	13	14	-53
-6	9	7	102	106	8
-5	9	7	23	13	-26
-4	9	7	45	45	14
-3	9	7	12	21	-50
-2	9	7	12	17	-50
-1	9	7	12	46	-50
0	9	7	100	94	10
1	9	7	19	26	-33
2	9	7	34	33	-20
3	9	7	24	32	-30
4	9	7	128	126	9
5	9	7	36	9	-21
6	9	7	33	24	-24
7	9	7	15	16	-62
8	9	7	26	3	-35
-8	10	7	28	6	-26
-7	10	7	23	6	-30
-6	10	7	64	80	12
-5	10	7	12	1	-51
-4	10	7	12	7	-50

Table 56. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-3	10	7	56	78	12
-2	10	7	12	17	-50
-1	10	7	36	56	-18
0	10	7	347	343	4
1	10	7	71	78	10
2	10	7	24	15	-26
3	10	7	13	9	-54
4	10	7	45	48	-17
5	10	7	13	10	-55
6	10	7	14	9	-58
7	10	7	15	26	-62
-8	11	7	32	33	-24
-7	11	7	48	41	-23
-6	11	7	68	67	12
-5	11	7	96	98	9
-4	11	7	41	47	-16
-3	11	7	168	175	6
-2	11	7	12	4	-51
-1	11	7	47	40	15
0	11	7	46	57	11
1	11	7	22	3	-30
2	11	7	13	1	-53
3	11	7	91	89	7
4	11	7	57	52	14
5	11	7	33	52	-25
6	11	7	14	36	-59
7	11	7	29	44	-34
-8	12	7	65	70	14
-7	12	7	100	88	9
-6	12	7	13	12	-38
-5	12	7	13	6	-53
-4	12	7	98	96	9
-3	12	7	21	6	-33
-2	12	7	35	31	-19
-1	12	7	40	23	-17
0	12	7	29	7	-21
1	12	7	31	42	-23
2	12	7	72	73	8
3	12	7	51	34	16
4	12	7	23	7	-35
5	12	7	14	23	-59
6	12	7	14	19	-59
7	12	7	34	34	-28
-8	13	7	15	17	-59
-7	13	7	50	29	17
-6	13	7	13	17	-55
-5	13	7	28	21	-22
-4	13	7	13	3	-54
-3	13	7	105	121	9
-2	13	7	69	73	11
-1	13	7	66	75	12
0	13	7	13	1	-38
1	13	7	26	34	-21
2	13	7	51	49	15
3	13	7	60	63	14
4	13	7	14	16	-58
5	13	7	34	7	-25
6	13	7	23	15	-38
-8	14	7	57	61	18
-7	14	7	14	42	-59
-6	14	7	14	21	-57
-5	14	7	60	78	15
-4	14	7	32	13	-24
-3	14	7	13	41	-55
-2	14	7	25	6	-24
-1	14	7	13	2	-54
0	14	7	68	56	10
1	14	7	20	17	-36
2	14	7	68	63	12
3	14	7	34	44	-24
4	14	7	14	19	-59
5	14	7	15	10	-60
6	14	7	15	1	-61
-8	15	7	35	24	-28
-7	15	7	40	38	-23
-6	15	7	31	22	-26
-5	15	7	63	62	14
-4	15	7	28	34	-29
-3	15	7	27	8	-27
-2	15	7	14	31	-56
-1	15	7	106	96	9
0	15	7	22	35	-29
1	15	7	21	22	-38
2	15	7	14	19	-58
3	15	7	29	3	-29
4	15	7	15	28	-60
5	15	7	40	42	-23
-8	16	7	38	9	-25
-7	16	7	15	1	-60
-6	16	7	15	6	-60
-5	16	7	54	51	17
-4	16	7	46	51	-19

Table 56. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-3	16	7	14	7	-57
-2	16	7	25	22	-33
-1	16	7	57	54	16
0	16	7	14	16	-41
1	16	7	14	30	-58
2	16	7	49	34	-18
3	16	7	14	2	-59
4	16	7	15	4	-60
-8	17	7	40	20	-24
-7	17	7	15	9	-62
-6	17	7	15	13	-61
-5	17	7	31	44	-29
-4	17	7	14	27	-59
-3	17	7	30	5	-27
-2	17	7	14	15	-59
-1	17	7	14	17	-59
0	17	7	22	19	-30
1	17	7	14	5	-59
2	17	7	15	1	-60
3	17	7	15	5	-60
-6	18	7	15	3	-61
-5	18	7	15	8	-60
-4	18	7	22	18	-40
-3	18	7	14	13	-59
-2	18	7	44	42	-22
-1	18	7	23	13	-38
0	18	7	26	3	-27
1	18	7	15	14	-60
-5	19	7	15	5	-61
-4	19	7	15	14	-62
-3	19	7	37	16	-25
-1	19	7	24	25	-39
0	19	7	15	4	-43
1	19	7	15	14	-61
-10	0	8	31	50	-25
-8	0	8	47	40	14
-6	0	8	199	187	5
-4	0	8	102	104	6
-2	0	8	327	377	4
0	0	8	124	103	4
2	0	8	61	62	11
4	0	8	407	386	5
6	0	8	36	35	-21
8	0	8	46	23	-19
-10	1	8	28	1	-27
-9	1	8	44	45	-16
-8	1	8	147	141	6
-7	1	8	39	22	-15
-6	1	8	268	268	4
-5	1	8	33	3	-16
-4	1	8	117	125	5
-3	1	8	12	37	-47
-2	1	8	29	28	-17
-1	1	8	124	137	5
0	1	8	183	213	3
1	1	8	296	289	1
2	1	8	108	78	7
3	1	8	31	28	-19
4	1	8	232	236	6
5	1	8	31	19	-21
6	1	8	20	1	-37
7	1	8	45	33	-20
8	1	8	28	29	-31
-10	2	8	39	36	-20
-9	2	8	102	94	8
-8	2	8	42	36	-15
-7	2	8	37	40	-16
-6	2	8	30	36	-19
-5	2	8	88	89	7
-4	2	8	63	57	9
-3	2	8	500	505	1
-2	2	8	143	154	5
-1	2	8	96	116	6
0	2	8	78	98	7
1	2	8	64	51	11
2	2	8	75	68	9
3	2	8	31	13	-20
4	2	8	142	149	7
5	2	8	13	2	-51
6	2	8	31	30	-24
7	2	8	95	85	11
8	2	8	26	15	-33
-9	3	8	90	98	10
-8	3	8	122	115	7
-7	3	8	62	62	10
-6	3	8	52	73	11
-5	3	8	24	13	-23
-4	3	8	244	222	4
-3	3	8	24	22	-25
-2	3	8	34	7	-14
-1	3	8	63	70	9
0	3	8	87	110	8

Table 56. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
1	3	8	325	316	4
2	3	8	119	158	7
3	3	8	30	33	-15
4	3	8	43	15	-18
5	3	8	35	23	-19
6	3	8	25	10	-30
7	3	8	49	43	-18
8	3	8	15	10	-60
-9	4	8	90	84	9
-8	4	8	13	19	-53
-7	4	8	94	91	8
-6	4	8	85	83	8
-5	4	8	60	52	10
-4	4	8	270	265	4
-3	4	8	264	247	3
-2	4	8	11	11	-45
-1	4	8	108	109	6
0	4	8	43	35	9
1	4	8	92	102	8
2	4	8	32	33	-22
3	4	8	76	79	7
4	4	8	78	71	10
5	4	8	13	2	-37
6	4	8	96	104	10
7	4	8	53	67	17
8	4	8	15	19	-60
-9	5	8	13	6	-54
-8	5	8	133	136	7
-7	5	8	157	145	6
-6	5	8	247	238	5
-5	5	8	106	110	7
-4	5	8	32	53	-19
-3	5	8	129	141	4
-2	5	8	11	11	-46
-1	5	8	118	123	6
0	5	8	94	77	5
1	5	8	40	31	-15
2	5	8	250	241	5
3	5	8	68	67	12
4	5	8	50	46	14
5	5	8	13	14	-52
6	5	8	37	2	-22
7	5	8	34	10	-24
8	5	8	25	16	-35
-9	6	8	13	21	-54
-8	6	8	13	11	-53
-7	6	8	63	73	11
-6	6	8	13	9	-51
-5	6	8	65	62	10
-4	6	8	136	153	6
-3	6	8	33	27	-19
-2	6	8	30	22	-19
-1	6	8	377	375	4
0	6	8	131	159	4
1	6	8	12	10	-50
2	6	8	19	7	-38
3	6	8	20	31	-32
4	6	8	81	92	10
5	6	8	26	49	-28
6	6	8	37	26	-23
7	6	8	14	14	-58
8	6	8	15	1	-60
-8	7	8	13	6	-53
-7	7	8	75	83	10
-6	7	8	99	115	8
-5	7	8	151	151	6
-4	7	8	173	195	5
-3	7	8	71	71	10
-2	7	8	117	126	6
-1	7	8	271	280	5
0	7	8	47	59	9
1	7	8	70	57	10
2	7	8	84	86	10
3	7	8	90	93	9
4	7	8	29	41	-21
5	7	8	33	18	-22
6	7	8	15	4	-60
7	7	8	14	2	-59
8	7	8	27	19	-33
-8	8	8	83	73	10
-7	8	8	13	11	-53
-6	8	8	87	100	9
-5	8	8	35	37	-18
-4	8	8	155	168	6
-3	8	8	127	132	6
-2	8	8	12	12	-50
-1	8	8	196	203	5
0	8	8	127	117	4
1	8	8	12	14	-51
2	8	8	101	107	9
3	8	8	22	18	-33
4	8	8	13	5	-53

Table 56. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
5	8	8	25	29	-31
6	8	8	89	86	12
7	8	8	28	16	-31
-8	9	8	90	97	12
-7	9	8	13	3	-53
-6	9	8	13	27	-53
-5	9	8	51	42	13
-4	9	8	121	111	7
-3	9	8	29	40	-22
-2	9	8	53	21	12
-1	9	8	73	77	10
0	9	8	42	41	11
1	9	8	28	9	-24
2	9	8	245	240	6
3	9	8	56	63	10
4	9	8	13	21	-54
5	9	8	39	21	-21
6	9	8	15	9	-60
7	9	8	24	1	-38
-8	10	8	50	51	16
-7	10	8	35	37	-21
-6	10	8	65	73	12
-5	10	8	67	70	11
-4	10	8	156	156	6
-3	10	8	12	2	-50
-1	10	8	88	93	9
0	10	8	33	47	-14
1	10	8	31	12	-22
2	10	8	23	24	-33
3	10	8	13	4	-54
4	10	8	21	13	-37
5	10	8	14	18	-58
6	10	8	74	84	14
7	10	8	15	6	-61
-8	11	8	34	33	-23
-7	11	8	30	20	-25
-6	11	8	40	48	-18
-5	11	8	13	4	-53
-4	11	8	13	23	-52
-3	11	8	46	40	15
-2	11	8	59	73	12
-1	11	8	134	126	7
0	11	8	18	0	-27
1	11	8	63	60	12
2	11	8	111	108	8
3	11	8	62	63	13
4	11	8	41	15	-19
5	11	8	14	9	-58
6	11	8	15	7	-62
-8	12	8	28	40	-30
-7	12	8	33	14	-23
-6	12	8	13	12	-55
-5	12	8	54	63	10
-4	12	8	21	20	-34
-3	12	8	34	35	-20
-2	12	8	84	80	10
-1	12	8	137	144	7
0	12	8	31	4	-17
1	12	8	22	20	-32
2	12	8	14	8	-56
3	12	8	14	24	-57
4	12	8	30	46	-29
5	12	8	26	36	-35
6	12	8	15	3	-61
-8	13	8	49	38	-19
-7	13	8	14	1	-57
-6	13	8	106	108	10
-5	13	8	81	85	11
-4	13	8	14	32	-55
-3	13	8	36	18	-21
-2	13	8	36	49	-15
-1	13	8	43	44	-18
0	13	8	28	29	-20
1	13	8	40	19	-19
2	13	8	23	9	-35
3	13	8	14	30	-58
4	13	8	52	50	-18
5	13	8	26	26	-34
-8	14	8	42	2	-22
-7	14	8	14	3	-58
-6	14	8	51	43	17
-5	14	8	14	5	-57
-4	14	8	31	9	-25
-3	14	8	73	63	12
-2	14	8	14	15	-56
-1	14	8	51	53	16
0	14	8	24	27	-22
1	14	8	30	44	-28
2	14	8	14	17	-58
3	14	8	44	28	-19
4	14	8	15	25	-61
5	14	8	15	15	-61

Table 56. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-8	15	8	38	32	-26
-7	15	8	15	4	-60
-6	15	8	14	21	-59
-5	15	8	48	53	-18
-4	15	8	60	55	15
-3	15	8	33	8	-24
-2	15	8	42	34	-21
-1	15	8	14	3	-58
0	15	8	37	7	-21
1	15	8	82	78	11
2	15	8	46	46	-19
3	15	8	15	5	-60
4	15	8	15	13	-61
-8	16	8	35	21	-28
-7	16	8	15	5	-62
-6	16	8	15	25	-61
-5	16	8	22	12	-37
-4	16	8	14	16	-58
-3	16	8	89	76	11
-2	16	8	41	50	-22
-1	16	8	34	5	-24
0	16	8	21	19	-31
1	16	8	15	30	-59
2	16	8	15	8	-60
3	16	8	15	6	-60
-7	17	8	15	8	-62
-6	17	8	15	38	-62
-5	17	8	29	10	-30
-4	17	8	30	11	-28
-3	17	8	15	3	-59
-2	17	8	47	16	-19
-1	17	8	44	2	-19
0	17	8	36	25	-23
1	17	8	30	36	-31
2	17	8	15	7	-61
-6	18	8	15	1	-61
-5	18	8	15	0	-60
-4	18	8	15	12	-60
-3	18	8	26	19	-34
-2	18	8	39	40	-24
-1	18	8	26	0	-33
0	18	8	15	7	-43
1	18	8	15	10	-61
-3	19	8	15	11	-61
-2	19	8	15	1	-61
-1	19	8	15	9	-61
-8	0	9	43	32	-16
-6	0	9	12	2	-49
-4	0	9	443	436	4
-2	0	9	149	157	5
0	0	9	266	272	4
2	0	9	71	68	9
4	0	9	13	2	-51
6	0	9	42	17	-22
8	0	9	15	4	-60
-9	1	9	32	51	-22
-8	1	9	109	101	8
-7	1	9	29	6	-22
-6	1	9	76	75	9
-5	1	9	66	41	9
-4	1	9	340	332	4
-3	1	9	11	4	-47
-2	1	9	120	118	6
-1	1	9	140	141	5
0	1	9	180	185	4
1	1	9	44	11	14
2	1	9	12	13	-49
3	1	9	57	68	17
4	1	9	13	12	-52
5	1	9	25	24	-29
6	1	9	130	120	8
7	1	9	15	6	-60
8	1	9	15	22	-60
-9	2	9	97	110	9
-8	2	9	40	11	-16
-7	2	9	226	228	5
-6	2	9	12	16	-50
-5	2	9	32	31	-19
-4	2	9	184	195	5
-3	2	9	31	41	-18
-2	2	9	137	151	5
-1	2	9	150	132	5
0	2	9	32	25	-19
1	2	9	87	65	8
2	2	9	57	57	11
3	2	9	313	307	5
4	2	9	13	3	-52
5	2	9	13	19	-55
6	2	9	14	14	-59
7	2	9	15	15	-60
8	2	9	15	2	-60
-9	3	9	32	31	-23

Table 56. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-8	3	9	95	101	8
-7	3	9	61	60	12
-6	3	9	51	34	12
-5	3	9	104	125	7
-4	3	9	102	93	7
-3	3	9	66	65	9
-2	3	9	326	314	4
-1	3	9	262	290	4
0	3	9	12	11	-36
1	3	9	36	32	-19
2	3	9	52	53	13
3	3	9	61	65	13
4	3	9	27	26	-21
5	3	9	14	10	-56
6	3	9	14	7	-59
7	3	9	14	29	-59
8	3	9	22	30	-41
-9	4	9	54	48	14
-8	4	9	13	11	-52
-7	4	9	110	118	7
-6	4	9	172	187	6
-5	4	9	12	6	-50
-4	4	9	48	46	14
-3	4	9	29	7	-15
-2	4	9	60	57	11
-1	4	9	12	7	-49
0	4	9	98	89	5
1	4	9	42	20	-17
2	4	9	31	24	-20
3	4	9	175	175	8
4	4	9	69	78	11
5	4	9	34	34	-22
6	4	9	22	13	-39
7	4	9	14	10	-58
-9	5	9	94	98	9
-7	5	9	57	68	12
-6	5	9	77	88	10
-5	5	9	38	36	-18
-4	5	9	223	223	5
-3	5	9	70	47	17
-2	5	9	287	299	4
-1	5	9	106	102	7
0	5	9	124	111	5
1	5	9	144	131	7
2	5	9	30	16	-21
3	5	9	13	1	-37
4	5	9	41	36	-18
5	5	9	36	59	-23
6	5	9	74	86	13
7	5	9	14	12	-59
-8	6	9	23	7	-29
-7	6	9	54	46	13
-6	6	9	54	53	12
-5	6	9	241	217	5
-4	6	9	166	169	6
-3	6	9	62	51	9
-2	6	9	65	63	11
-1	6	9	78	74	8
0	6	9	31	10	-15
1	6	9	289	325	5
2	6	9	31	48	-21
3	6	9	13	25	-53
4	6	9	39	49	-20
5	6	9	37	64	-23
6	6	9	14	19	-58
7	6	9	26	20	-34
-8	7	9	61	61	13
-7	7	9	13	2	-53
-6	7	9	47	41	14
-5	7	9	67	58	10
-4	7	9	72	76	10
-3	7	9	34	14	-18
-2	7	9	104	105	7
-1	7	9	53	49	12
0	7	9	12	10	-36
1	7	9	120	135	8
2	7	9	13	20	-52
3	7	9	13	13	-38
5	7	9	97	81	10
6	7	9	14	17	-59
7	7	9	23	9	-38
-8	8	9	25	16	-24
-7	8	9	44	46	-17
-6	8	9	128	137	7
-5	8	9	12	16	-50
-4	8	9	98	98	8
-3	8	9	19	3	-32
-2	8	9	35	25	-20
-1	8	9	12	6	-50
0	8	9	13	13	-36
1	8	9	185	182	6
2	8	9	106	105	8

Table 56. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
3	8	9	24	33	-30
4	8	9	48	33	-16
5	8	9	14	21	-59
6	8	9	14	6	-59
7	8	9	15	9	-60
-8	9	9	13	20	-55
-7	9	9	13	0	-53
-6	9	9	13	3	-54
-5	9	9	69	44	10
-4	9	9	28	25	-22
-3	9	9	30	4	-20
-2	9	9	289	293	5
-1	9	9	42	46	-16
0	9	9	19	17	-24
1	9	9	44	38	-18
2	9	9	32	18	-20
3	9	9	37	13	-19
4	9	9	66	61	13
5	9	9	15	15	-60
6	9	9	32	15	-28
-8	10	9	39	31	-20
-7	10	9	63	64	13
-6	10	9	123	113	8
-5	10	9	69	74	11
-4	10	9	13	11	-51
-3	10	9	47	32	14
-2	10	9	13	18	-54
-1	10	9	30	18	-22
0	10	9	35	37	-14
1	10	9	49	55	-17
2	10	9	34	24	-21
4	10	9	62	56	14
5	10	9	57	24	16
6	10	9	40	3	-22
-8	11	9	14	9	-56
-7	11	9	22	4	-33
-6	11	9	48	49	16
-5	11	9	13	12	-38
-4	11	9	28	26	-25
-3	11	9	48	35	15
-2	11	9	108	110	8
-1	11	9	13	1	-53
0	11	9	64	72	6
1	11	9	65	71	13
2	11	9	29	23	-26
3	11	9	14	17	-57
4	11	9	37	19	-23
5	11	9	45	42	-21
6	11	9	15	7	-61
-8	12	9	22	4	-39
-7	12	9	55	57	16
-6	12	9	34	43	-23
-5	12	9	26	42	-30
-4	12	9	92	91	10
-3	12	9	29	35	-18
-2	12	9	26	3	-23
-1	12	9	13	26	-55
0	12	9	27	12	-23
1	12	9	102	96	9
2	12	9	14	17	-56
3	12	9	37	13	-23
4	12	9	32	27	-28
-8	13	9	15	3	-60
-7	13	9	15	44	-61
-6	13	9	51	44	16
-5	13	9	21	12	-35
-4	13	9	92	88	10
-3	13	9	31	38	-25
-2	13	9	33	42	-23
-1	13	9	13	2	-55
0	13	9	65	61	12
1	13	9	65	57	13
2	13	9	32	21	-26
3	13	9	15	5	-59
4	13	9	15	19	-61
5	13	9	15	26	-61
-8	14	9	15	15	-62
-7	14	9	50	40	-19
-6	14	9	29	36	-30
-5	14	9	14	19	-57
-4	14	9	65	46	13
-3	14	9	95	83	10
-2	14	9	14	25	-56
-1	14	9	14	11	-56
0	14	9	35	17	-22
1	14	9	32	32	-27
2	14	9	15	1	-60
3	14	9	48	52	-20
4	14	9	15	19	-61
-8	15	9	42	3	-22
-7	15	9	41	36	-23
-6	15	9	15	2	-60

Table 56. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-5	15	9	14	10	-58
-4	15	9	41	42	-22
-3	15	9	40	22	-21
-2	15	9	42	33	-20
-1	15	9	38	43	-23
0	15	9	42	2	-21
1	15	9	15	23	-60
2	15	9	15	12	-60
3	15	9	40	3	-22
-8	16	9	15	3	-62
-7	16	9	55	45	19
-6	16	9	41	34	-23
-5	16	9	27	8	-32
-4	16	9	15	19	-60
-3	16	9	14	21	-59
-2	16	9	15	18	-59
-1	16	9	15	15	-59
0	16	9	15	7	-42
1	16	9	35	19	-25
2	16	9	23	1	-38
-6	17	9	15	14	-61
-5	17	9	15	3	-60
-4	17	9	15	15	-59
-3	17	9	29	3	-29
-2	17	9	15	3	-60
-1	17	9	28	36	-33
0	17	9	38	44	-19
1	17	9	15	2	-60
-5	18	9	15	12	-61
-4	18	9	15	29	-62
-3	18	9	42	12	-21
-2	18	9	25	7	-37
-1	18	9	22	5	-42
-8	0	10	127	132	7
-6	0	10	13	2	-52
-4	0	10	25	41	-25
-2	0	10	350	364	4
0	0	10	31	16	-14
2	0	10	72	71	12
4	0	10	13	17	-54
6	0	10	14	18	-59
-9	1	10	13	12	-54
-8	1	10	66	52	11
-7	1	10	85	92	9
-6	1	10	23	4	-28
-5	1	10	226	238	5
-4	1	10	100	101	7
-3	1	10	12	14	-48
-2	1	10	96	86	8
-1	1	10	56	66	11
0	1	10	45	33	-18
1	1	10	130	124	6
2	1	10	203	204	6
3	1	10	31	31	-22
4	1	10	13	17	-55
5	1	10	57	51	16
6	1	10	14	3	-58
7	1	10	15	11	-60
-9	2	10	47	38	16
-8	2	10	92	84	9
-7	2	10	13	1	-52
-6	2	10	97	74	8
-5	2	10	79	80	10
-4	2	10	56	44	11
-3	2	10	103	110	7
-2	2	10	119	103	7
-1	2	10	136	119	6
0	2	10	126	154	5
1	2	10	71	70	10
2	2	10	40	35	-19
3	2	10	13	5	-53
4	2	10	13	3	-55
5	2	10	89	91	11
6	2	10	38	33	-22
7	2	10	14	35	-59
-9	3	10	13	1	-54
-8	3	10	60	46	12
-7	3	10	121	117	7
-6	3	10	46	32	15
-5	3	10	339	334	5
-4	3	10	12	33	-50
-3	3	10	78	81	9
-2	3	10	98	115	8
-1	3	10	12	31	-50
0	3	10	13	10	-37
1	3	10	87	87	9
2	3	10	83	58	10
3	3	10	29	39	-19
4	3	10	14	46	-56
5	3	10	100	103	10
6	3	10	14	17	-59
7	3	10	15	4	-60

Table 56. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-8	4	10	13	23	-54
-7	4	10	93	93	8
-6	4	10	13	44	-52
-5	4	10	55	56	14
-4	4	10	28	35	-23
-3	4	10	13	5	-36
-2	4	10	175	185	5
-1	4	10	93	97	8
0	4	10	202	214	8
1	4	10	117	119	7
2	4	10	61	64	12
3	4	10	13	1	-55
4	4	10	14	12	-56
5	4	10	75	65	12
6	4	10	40	22	-22
7	4	10	14	7	-59
-8	5	10	58	59	13
-7	5	10	71	68	11
-6	5	10	46	46	15
-5	5	10	165	164	6
-4	5	10	22	32	-29
-3	5	10	243	250	4
-2	5	10	27	51	-24
-1	5	10	28	38	-23
0	5	10	185	195	4
1	5	10	26	31	-26
2	5	10	98	100	9
3	5	10	93	98	9
4	5	10	26	11	-30
5	5	10	37	22	-23
6	5	10	14	2	-59
7	5	10	15	3	-60
-8	6	10	44	46	15
-7	6	10	104	103	9
-6	6	10	72	70	10
-5	6	10	81	88	9
-4	6	10	59	67	11
-3	6	10	178	177	4
-2	6	10	151	159	6
-1	6	10	13	3	-51
0	6	10	60	52	9
1	6	10	33	45	-21
2	6	10	65	60	8
3	6	10	30	2	-26
4	6	10	35	8	-23
5	6	10	26	24	-34
6	6	10	15	4	-60
-8	7	10	26	9	-28
-7	7	10	138	145	8
-6	7	10	13	52	-53
-5	7	10	13	4	-51
-4	7	10	46	66	14
-3	7	10	148	144	6
-2	7	10	47	57	14
-1	7	10	13	5	-51
0	7	10	24	1	-26
1	7	10	13	18	-53
2	7	10	47	48	15
3	7	10	152	147	7
4	7	10	62	51	14
5	7	10	14	32	-58
6	7	10	15	19	-60
-8	8	10	13	9	-55
-7	8	10	48	43	14
-6	8	10	29	43	-25
-5	8	10	13	18	-52
-4	8	10	53	49	13
-3	8	10	135	143	7
-2	8	10	13	18	-51
-1	8	10	28	29	-24
0	8	10	172	168	5
1	8	10	30	1	-21
2	8	10	13	28	-54
3	8	10	14	18	-58
4	8	10	34	1	-25
5	8	10	15	20	-59
6	8	10	25	16	-36
-8	9	10	35	37	-23
-7	9	10	24	21	-31
-6	9	10	13	21	-38
-5	9	10	13	14	-53
-4	9	10	67	78	11
-3	9	10	29	21	-24
-2	9	10	13	15	-52
-1	9	10	13	48	-53
0	9	10	65	69	7
1	9	10	13	24	-54
2	9	10	14	27	-55
3	9	10	39	38	-22
4	9	10	51	61	-18
5	9	10	33	10	-26
-8	10	10	23	11	-34

Table 56. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-7	10	10	13	9	-55
-6	10	10	27	11	-27
-5	10	10	31	31	-17
-4	10	10	41	30	-18
-3	10	10	33	34	-22
-2	10	10	13	12	-53
-1	10	10	27	19	-21
0	10	10	169	169	5
1	10	10	28	19	-27
2	10	10	14	35	-56
3	10	10	15	26	-60
4	10	10	15	25	-60
5	10	10	22	4	-40
-8	11	10	30	3	-27
-7	11	10	48	45	-17
-6	11	10	14	23	-56
-5	11	10	100	92	10
-4	11	10	93	87	9
-3	11	10	57	80	15
-2	11	10	21	18	-33
-1	11	10	13	8	-54
0	11	10	14	11	-40
1	11	10	35	10	-22
2	11	10	39	26	-21
3	11	10	70	58	13
4	11	10	15	21	-60
5	11	10	15	14	-61
-8	12	10	47	56	-21
-7	12	10	47	51	-19
-6	12	10	14	3	-56
-5	12	10	56	58	15
-4	12	10	14	34	-57
-3	12	10	57	50	14
-2	12	10	44	47	-18
-1	12	10	39	30	-19
0	12	10	36	7	-21
1	12	10	14	3	-57
2	12	10	43	38	-20
3	12	10	34	7	-26
4	12	10	15	15	-61
-8	13	10	41	41	-23
-7	13	10	51	36	-18
-6	13	10	14	10	-58
-5	13	10	14	18	-58
-4	13	10	31	32	-26
-3	13	10	57	58	15
-2	13	10	22	6	-35
-1	13	10	33	22	-25
0	13	10	28	16	-26
1	13	10	26	19	-32
2	13	10	51	45	-18
3	13	10	70	54	14
4	13	10	24	20	-38
-8	14	10	35	22	-27
-7	14	10	32	46	-30
-6	14	10	15	11	-60
-5	14	10	25	29	-35
-3	14	10	23	2	-35
-2	14	10	62	62	14
-1	14	10	60	57	15
0	14	10	47	45	-19
1	14	10	29	8	-30
2	14	10	15	14	-60
3	14	10	15	11	-61
-8	15	10	41	21	-23
-7	15	10	28	5	-32
-6	15	10	15	8	-61
-5	15	10	55	69	18
-4	15	10	49	35	-18
-3	15	10	14	5	-59
-2	15	10	14	3	-59
-1	15	10	14	19	-58
0	15	10	25	17	-27
1	15	10	15	18	-60
2	15	10	15	6	-61
-7	16	10	15	7	-62
-6	16	10	15	0	-60
-5	16	10	15	5	-61
-4	16	10	15	1	-59
-3	16	10	14	2	-59
-2	16	10	15	1	-60
-1	16	10	54	36	17
0	16	10	28	21	-27
1	16	10	47	15	-19
-5	17	10	15	31	-62
-4	17	10	28	21	-32
-3	17	10	15	2	-60
-2	17	10	38	12	-24
-1	17	10	32	4	-29
-8	0	11	92	88	9
-6	0	11	225	223	6
-4	0	11	23	13	-28

Table 56. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-2	0	11	43	4	-15
0	0	11	71	66	9
2	0	11	29	5	-21
4	0	11	153	147	8
6	0	11	15	14	-60
-9	1	11	13	27	-55
-8	1	11	22	26	-33
-7	1	11	13	4	-54
-6	1	11	147	145	7
-5	1	11	31	9	-22
-4	1	11	42	46	-16
-3	1	11	131	118	7
-2	1	11	26	20	-25
-1	1	11	109	89	7
0	1	11	249	251	7
1	1	11	68	71	11
2	1	11	43	38	-16
3	1	11	37	7	-20
4	1	11	15	15	-60
5	1	11	14	15	-59
6	1	11	15	7	-59
-9	2	11	33	8	-23
-8	2	11	59	50	13
-7	2	11	35	27	-19
-6	2	11	71	72	11
-5	2	11	72	85	10
-4	2	11	69	76	10
-3	2	11	202	201	6
-2	2	11	62	49	11
-1	2	11	21	16	-31
0	2	11	53	58	10
1	2	11	87	83	9
2	2	11	43	46	12
3	2	11	46	22	-17
4	2	11	81	75	12
5	2	11	14	22	-59
6	2	11	15	22	-60
-8	3	11	92	89	7
-7	3	11	13	47	-53
-6	3	11	82	81	9
-5	3	11	46	56	15
-4	3	11	19	3	-33
-3	3	11	172	182	6
-2	3	11	12	6	-51
-1	3	11	79	84	9
0	3	11	72	65	11
1	3	11	107	102	8
2	3	11	85	88	10
3	3	11	24	20	-31
4	3	11	15	1	-60
5	3	11	14	1	-59
6	3	11	40	23	-22
-8	4	11	72	79	10
-7	4	11	30	5	-23
-6	4	11	82	77	9
-5	4	11	38	19	-17
-4	4	11	122	122	7
-3	4	11	236	235	5
-2	4	11	12	11	-51
-1	4	11	124	116	7
0	4	11	56	57	10
1	4	11	19	5	-36
2	4	11	122	130	8
3	4	11	32	42	-24
4	4	11	78	73	13
5	4	11	15	20	-60
6	4	11	15	23	-60
-8	5	11	72	72	12
-7	5	11	82	75	10
-6	5	11	34	29	-21
-5	5	11	46	47	15
-4	5	11	92	99	8
-3	5	11	13	10	-38
-2	5	11	13	8	-51
-1	5	11	123	127	8
0	5	11	84	84	7
1	5	11	18	10	-30
2	5	11	66	67	13
3	5	11	20	36	-40
4	5	11	15	22	-59
5	5	11	15	16	-59
6	5	11	15	17	-60
-8	6	11	63	66	13
-7	6	11	13	4	-38
-6	6	11	47	50	16
-5	6	11	145	146	7
-4	6	11	13	20	-52
-3	6	11	43	35	12
-2	6	11	48	44	14
-1	6	11	38	44	-20
0	6	11	13	12	-38
1	6	11	25	12	-28

Table 56. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
2	6	11	62	42	14
3	6	11	14	27	-57
4	6	11	63	72	14
5	6	11	15	29	-60
-8	7	11	59	59	14
-7	7	11	13	1	-54
-6	7	11	45	43	-16
-5	7	11	13	5	-54
-4	7	11	76	85	10
-3	7	11	88	73	9
-2	7	11	13	15	-52
-1	7	11	165	181	7
0	7	11	64	62	7
1	7	11	14	32	-56
2	7	11	15	29	-60
3	7	11	28	7	-29
4	7	11	14	4	-58
5	7	11	23	16	-39
-8	8	11	39	17	-21
-7	8	11	35	39	-22
-6	8	11	48	55	-16
-5	8	11	83	82	10
-4	8	11	106	108	8
-3	8	11	13	16	-53
-2	8	11	13	11	-53
-1	8	11	22	11	-27
0	8	11	13	1	-38
1	8	11	14	24	-56
2	8	11	94	82	10
3	8	11	36	10	-23
4	8	11	14	8	-59
5	8	11	35	43	-28
-8	9	11	107	98	10
-7	9	11	37	40	-22
-6	9	11	14	16	-57
-5	9	11	14	25	-55
-4	9	11	36	22	-17
-3	9	11	13	1	-38
-2	9	11	46	57	-16
-1	9	11	27	19	-28
0	9	11	21	9	-28
1	9	11	14	12	-56
2	9	11	80	84	13
3	9	11	15	25	-59
4	9	11	39	1	-22
5	9	11	15	2	-62
-8	10	11	15	9	-60
-7	10	11	14	6	-57
-6	10	11	51	49	17
-5	10	11	32	20	-24
-4	10	11	39	58	-20
-3	10	11	35	35	-22
-2	10	11	62	76	13
-1	10	11	32	31	-25
0	10	11	30	18	-23
1	10	11	14	10	-56
2	10	11	90	81	11
3	10	11	40	9	-21
4	10	11	15	14	-60
-8	11	11	65	58	15
-7	11	11	14	15	-58
-6	11	11	28	43	-29
-5	11	11	24	19	-34
-4	11	11	23	11	-33
-3	11	11	36	42	-22
-2	11	11	53	42	15
-1	11	11	111	107	9
0	11	11	40	8	-21
1	11	11	14	8	-57
2	11	11	62	54	15
3	11	11	38	18	-23
4	11	11	15	2	-61
-8	12	11	15	6	-60
-7	12	11	15	11	-59
-6	12	11	31	54	-30
-5	12	11	91	74	11
-4	12	11	40	13	-20
-3	12	11	20	10	-40
-2	12	11	29	51	-29
-1	12	11	31	40	-27
0	12	11	31	20	-24
1	12	11	23	9	-37
2	12	11	15	1	-61
3	12	11	15	17	-61
-8	13	11	15	0	-61
-7	13	11	25	7	-35
-6	13	11	15	28	-60
-5	13	11	43	25	-21
-4	13	11	14	4	-58
-3	13	11	33	20	-25
-2	13	11	14	10	-59
-1	13	11	56	58	17

Table 56. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
0	13	11	41	26	-15
1	13	11	44	33	-21
2	13	11	15	2	-61
-8	14	11	15	6	-61
-7	14	11	15	6	-61
-6	14	11	42	49	-23
-5	14	11	53	41	18
-4	14	11	22	25	-39
-3	14	11	49	37	-18
-2	14	11	14	4	-59
-1	14	11	29	10	-29
0	14	11	15	1	-42
1	14	11	15	6	-61
2	14	11	59	37	16
-7	15	11	15	5	-60
-6	15	11	15	18	-61
-5	15	11	15	21	-61
-4	15	11	15	9	-59
-3	15	11	15	23	-60
-2	15	11	15	1	-60
-1	15	11	15	1	-59
0	15	11	15	17	-43
1	15	11	15	41	-62
-6	16	11	15	1	-60
-5	16	11	15	4	-61
-4	16	11	28	1	-32
-3	16	11	49	47	-20
-2	16	11	35	29	-26
-1	16	11	15	8	-61
-8	0	12	50	68	16
-6	0	12	47	65	16
-4	0	12	14	22	-58
-2	0	12	66	59	11
0	0	12	77	63	7
2	0	12	69	81	12
4	0	12	33	6	-26
-9	1	12	14	11	-57
-8	1	12	14	5	-56
-7	1	12	52	40	14
-6	1	12	64	71	12
-5	1	12	13	31	-53
-4	1	12	268	273	5
-3	1	12	47	48	15
-2	1	12	13	8	-52
-1	1	12	22	19	-35
0	1	12	21	11	-19
1	1	12	22	31	-31
2	1	12	37	29	-22
3	1	12	59	50	16
4	1	12	15	20	-60
5	1	12	45	12	-19
-9	2	12	83	83	11
-8	2	12	52	49	15
-7	2	12	70	70	11
-6	2	12	110	99	8
-5	2	12	13	5	-52
-4	2	12	66	80	12
-3	2	12	42	37	-16
-2	2	12	13	2	-53
-1	2	12	175	186	6
0	2	12	33	13	-14
1	2	12	33	41	-22
2	2	12	35	53	-23
3	2	12	59	60	16
4	2	12	15	0	-60
5	2	12	23	5	-38
-8	3	12	49	33	16
-7	3	12	14	17	-39
-6	3	12	33	48	-23
-5	3	12	43	25	-16
-4	3	12	59	48	13
-3	3	12	43	20	-16
-2	3	12	97	107	9
-1	3	12	126	127	8
0	3	12	38	26	10
1	3	12	45	50	-18
2	3	12	14	2	-57
3	3	12	110	110	10
4	3	12	46	46	-20
5	3	12	15	17	-60
-8	4	12	14	20	-56
-7	4	12	59	55	13
-6	4	12	89	97	10
-5	4	12	34	61	-21
-4	4	12	73	71	11
-3	4	12	36	37	-14
-2	4	12	82	89	10
-1	4	12	119	125	8
0	4	12	53	50	12
1	4	12	59	52	14
2	4	12	14	4	-57
3	4	12	15	38	-60

Table 56. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
4	4	12	14	5	-58
5	4	12	15	0	-60
-8	5	12	14	4	-57
-7	5	12	39	35	-20
-6	5	12	94	92	7
-5	5	12	13	23	-54
-4	5	12	115	122	8
-3	5	12	60	64	12
-2	5	12	31	7	-23
-1	5	12	104	95	6
0	5	12	26	6	-20
1	5	12	14	5	-58
2	5	12	49	35	17
3	5	12	25	28	-35
4	5	12	24	30	-38
5	5	12	33	34	-27
-8	6	12	74	66	12
-7	6	12	38	17	-21
-6	6	12	14	10	-55
-5	6	12	34	41	-18
-4	6	12	13	9	-54
-3	6	12	29	16	-17
-2	6	12	51	59	11
-1	6	12	23	15	-31
0	6	12	28	31	-20
1	6	12	158	154	7
2	6	12	14	29	-58
3	6	12	14	6	-59
4	6	12	24	4	-36
-8	7	12	14	24	-58
-7	7	12	42	36	-19
-6	7	12	35	30	-23
-5	7	12	28	10	-26
-4	7	12	48	30	15
-3	7	12	69	67	11
-2	7	12	65	80	13
-1	7	12	27	16	-27
0	7	12	22	18	-27
1	7	12	55	33	17
2	7	12	14	0	-58
3	7	12	33	23	-26
4	7	12	24	5	-37
-8	8	12	46	18	-18
-7	8	12	29	19	-29
-6	8	12	78	73	12
-5	8	12	49	34	15
-4	8	12	32	38	-24
-3	8	12	14	28	-55
-2	8	12	58	56	14
-1	8	12	40	28	-19
0	8	12	42	13	-20
1	8	12	89	88	11
2	8	12	47	23	-18
3	8	12	14	1	-59
4	8	12	15	8	-61
-8	9	12	31	36	-28
-7	9	12	27	1	-31
-6	9	12	89	89	11
-5	9	12	14	20	-56
-4	9	12	43	34	-18
-3	9	12	54	56	15
-2	9	12	119	118	9
-1	9	12	46	5	-17
0	9	12	14	5	-40
1	9	12	15	11	-61
2	9	12	15	7	-59
3	9	12	29	16	-30
-8	10	12	36	15	-24
-7	10	12	43	36	-21
-6	10	12	85	76	12
-5	10	12	21	39	-39
-4	10	12	28	37	-29
-3	10	12	14	14	-57
-2	10	12	61	57	15
-1	10	12	14	21	-58
0	10	12	48	36	-18
1	10	12	48	42	-20
2	10	12	15	1	-60
3	10	12	35	11	-25
-8	11	12	29	18	-30
-7	11	12	47	43	-19
-6	11	12	24	41	-38
-5	11	12	14	20	-58
-4	11	12	34	26	-24
-3	11	12	28	29	-29
-2	11	12	42	39	-20
-1	11	12	14	13	-58
0	11	12	14	12	-41
1	11	12	15	18	-61
2	11	12	15	9	-61
-8	12	12	15	9	-60
-7	12	12	26	6	-33

Table 56. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-6	12	12	32	41	-28
-5	12	12	14	27	-59
-4	12	12	14	19	-59
-3	12	12	14	6	-58
-2	12	12	38	3	-23
-1	12	12	14	24	-59
0	12	12	32	41	-20
1	12	12	72	73	14
2	12	12	15	4	-61
-8	13	12	33	6	-28
-7	13	12	15	22	-62
-6	13	12	26	8	-34
-5	13	12	14	1	-59
-4	13	12	42	54	-23
-3	13	12	37	46	-25
-2	13	12	15	22	-60
-1	13	12	14	6	-58
0	13	12	15	9	-42
1	13	12	33	9	-28
-7	14	12	15	40	-62
-6	14	12	15	12	-61
-5	14	12	15	8	-60
-4	14	12	15	7	-60
-3	14	12	30	18	-30
-2	14	12	15	13	-60
-1	14	12	38	10	-23
0	14	12	32	12	-24
-5	15	12	33	0	-27
-4	15	12	15	16	-61
-3	15	12	29	23	-32
-2	15	12	26	7	-35
-8	0	13	28	5	-28
-6	0	13	13	4	-55
-4	0	13	69	73	11
-2	0	13	169	181	7
0	0	13	14	18	-39
2	0	13	35	17	-25
4	0	13	30	18	-31
-9	1	13	51	29	17
-8	1	13	14	22	-57
-7	1	13	23	45	-34
-6	1	13	19	3	-36
-5	1	13	46	45	13
-4	1	13	64	63	9
-3	1	13	35	14	-15
-2	1	13	47	76	-18
-1	1	13	32	13	-22
0	1	13	32	29	-18
1	1	13	43	59	-21
2	1	13	80	82	12
3	1	13	40	12	-22
4	1	13	21	21	-42
-9	2	13	37	26	-24
-8	2	13	14	7	-56
-7	2	13	88	80	10
-6	2	13	13	0	-54
-5	2	13	107	104	6
-4	2	13	21	17	-28
-3	2	13	42	37	12
-2	2	13	124	122	8
-1	2	13	41	22	-18
0	2	13	33	26	-20
1	2	13	26	0	-33
2	2	13	27	20	-31
3	2	13	34	39	-26
4	2	13	36	31	-25
-8	3	13	14	5	-56
-7	3	13	37	8	-22
-6	3	13	13	12	-54
-5	3	13	104	107	9
-4	3	13	61	57	-23
-3	3	13	42	47	-17
-2	3	13	14	33	-57
-1	3	13	13	14	-55
0	3	13	65	66	9
1	3	13	91	95	10
2	3	13	14	1	-58
3	3	13	15	10	-60
4	3	13	15	14	-60
-8	4	13	14	7	-58
-7	4	13	75	71	12
-6	4	13	30	13	-25
-5	4	13	65	72	13
-4	4	13	78	78	11
-3	4	13	74	72	11
-2	4	13	41	51	-20
-1	4	13	55	42	14
0	4	13	18	9	-33
1	4	13	14	9	-58
2	4	13	27	22	-32
3	4	13	15	12	-60
4	4	13	15	6	-60

Table 56. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-8	5	13	35	26	-24
-7	5	13	114	111	9
-6	5	13	60	45	13
-5	5	13	74	77	11
-4	5	13	31	6	-23
-3	5	13	36	37	-22
-2	5	13	51	46	16
-1	5	13	14	17	-55
0	5	13	76	73	8
1	5	13	39	39	-22
2	5	13	29	34	-29
3	5	13	30	36	-30
4	5	13	15	1	-60
-8	6	13	14	13	-59
-7	6	13	15	1	-60
-6	6	13	29	11	-28
-5	6	13	52	49	15
-4	6	13	33	30	-23
-3	6	13	86	90	11
-2	6	13	80	81	11
-1	6	13	29	30	-26
0	6	13	38	37	-22
1	6	13	21	38	-40
2	6	13	14	16	-58
3	6	13	23	32	-39
-8	7	13	14	9	-59
-7	7	13	106	110	11
-6	7	13	64	63	14
-5	7	13	41	7	-19
-4	7	13	13	9	-55
-3	7	13	37	8	-21
-2	7	13	39	22	-20
-1	7	13	14	27	-56
0	7	13	50	40	12
1	7	13	14	13	-59
2	7	13	25	11	-35
3	7	13	55	51	18
-8	8	13	32	7	-26
-7	8	13	15	12	-60
-6	8	13	14	11	-57
-5	8	13	14	22	-57
-4	8	13	53	44	15
-3	8	13	33	38	-25
-2	8	13	31	8	-26
-1	8	13	26	42	-32
0	8	13	64	68	11
1	8	13	24	8	-37
2	8	13	15	13	-60
3	8	13	26	34	-38
-8	9	13	41	29	-21
-7	9	13	34	31	-26
-6	9	13	14	21	-58
-5	9	13	14	9	-57
-4	9	13	14	18	-59
-3	9	13	14	23	-59
-2	9	13	47	52	-19
-1	9	13	32	16	-25
0	9	13	96	97	8
1	9	13	24	13	-38
2	9	13	38	5	-23
-8	10	13	15	19	-60
-7	10	13	15	0	-59
-6	10	13	14	11	-58
-5	10	13	26	39	-34
-4	10	13	69	73	14
-3	10	13	33	40	-26
-2	10	13	14	6	-58
-1	10	13	36	19	-24
0	10	13	35	37	-19
1	10	13	41	4	-22
2	10	13	22	7	-41
-8	11	13	15	12	-61
-7	11	13	15	31	-61
-6	11	13	14	1	-59
-5	11	13	14	5	-59
-4	11	13	37	31	-24
-3	11	13	41	10	-21
-2	11	13	14	20	-59
-1	11	13	14	8	-59
0	11	13	53	43	16
1	11	13	15	3	-60
-8	12	13	45	14	-21
-7	12	13	28	4	-34
-6	12	13	15	0	-60
-5	12	13	44	28	-20
-4	12	13	15	11	-60
-3	12	13	15	41	-61
-2	12	13	27	24	-33
-1	12	13	15	14	-59
0	12	13	15	4	-43
-7	13	13	51	34	-19
-6	13	13	25	4	-36

Table 56. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-5	13	13	33	32	-28
-4	13	13	15	14	-61
-3	13	13	23	4	-40
-2	13	13	34	6	-26
-1	13	13	15	11	-60
-5	14	13	15	10	-62
-4	14	13	28	17	-35
-3	14	13	26	3	-34
-8	0	14	68	62	14
-6	0	14	69	75	13
-4	0	14	27	25	-28
-2	0	14	22	41	-35
0	0	14	106	108	7
2	0	14	30	12	-29
-9	1	14	31	2	-28
-8	1	14	51	52	17
-7	1	14	14	0	-56
-6	1	14	43	20	-18
-5	1	14	45	57	-18
-4	1	14	14	6	-55
-3	1	14	67	68	13
-2	1	14	53	42	15
-1	1	14	14	11	-58
0	1	14	66	75	13
1	1	14	14	21	-58
2	1	14	15	22	-59
3	1	14	15	0	-60
-9	2	14	14	5	-59
-8	2	14	14	6	-58
-7	2	14	51	42	16
-6	2	14	42	42	-19
-5	2	14	37	17	-21
-4	2	14	52	49	15
-3	2	14	14	12	-58
-2	2	14	49	33	16
-1	2	14	33	44	-25
0	2	14	49	48	14
1	2	14	39	36	-22
2	2	14	15	22	-60
3	2	14	52	27	17
-8	3	14	49	44	-18
-7	3	14	14	12	-58
-6	3	14	14	4	-56
-5	3	14	61	56	13
-4	3	14	33	28	-24
-3	3	14	127	129	8
-2	3	14	64	60	13
-1	3	14	23	5	-34
0	3	14	15	14	-59
1	3	14	33	9	-25
2	3	14	28	9	-32
3	3	14	22	14	-39
-8	4	14	75	79	13
-7	4	14	58	57	15
-6	4	14	14	33	-57
-5	4	14	46	52	-18
-4	4	14	14	19	-56
-3	4	14	52	44	16
-2	4	14	14	3	-56
-1	4	14	21	17	-39
0	4	14	37	43	-17
1	4	14	34	22	-25
2	4	14	44	53	-21
-8	5	14	15	4	-59
-7	5	14	15	36	-60
-6	5	14	14	4	-59
-5	5	14	31	9	-26
-4	5	14	14	2	-55
-3	5	14	14	19	-58
-2	5	14	50	42	16
-1	5	14	73	68	12
0	5	14	33	20	-24
1	5	14	15	11	-59
2	5	14	15	1	-61
-8	6	14	15	33	-60
-7	6	14	22	7	-39
-6	6	14	42	37	-21
-5	6	14	81	81	12
-4	6	14	35	42	-23
-3	6	14	29	35	-28
-2	6	14	14	7	-57
-1	6	14	21	35	-41
0	6	14	26	40	-25
1	6	14	15	1	-60
2	6	14	15	8	-62
-8	7	14	28	29	-32
-7	7	14	43	26	-20
-6	7	14	26	36	-34
-5	7	14	15	44	-60
-4	7	14	24	17	-34
-3	7	14	62	47	14
-2	7	14	14	6	-57

Table 56. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-1	7	14	64	66	15
0	7	14	27	39	-28
1	7	14	42	14	-21
2	7	14	15	9	-63
-8	8	14	15	27	-60
-7	8	14	15	26	-60
-6	8	14	28	10	-30
-5	8	14	60	50	15
-4	8	14	39	49	-23
-3	8	14	38	8	-22
-2	8	14	14	3	-59
-1	8	14	15	37	-61
0	8	14	32	8	-20
1	8	14	15	12	-60
-8	9	14	15	31	-62
-7	9	14	15	1	-60
-6	9	14	27	39	-32
-5	9	14	14	13	-59
-4	9	14	36	31	-24
-3	9	14	14	2	-59
-2	9	14	30	42	-30
-1	9	14	15	14	-61
0	9	14	15	16	-43
1	9	14	15	2	-61
-8	10	14	15	27	-62
-7	10	14	15	1	-60
-6	10	14	14	6	-59
-5	10	14	15	4	-60
-4	10	14	42	19	-21
-3	10	14	14	8	-59
-2	10	14	15	0	-60
-1	10	14	15	1	-60
0	10	14	26	11	-25
-7	11	14	15	6	-61
-6	11	14	15	15	-61
-5	11	14	46	30	-20
-4	11	14	15	9	-60
-3	11	14	15	19	-60
-2	11	14	45	32	-20
-1	11	14	15	42	-62
-6	12	14	15	37	-63
-5	12	14	57	35	17
-4	12	14	15	4	-60
-3	12	14	15	14	-60
-2	12	14	15	15	-61
-8	0	15	62	60	16
-6	0	15	77	69	12
-4	0	15	78	70	12
-2	0	15	22	5	-38
0	0	15	15	36	-60
-9	1	15	15	29	-61
-8	1	15	15	22	-61
-7	1	15	15	8	-59
-6	1	15	32	1	-25
-5	1	15	14	3	-57
-4	1	15	58	58	15
-3	1	15	14	6	-58
-2	1	15	14	34	-58
-1	1	15	15	21	-61
0	1	15	28	0	-26
1	1	15	48	18	-19
-9	2	15	15	21	-62
-8	2	15	39	49	-24
-7	2	15	14	13	-59
-6	2	15	24	35	-36
-5	2	15	14	7	-57
-4	2	15	26	27	-32
-3	2	15	44	36	-20
-2	2	15	37	16	-23
-1	2	15	92	96	11
0	2	15	15	11	-42
1	2	15	15	12	-60
-8	3	15	27	12	-32
-7	3	15	14	18	-58
-6	3	15	83	70	12
-5	3	15	38	36	-21
-4	3	15	14	4	-58
-3	3	15	14	28	-59
-2	3	15	28	23	-30
-1	3	15	15	25	-62
0	3	15	26	0	-28
1	3	15	15	10	-60
-8	4	15	28	12	-31
-7	4	15	14	10	-59
-6	4	15	15	7	-59
-5	4	15	14	8	-58
-4	4	15	41	44	-22
-3	4	15	34	7	-24
-2	4	15	15	38	-60
-1	4	15	74	67	14
0	4	15	28	13	-22
1	4	15	45	23	-20

Table 56. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-8	5	15	41	41	-22
-7	5	15	34	6	-26
-6	5	15	56	55	17
-5	5	15	55	46	16
-4	5	15	43	47	-21
-3	5	15	49	40	-18
-2	5	15	21	6	-40
-1	5	15	15	18	-62
0	5	15	40	4	-22
1	5	15	41	39	-24
-8	6	15	15	19	-61
-7	6	15	14	8	-59
-6	6	15	15	24	-60
-5	6	15	35	22	-24
-4	6	15	14	23	-59
-3	6	15	38	41	-24
-2	6	15	15	3	-59
-1	6	15	36	15	-25
0	6	15	15	10	-43
-8	7	15	15	12	-61
-7	7	15	26	17	-34
-6	7	15	15	19	-61
-5	7	15	15	10	-60
-4	7	15	38	33	-24
-3	7	15	31	30	-29
-2	7	15	23	22	-39
-1	7	15	23	26	-41
0	7	15	15	9	-43
-8	8	15	15	16	-61
-7	8	15	15	1	-60
-6	8	15	15	16	-61
-5	8	15	14	2	-59
-4	8	15	15	21	-59
-3	8	15	50	37	-18

APPENDIX I

TABLE 57

Table 57. 1,2,4-Trimethybenzene Thiourea Host/Guest Adduct F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
2	0	0	489	390	6
4	0	0	115	127	10
6	0	0	229	223	9
8	0	0	87	96	22
10	0	0	171	161	16
12	0	0	97	53	-31
1	1	0	80	76	5
2	1	0	293	240	6
3	1	0	601	504	20
4	1	0	237	277	10
5	1	0	163	165	7
6	1	0	192	192	14
7	1	0	207	188	8
8	1	0	92	73	15
9	1	0	44	13	-31
10	1	0	48	8	-41
11	1	0	46	9	-42
12	1	0	70	30	-40
0	2	0	409	484	4
1	2	0	11	24	-30
2	2	0	90	100	11
3	2	0	603	552	8
4	2	0	17	19	-64
5	2	0	35	29	-36
6	2	0	20	19	-77
7	2	0	294	286	9
8	2	0	22	13	-84
9	2	0	58	18	-34
10	2	0	65	48	-37
11	2	0	27	15	-102
1	3	0	29	21	-22
2	3	0	403	417	8
3	3	0	837	764	8
4	3	0	98	86	12
5	3	0	130	147	12
6	3	0	21	5	-80
7	3	0	285	275	9
8	3	0	32	17	-58
9	3	0	41	43	-49
10	3	0	25	8	-96
11	3	0	27	22	-102
0	4	0	574	390	7
1	4	0	940	791	23
2	4	0	589	540	8
3	4	0	201	190	8
4	4	0	41	65	-28
5	4	0	19	30	-72
6	4	0	34	8	-50
7	4	0	202	200	11
8	4	0	207	181	11
9	4	0	41	24	-49
10	4	0	130	104	20
11	4	0	27	6	-102
1	5	0	192	161	6
2	5	0	447	410	7
3	5	0	155	133	8
4	5	0	246	250	7
5	5	0	343	325	8
6	5	0	21	23	-80
7	5	0	22	18	-84
8	5	0	110	127	18
9	5	0	77	22	-26
10	5	0	55	36	-45
11	5	0	78	48	-36
0	6	0	177	240	7
1	6	0	141	158	9
2	6	0	257	272	7
3	6	0	44	42	-27
4	6	0	138	156	11
5	6	0	156	145	12
6	6	0	32	40	-54
7	6	0	82	79	24
8	6	0	72	68	-27
9	6	0	86	100	25
10	6	0	95	89	27
11	6	0	53	20	-53
1	7	0	104	108	8
2	7	0	45	1	-26
3	7	0	86	98	16
4	7	0	118	128	14
5	7	0	575	589	9
6	7	0	48	53	-38
7	7	0	102	110	19
8	7	0	61	73	-33
9	7	0	23	2	-89
10	7	0	39	33	-66
11	7	0	52	34	-56
0	8	0	364	346	7
1	8	0	67	46	13
2	8	0	549	548	9
3	8	0	85	88	18
4	8	0	215	220	10

Table 57. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
5	8	0	21	30	-81
6	8	0	57	29	-33
7	8	0	83	64	23
8	8	0	127	125	17
9	8	0	68	60	-36
10	8	0	26	41	-101
11	8	0	28	30	-106
1	9	0	61	57	16
2	9	0	350	364	8
3	9	0	37	15	-42
4	9	0	63	87	-26
5	9	0	164	160	13
6	9	0	22	38	-84
7	9	0	52	23	-37
8	9	0	23	32	-89
9	9	0	26	35	-98
10	9	0	69	14	-40
0	10	0	200	217	9
1	10	0	103	89	11
2	10	0	385	392	9
3	10	0	20	12	-78
4	10	0	43	28	-40
5	10	0	22	19	-84
6	10	0	49	3	-38
7	10	0	23	0	-86
8	10	0	99	96	25
9	10	0	26	1	-99
10	10	0	58	46	-49
1	11	0	132	138	9
2	11	0	212	197	10
3	11	0	101	100	17
4	11	0	48	30	-37
5	11	0	226	219	10
6	11	0	22	35	-85
7	11	0	23	29	-89
8	11	0	26	43	-98
9	11	0	40	36	-67
10	11	0	28	13	-105
0	12	0	261	270	9
1	12	0	98	110	21
2	12	0	96	95	19
3	12	0	52	37	-34
4	12	0	22	3	-82
5	12	0	22	1	-85
6	12	0	96	104	22
7	12	0	25	38	-95
8	12	0	26	20	-99
9	12	0	27	36	-102
1	13	0	21	3	-57
2	13	0	21	20	-82
3	13	0	21	3	-82
4	13	0	22	43	-84
5	13	0	145	157	15
6	13	0	42	13	-49
7	13	0	25	5	-96
8	13	0	27	16	-102
9	13	0	73	2	-39
0	14	0	150	156	13
1	14	0	105	109	13
2	14	0	83	76	22
3	14	0	35	15	-51
4	14	0	22	23	-86
5	14	0	23	43	-88
6	14	0	53	25	-45
7	14	0	47	32	-55
8	14	0	62	35	-46
1	15	0	22	43	-59
2	15	0	53	55	-36
3	15	0	127	128	16
4	15	0	58	36	-39
5	15	0	50	33	-48
6	15	0	26	28	-99
7	15	0	86	48	-32
0	16	0	22	6	-86
1	16	0	22	14	-61
2	16	0	23	11	-86
3	16	0	25	51	-94
4	16	0	25	15	-97
5	16	0	39	10	-65
6	16	0	54	47	-50
7	16	0	41	31	-71
1	17	0	24	7	-64
2	17	0	25	44	-95
3	17	0	25	75	-98
4	17	0	26	19	-99
5	17	0	54	12	-49
6	17	0	27	1	-104
0	18	0	74	86	-32
1	18	0	44	23	-37
2	18	0	26	20	-98
3	18	0	63	53	-42
4	18	0	27	34	-102

Table 57. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
1	19	0	66	21	-29
2	19	0	26	10	-101
3	19	0	27	4	-103
-12	0	1	69	13	-42
-10	0	1	23	28	-89
-8	0	1	74	40	-26
-6	0	1	107	104	14
-2	0	1	195	158	5
2	0	1	797	713	6
4	0	1	480	493	8
6	0	1	346	342	9
8	0	1	22	19	-85
10	0	1	25	8	-97
-12	1	1	75	11	-39
-11	1	1	89	54	-37
-10	1	1	42	46	-36
-9	1	1	38	54	-36
-8	1	1	428	412	19
-7	1	1	21	21	-56
-6	1	1	280	250	15
-5	1	1	108	87	12
-4	1	1	56	40	-24
-3	1	1	232	173	8
-2	1	1	36	65	-13
-1	1	1	345	409	22
1	1	1	164	182	3
2	1	1	1384	1315	6
4	1	1	242	218	6
5	1	1	156	141	8
6	1	1	52	54	-22
7	1	1	22	9	-58
8	1	1	79	58	17
9	1	1	115	105	19
10	1	1	39	26	-49
11	1	1	52	48	-45
-12	2	1	28	21	-106
-11	2	1	42	70	-62
-10	2	1	62	45	-33
-9	2	1	22	17	-85
-8	2	1	44	14	-43
-7	2	1	48	44	-36
-6	2	1	116	103	14
-5	2	1	385	391	7
-4	2	1	422	377	8
-3	2	1	284	251	7
-2	2	1	330	332	6
-1	2	1	842	867	5
0	2	1	11	17	-29
1	2	1	104	85	5
2	2	1	328	315	7
3	2	1	334	293	7
4	2	1	149	137	9
5	2	1	494	484	9
6	2	1	71	68	-24
7	2	1	181	186	12
8	2	1	22	6	-85
9	2	1	85	76	25
10	2	1	25	20	-97
11	2	1	27	2	-103
-12	3	1	28	14	-106
-11	3	1	113	82	24
-10	3	1	92	51	23
-9	3	1	111	101	18
-8	3	1	22	13	-84
-7	3	1	82	77	22
-6	3	1	360	370	8
-5	3	1	90	95	15
-4	3	1	122	116	10
-3	3	1	330	296	7
-1	3	1	1847	1635	52
0	3	1	150	123	5
1	3	1	191	205	6
2	3	1	56	76	-21
3	3	1	249	210	7
4	3	1	182	184	8
5	3	1	129	97	12
6	3	1	21	7	-79
7	3	1	79	26	23
8	3	1	44	41	-44
9	3	1	213	201	12
10	3	1	43	62	-57
11	3	1	27	53	-104
-12	4	1	62	15	-48
-11	4	1	57	51	-47
-10	4	1	54	44	-44
-9	4	1	42	28	-46
-8	4	1	96	99	20
-7	4	1	21	10	-81
-6	4	1	304	289	8
-5	4	1	166	162	10
-4	4	1	196	212	7
-3	4	1	158	170	8

Table 57. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-2	4	1	222	203	8
-1	4	1	1589	1241	6
0	4	1	434	350	5
1	4	1	151	152	7
2	4	1	232	225	8
3	4	1	312	300	7
4	4	1	269	267	8
5	4	1	376	372	8
6	4	1	238	242	10
7	4	1	36	46	-51
8	4	1	32	2	-58
9	4	1	55	12	-38
10	4	1	26	9	-99
11	4	1	27	9	-103
-11	5	1	26	6	-101
-10	5	1	88	95	-29
-9	5	1	23	27	-88
-8	5	1	185	164	12
-7	5	1	22	61	-83
-6	5	1	300	313	9
-5	5	1	103	99	15
-4	5	1	50	49	-24
-3	5	1	64	59	17
-2	5	1	70	62	16
0	5	1	789	710	5
1	5	1	465	414	12
2	5	1	567	501	9
3	5	1	17	33	-67
4	5	1	29	41	-44
5	5	1	60	9	-26
6	5	1	21	49	-82
7	5	1	186	164	12
8	5	1	23	29	-86
9	5	1	77	45	-28
10	5	1	60	48	-43
11	5	1	53	10	-54
-11	6	1	27	23	-102
-10	6	1	57	2	-44
-9	6	1	79	41	-25
-8	6	1	41	10	-46
-7	6	1	68	43	-27
-6	6	1	184	195	12
-5	6	1	168	168	10
-4	6	1	158	135	10
-2	6	1	74	108	15
-1	6	1	16	33	-43
0	6	1	401	375	5
1	6	1	96	62	14
2	6	1	169	130	8
3	6	1	318	310	8
4	6	1	135	137	12
5	6	1	39	69	-43
6	6	1	160	165	14
7	6	1	242	237	11
8	6	1	23	26	-86
9	6	1	63	63	-38
10	6	1	26	23	-100
11	6	1	40	12	-73
-11	7	1	27	36	-104
-10	7	1	26	4	-98
-9	7	1	103	92	21
-8	7	1	131	137	16
-7	7	1	43	3	-44
-6	7	1	131	122	15
-5	7	1	35	23	-46
-4	7	1	31	15	-46
-3	7	1	349	342	8
-2	7	1	192	196	8
-1	7	1	54	17	-22
0	7	1	233	229	14
1	7	1	651	646	28
2	7	1	112	100	12
3	7	1	66	46	20
4	7	1	44	16	-37
5	7	1	53	60	-32
6	7	1	141	140	15
7	7	1	153	161	14
8	7	1	23	6	-87
9	7	1	58	72	-44
10	7	1	27	21	-102
-11	8	1	82	27	-36
-10	8	1	26	29	-99
-9	8	1	43	25	-56
-8	8	1	61	54	-32
-7	8	1	22	13	-84
-6	8	1	168	170	13
-5	8	1	52	85	-33
-4	8	1	56	0	-27
-3	8	1	571	558	9
-2	8	1	246	231	8
-1	8	1	70	74	12
0	8	1	255	254	5

Table 57. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
1	8	1	145	131	7
2	8	1	47	20	-27
3	8	1	158	159	11
4	8	1	334	334	9
5	8	1	80	49	22
6	8	1	40	10	-46
7	8	1	241	240	10
8	8	1	53	58	-39
9	8	1	44	39	-57
10	8	1	27	19	-102
-11	9	1	47	11	-63
-10	9	1	67	52	-39
-9	9	1	25	12	-96
-8	9	1	23	26	-87
-7	9	1	47	18	-41
-6	9	1	232	230	11
-5	9	1	112	121	17
-4	9	1	31	2	-53
-3	9	1	36	65	-42
-2	9	1	102	101	15
-1	9	1	18	1	-50
0	9	1	455	449	11
1	9	1	94	106	12
2	9	1	96	71	16
3	9	1	145	139	12
4	9	1	273	280	9
5	9	1	76	83	24
6	9	1	22	13	-84
7	9	1	38	29	-52
8	9	1	54	2	-44
9	9	1	26	19	-99
10	9	1	64	64	-45
-10	10	1	54	42	-51
-9	10	1	26	35	-98
-8	10	1	59	30	-35
-7	10	1	43	58	-46
-6	10	1	253	262	10
-5	10	1	22	9	-83
-4	10	1	21	4	-80
-3	10	1	55	64	-29
-2	10	1	71	71	22
-1	10	1	52	47	-30
0	10	1	40	19	-31
1	10	1	134	134	9
2	10	1	51	37	-31
3	10	1	98	87	17
4	10	1	367	365	9
5	10	1	43	68	-43
6	10	1	22	44	-85
7	10	1	23	18	-88
8	10	1	25	37	-97
9	10	1	26	30	-101
10	10	1	28	8	-106
-10	11	1	27	24	-105
-9	11	1	26	30	-99
-8	11	1	42	16	-58
-7	11	1	33	28	-61
-6	11	1	88	107	22
-5	11	1	41	32	-46
-4	11	1	78	80	23
-3	11	1	21	17	-80
-2	11	1	91	112	20
-1	11	1	142	155	15
0	11	1	175	193	8
1	11	1	205	212	7
2	11	1	21	19	-80
3	11	1	21	27	-81
4	11	1	133	136	15
5	11	1	39	33	-48
6	11	1	34	4	-58
7	11	1	68	79	-32
8	11	1	26	40	-99
9	11	1	27	39	-102
-9	12	1	27	17	-102
-8	12	1	26	6	-98
-7	12	1	39	18	-53
-6	12	1	53	57	-38
-5	12	1	61	61	-31
-4	12	1	69	62	-26
-3	12	1	271	284	9
-2	12	1	72	2	-24
-1	12	1	27	13	-44
0	12	1	54	63	-23
1	12	1	67	69	19
2	12	1	45	24	-38
3	12	1	21	25	-82
4	12	1	90	76	21
5	12	1	80	63	24
6	12	1	23	29	-88
7	12	1	66	74	-37
8	12	1	26	14	-101
9	12	1	41	43	-70

Table 57. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-9	13	1	91	28	-31
-8	13	1	117	95	24
-7	13	1	42	47	-57
-6	13	1	23	11	-88
-5	13	1	23	9	-86
-4	13	1	70	73	-26
-3	13	1	66	12	-26
-2	13	1	107	100	17
-1	13	1	61	57	-21
0	13	1	21	12	-57
1	13	1	173	189	9
2	13	1	154	146	12
3	13	1	50	49	-35
4	13	1	97	80	20
5	13	1	85	87	24
6	13	1	65	31	-37
7	13	1	81	81	-31
8	13	1	27	33	-103
-8	14	1	27	32	-104
-7	14	1	68	37	-37
-6	14	1	25	11	-96
-5	14	1	34	21	-60
-4	14	1	86	94	23
-3	14	1	115	125	16
-2	14	1	22	5	-83
-1	14	1	97	94	13
0	14	1	38	3	-38
1	14	1	21	38	-58
2	14	1	43	47	-43
3	14	1	22	9	-84
4	14	1	60	63	-33
5	14	1	25	45	-95
6	14	1	25	44	-97
7	14	1	54	19	-49
8	14	1	28	13	-105
-8	15	1	27	35	-105
-7	15	1	27	48	-102
-6	15	1	54	61	-48
-5	15	1	52	25	-46
-4	15	1	61	12	-33
-3	15	1	53	49	-36
-2	15	1	33	24	-57
-1	15	1	120	98	11
0	15	1	92	87	15
1	15	1	41	19	-37
2	15	1	107	115	19
3	15	1	59	55	-33
4	15	1	58	4	-40
5	15	1	88	55	28
6	15	1	26	7	-99
7	15	1	47	14	-59
-7	16	1	27	13	-104
-6	16	1	54	1	-48
-5	16	1	56	66	-46
-4	16	1	25	2	-96
-3	16	1	40	4	-58
-2	16	1	23	24	-87
-1	16	1	109	115	13
0	16	1	33	20	-45
1	16	1	22	36	-61
2	16	1	24	50	-92
3	16	1	25	9	-95
4	16	1	25	42	-96
5	16	1	46	74	-57
6	16	1	27	8	-103
-6	17	1	58	8	-48
-5	17	1	26	17	-101
-4	17	1	70	47	-36
-3	17	1	25	19	-96
-2	17	1	25	27	-95
-1	17	1	69	87	-23
0	17	1	24	4	-64
1	17	1	24	0	-64
2	17	1	25	27	-94
3	17	1	25	40	-97
4	17	1	66	3	-39
5	17	1	27	21	-102
-5	18	1	49	19	-57
-4	18	1	48	50	-56
-3	18	1	26	4	-98
-2	18	1	26	4	-98
-1	18	1	37	32	-48
0	18	1	39	25	-46
1	18	1	38	10	-47
2	18	1	41	56	-63
3	18	1	39	17	-69
4	18	1	27	1	-102
-3	19	1	27	15	-103
-2	19	1	57	35	-47
-1	19	1	62	29	-38
0	19	1	57	17	-38
1	19	1	25	15	-68

Table 57. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
2	19	1	84	67	-34
-12	0	2	63	9	-45
-10	0	2	77	4	-26
-8	0	2	69	70	-27
-6	0	2	400	370	8
-4	0	2	54	25	-19
0	0	2	140	156	4
2	0	2	349	288	7
4	0	2	599	547	10
6	0	2	100	106	18
8	0	2	214	239	11
10	0	2	26	18	-99
-12	1	2	81	70	-27
-11	1	2	59	42	-31
-10	1	2	44	1	-33
-9	1	2	83	62	17
-8	1	2	63	48	-31
-7	1	2	84	77	14
-6	1	2	251	245	19
-5	1	2	182	170	15
-4	1	2	100	81	8
-3	1	2	526	484	8
-1	1	2	24	35	-13
0	1	2	183	161	6
1	1	2	272	197	4
2	1	2	152	138	7
3	1	2	39	52	-20
4	1	2	789	696	15
5	1	2	137	132	9
6	1	2	21	37	-57
7	1	2	83	80	16
8	1	2	223	211	8
9	1	2	55	33	-27
10	1	2	46	31	-40
11	1	2	86	1	24
-12	2	2	27	6	-105
-11	2	2	86	64	-30
-10	2	2	42	25	-48
-9	2	2	258	238	10
-7	2	2	115	99	16
-6	2	2	180	153	10
-5	2	2	156	133	9
-4	2	2	357	364	7
-3	2	2	399	393	7
-1	2	2	192	174	6
0	2	2	481	372	4
1	2	2	1586	1455	6
2	2	2	710	562	8
3	2	2	468	451	7
4	2	2	433	405	8
5	2	2	20	35	-75
6	2	2	21	26	-80
7	2	2	22	2	-84
8	2	2	158	154	14
9	2	2	94	102	23
10	2	2	73	39	-36
11	2	2	116	100	26
-12	3	2	27	1	-105
-11	3	2	61	48	-42
-10	3	2	51	43	-41
-9	3	2	139	138	15
-8	3	2	47	20	-39
-7	3	2	158	149	12
-6	3	2	174	179	11
-5	3	2	188	181	8
-4	3	2	341	384	7
-3	3	2	561	549	8
-1	3	2	44	78	-16
0	3	2	187	144	6
1	3	2	247	248	6
2	3	2	235	197	8
3	3	2	148	126	9
4	3	2	135	97	11
5	3	2	141	163	12
6	3	2	249	251	9
7	3	2	104	81	18
8	3	2	42	23	-46
9	3	2	52	67	-41
10	3	2	51	2	-51
11	3	2	49	6	-59
-12	4	2	62	14	-47
-11	4	2	26	48	-100
-10	4	2	23	16	-89
-9	4	2	155	131	13
-8	4	2	37	48	-50
-7	4	2	22	52	-84
-6	4	2	173	200	11
-5	4	2	214	219	8
-4	4	2	191	220	8
-3	4	2	319	279	6
-2	4	2	301	207	7
-1	4	2	42	12	-23

Table 57. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
0	4	2	44	46	-20
1	4	2	925	874	8
2	4	2	415	352	8
3	4	2	33	5	-35
4	4	2	234	229	8
5	4	2	62	23	-25
6	4	2	42	14	-42
7	4	2	22	13	-84
8	4	2	23	3	-87
9	4	2	25	6	-96
10	4	2	70	50	-38
11	4	2	78	74	-39
-12	5	2	53	48	-54
-11	5	2	26	38	-100
-10	5	2	47	25	-45
-9	5	2	116	100	18
-8	5	2	37	20	-50
-7	5	2	114	120	17
-6	5	2	224	236	10
-5	5	2	19	19	-72
-3	5	2	272	298	7
-2	5	2	96	134	12
-1	5	2	567	528	17
1	5	2	180	180	6
2	5	2	112	107	11
3	5	2	103	84	13
4	5	2	175	190	10
5	5	2	21	37	-81
6	5	2	287	307	10
7	5	2	38	19	-49
8	5	2	120	120	17
9	5	2	25	11	-95
10	5	2	27	21	-101
-12	6	2	28	12	-107
-11	6	2	26	29	-101
-10	6	2	25	15	-97
-9	6	2	23	26	-87
-8	6	2	22	27	-84
-7	6	2	355	360	9
-6	6	2	226	241	10
-5	6	2	20	4	-77
-4	6	2	54	52	-25
-3	6	2	88	100	14
-2	6	2	76	103	15
-1	6	2	805	766	10
0	6	2	160	198	9
1	6	2	95	81	18
2	6	2	161	168	9
3	6	2	192	206	9
4	6	2	221	218	10
5	6	2	209	201	11
6	6	2	111	92	17
7	6	2	22	47	-85
8	6	2	92	97	23
9	6	2	89	70	-29
10	6	2	27	22	-102
-11	7	2	27	68	-103
-10	7	2	84	40	-30
-9	7	2	65	11	-31
-8	7	2	36	3	-51
-7	7	2	42	55	-45
-6	7	2	21	39	-82
-5	7	2	20	31	-78
-4	7	2	19	18	-75
-3	7	2	125	110	11
-2	7	2	551	510	8
-1	7	2	814	754	9
0	7	2	301	308	5
1	7	2	41	51	-26
2	7	2	75	83	18
3	7	2	239	246	9
4	7	2	74	78	23
5	7	2	58	30	-30
6	7	2	83	94	23
7	7	2	22	18	-86
8	7	2	23	7	-88
9	7	2	57	74	-46
10	7	2	44	1	-63
-11	8	2	27	29	-103
-10	8	2	26	23	-98
-9	8	2	49	52	-43
-8	8	2	88	91	22
-7	8	2	189	209	12
-6	8	2	53	58	-35
-5	8	2	21	38	-80
-4	8	2	115	118	15
-3	8	2	19	10	-72
-2	8	2	96	79	14
-1	8	2	334	325	7
0	8	2	209	216	6
1	8	2	152	144	8
2	8	2	19	37	-73

Table 57. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
3	8	2	347	349	9
4	8	2	21	24	-79
5	8	2	22	8	-83
6	8	2	68	55	-28
7	8	2	59	18	-33
8	8	2	74	37	-32
9	8	2	26	55	-100
10	8	2	27	9	-105
-11	9	2	58	24	-51
-10	9	2	54	25	-48
-9	9	2	69	8	-35
-8	9	2	48	31	-41
-7	9	2	121	95	16
-6	9	2	43	19	-43
-5	9	2	21	1	-82
-4	9	2	414	426	9
-3	9	2	20	2	-75
-2	9	2	128	121	13
-1	9	2	305	287	7
0	9	2	227	219	6
1	9	2	112	111	10
2	9	2	75	77	22
3	9	2	83	71	20
4	9	2	46	52	-38
5	9	2	22	35	-84
6	9	2	332	329	10
7	9	2	23	13	-88
8	9	2	80	73	-31
9	9	2	74	45	-37
-10	10	2	43	12	-62
-9	10	2	73	63	-34
-8	10	2	23	56	-89
-7	10	2	22	36	-86
-6	10	2	22	38	-84
-5	10	2	69	70	-26
-4	10	2	188	197	11
-3	10	2	50	52	-32
-2	10	2	243	243	9
-1	10	2	167	156	8
0	10	2	218	214	6
1	10	2	83	59	-32
2	10	2	299	315	9
3	10	2	137	141	14
4	10	2	75	87	-25
5	10	2	38	44	-49
6	10	2	57	21	-35
7	10	2	53	37	-39
8	10	2	26	14	-99
9	10	2	27	38	-103
-10	11	2	42	3	-67
-9	11	2	54	8	-47
-8	11	2	82	42	-30
-7	11	2	23	21	-87
-6	11	2	22	1	-84
-5	11	2	22	1	-84
-4	11	2	228	203	10
-3	11	2	45	4	-37
-2	11	2	73	62	23
-1	11	2	68	69	17
0	11	2	35	15	-32
1	11	2	105	112	12
2	11	2	57	44	-30
3	11	2	81	77	22
4	11	2	52	37	-36
5	11	2	22	5	-85
6	11	2	184	190	13
7	11	2	25	18	-95
8	11	2	26	4	-100
9	11	2	51	16	-55
-10	12	2	70	13	-42
-9	12	2	84	83	-33
-8	12	2	25	29	-97
-7	12	2	78	87	-27
-6	12	2	61	50	-32
-5	12	2	22	3	-84
-4	12	2	52	23	-35
-3	12	2	21	37	-82
-2	12	2	41	9	-43
-1	12	2	211	225	10
0	12	2	108	114	12
1	12	2	90	70	-31
2	12	2	53	38	-33
3	12	2	253	245	10
4	12	2	22	37	-84
5	12	2	23	12	-87
6	12	2	25	19	-94
7	12	2	25	4	-97
8	12	2	27	25	-103
-9	13	2	27	27	-103
-8	13	2	26	51	-101
-7	13	2	25	24	-95
-6	13	2	45	60	-45

Table 57. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-5	13	2	59	20	-33
-4	13	2	65	51	-29
-3	13	2	21	19	-82
-2	13	2	179	183	12
-1	13	2	165	174	11
0	13	2	105	112	12
1	13	2	21	37	-57
2	13	2	66	55	-27
3	13	2	86	101	22
4	13	2	98	95	20
5	13	2	55	5	-37
6	13	2	25	20	-96
7	13	2	26	3	-99
8	13	2	27	34	-104
-8	14	2	68	19	-40
-7	14	2	25	43	-97
-6	14	2	39	71	-64
-5	14	2	96	84	21
-4	14	2	23	17	-86
-3	14	2	76	81	-24
-2	14	2	45	12	-40
-1	14	2	73	86	-25
0	14	2	42	19	-31
1	14	2	77	73	20
2	14	2	60	19	-30
3	14	2	22	18	-85
4	14	2	89	108	23
5	14	2	25	10	-95
6	14	2	26	3	-98
7	14	2	27	43	-101
-8	15	2	54	1	-53
-7	15	2	26	4	-101
-6	15	2	57	44	-44
-5	15	2	25	13	-95
-4	15	2	84	75	25
-3	15	2	63	55	-30
-2	15	2	22	46	-85
-1	15	2	43	44	-35
0	15	2	66	49	-31
1	15	2	34	7	-42
2	15	2	22	2	-85
3	15	2	79	67	-25
4	15	2	57	15	-41
5	15	2	61	32	-41
6	15	2	26	51	-101
7	15	2	27	10	-104
-7	16	2	27	14	-103
-6	16	2	26	8	-100
-5	16	2	26	59	-98
-4	16	2	54	36	-44
-3	16	2	57	14	-40
-2	16	2	45	53	-45
-1	16	2	38	29	-39
0	16	2	23	1	-61
1	16	2	153	157	17
2	16	2	66	20	-34
3	16	2	25	12	-95
4	16	2	51	65	-50
5	16	2	26	42	-100
6	16	2	27	15	-103
-6	17	2	27	20	-103
-5	17	2	26	30	-100
-4	17	2	26	3	-98
-3	17	2	80	54	-31
-2	17	2	25	50	-95
-1	17	2	45	11	-39
0	17	2	24	9	-64
1	17	2	53	30	-36
2	17	2	48	34	-50
3	17	2	26	4	-98
4	17	2	27	52	-102
5	17	2	65	31	-43
-5	18	2	27	11	-104
-4	18	2	26	18	-101
-3	18	2	26	4	-100
-2	18	2	26	15	-98
-1	18	2	39	13	-45
0	18	2	40	11	-46
1	18	2	55	63	-31
2	18	2	63	36	-42
3	18	2	27	4	-102
4	18	2	64	21	-43
-3	19	2	26	13	-101
-2	19	2	90	71	-31
-1	19	2	25	7	-69
0	19	2	55	17	-39
1	19	2	26	3	-69
2	19	2	55	16	-50
-12	0	3	61	74	-46
-10	0	3	196	165	12
-8	0	3	22	22	-83
-6	0	3	87	85	16

Table 57. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
2	0	3	109	112	11
4	0	3	203	222	9
6	0	3	233	209	11
8	0	3	145	169	15
10	0	3	103	74	27
-12	1	3	53	8	-44
-11	1	3	57	12	-39
-10	1	3	64	70	-26
-9	1	3	62	50	-31
-8	1	3	88	90	15
-7	1	3	295	276	15
-6	1	3	48	40	-27
-5	1	3	308	312	40
-3	1	3	434	351	14
-2	1	3	86	76	12
-1	1	3	291	312	14
1	1	3	344	288	9
2	1	3	16	5	-44
3	1	3	326	336	9
4	1	3	159	168	8
5	1	3	135	138	9
6	1	3	102	95	14
7	1	3	74	59	-31
8	1	3	56	46	-33
9	1	3	25	5	-68
10	1	3	128	97	19
-12	2	3	27	13	-103
-11	2	3	25	16	-97
-10	2	3	87	56	24
-9	2	3	39	22	-48
-8	2	3	68	31	-27
-7	2	3	66	24	-25
-6	2	3	46	14	-30
-5	2	3	176	214	9
-4	2	3	274	301	6
-3	2	3	228	237	7
-1	2	3	43	18	-19
0	2	3	543	496	5
1	2	3	59	48	14
2	2	3	145	123	9
3	2	3	218	213	8
4	2	3	127	120	12
5	2	3	135	117	13
6	2	3	56	37	-32
7	2	3	251	263	10
8	2	3	50	30	-40
9	2	3	57	10	-43
10	2	3	26	15	-101
-12	3	3	44	3	-64
-11	3	3	26	10	-98
-10	3	3	45	47	-46
-9	3	3	74	54	-26
-8	3	3	86	77	22
-7	3	3	477	485	8
-6	3	3	19	3	-74
-5	3	3	18	49	-68
-2	3	3	317	286	7
-1	3	3	42	38	-24
0	3	3	74	56	11
2	3	3	483	478	7
4	3	3	120	141	13
5	3	3	63	90	-28
6	3	3	22	11	-82
7	3	3	51	55	-37
8	3	3	58	47	-35
9	3	3	42	41	-59
10	3	3	70	2	-39
-12	4	3	101	66	29
-11	4	3	42	40	-61
-10	4	3	48	51	-43
-9	4	3	39	35	-49
-8	4	3	53	49	-35
-7	4	3	78	76	23
-6	4	3	59	60	-26
-5	4	3	230	242	8
-4	4	3	135	160	10
-3	4	3	283	324	6
-1	4	3	49	45	-21
0	4	3	478	429	17
1	4	3	98	61	8
2	4	3	124	128	10
3	4	3	78	44	17
4	4	3	101	108	16
5	4	3	67	63	-25
6	4	3	156	157	13
7	4	3	201	212	12
8	4	3	147	152	15
9	4	3	41	32	-61
10	4	3	58	58	-48
-12	5	3	61	16	-48
-11	5	3	65	28	-40
-10	5	3	46	43	-46

Table 57. (cont).
F(obs), F(calc), and σ_F

($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-9	5	3	60	55	-33
-8	5	3	180	177	12
-7	5	3	145	173	14
-6	5	3	76	62	21
-5	5	3	276	305	8
-3	5	3	94	60	12
-2	5	3	332	318	7
-1	5	3	78	83	10
0	5	3	624	568	12
1	5	3	81	107	10
2	5	3	164	159	9
3	5	3	156	172	10
4	5	3	30	3	-50
5	5	3	106	101	17
6	5	3	46	19	-40
7	5	3	83	92	24
8	5	3	45	9	-46
9	5	3	49	31	-51
10	5	3	78	86	-36
-12	6	3	61	36	-49
-11	6	3	26	29	-100
-10	6	3	67	61	-36
-9	6	3	124	99	17
-8	6	3	93	82	21
-7	6	3	149	114	14
-6	6	3	64	88	-27
-5	6	3	191	209	10
-4	6	3	135	137	11
-3	6	3	516	471	8
-2	6	3	429	421	8
-1	6	3	49	47	-20
0	6	3	470	432	16
1	6	3	166	177	6
2	6	3	39	35	-31
3	6	3	69	22	21
4	6	3	68	46	-25
5	6	3	332	375	10
6	6	3	119	131	16
7	6	3	53	22	-36
8	6	3	113	95	19
9	6	3	26	42	-99
10	6	3	43	37	-66
-11	7	3	27	11	-102
-10	7	3	25	11	-97
-9	7	3	126	115	17
-8	7	3	60	49	-31
-7	7	3	97	83	20
-6	7	3	21	11	-81
-5	7	3	299	318	9
-4	7	3	89	85	17
-3	7	3	379	332	7
-2	7	3	18	1	-69
-1	7	3	126	112	8
0	7	3	182	165	6
1	7	3	392	405	14
2	7	3	50	27	-29
3	7	3	181	221	11
4	7	3	165	163	12
5	7	3	223	225	11
6	7	3	22	12	-84
7	7	3	42	35	-47
8	7	3	25	53	-96
9	7	3	26	11	-101
10	7	3	27	19	-105
-11	8	3	63	9	-44
-10	8	3	26	22	-98
-9	8	3	71	57	-29
-8	8	3	99	105	20
-7	8	3	60	28	-32
-6	8	3	22	10	-82
-5	8	3	194	195	10
-4	8	3	65	52	-25
-3	8	3	35	62	-40
-2	8	3	480	458	8
-1	8	3	64	63	15
0	8	3	81	68	12
1	8	3	251	222	6
2	8	3	51	56	-30
3	8	3	82	78	20
4	8	3	97	124	19
5	8	3	239	246	10
6	8	3	22	23	-84
7	8	3	23	19	-88
8	8	3	65	64	-38
9	8	3	72	24	-38
-11	9	3	27	3	-104
-10	9	3	69	56	-38
-9	9	3	39	9	-62
-8	9	3	78	47	-25
-7	9	3	65	23	-29
-6	9	3	69	66	-27
-5	9	3	98	110	19

Table 57. (cont).
F(obs), F(calc), and σ_F

($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-4	9	3	21	65	-79
-3	9	3	145	153	12
-2	9	3	20	5	-75
-1	9	3	126	125	21
0	9	3	26	41	-40
1	9	3	141	150	9
2	9	3	403	408	9
3	9	3	50	37	-33
4	9	3	22	35	-83
5	9	3	72	56	-26
6	9	3	22	3	-86
7	9	3	23	16	-89
8	9	3	26	72	-100
9	9	3	27	33	-103
-11	10	3	64	12	-46
-10	10	3	26	38	-101
-9	10	3	54	25	-46
-8	10	3	48	37	-42
-7	10	3	22	12	-85
-6	10	3	22	8	-84
-5	10	3	78	44	23
-4	10	3	21	16	-81
-3	10	3	62	27	-26
-2	10	3	528	523	9
-1	10	3	90	86	12
0	10	3	57	58	-21
1	10	3	93	100	24
2	10	3	53	18	-31
3	10	3	62	2	-28
4	10	3	53	23	-34
5	10	3	51	18	-37
6	10	3	23	22	-87
7	10	3	25	30	-95
8	10	3	112	109	25
9	10	3	27	3	-105
-10	11	3	27	32	-104
-9	11	3	65	56	-40
-8	11	3	65	15	-37
-7	11	3	79	76	-26
-6	11	3	118	92	17
-5	11	3	181	185	12
-4	11	3	39	15	-46
-3	11	3	21	39	-80
-2	11	3	75	82	23
-1	11	3	73	80	16
0	11	3	63	47	-24
1	11	3	223	230	9
2	11	3	231	241	10
3	11	3	21	15	-81
4	11	3	82	75	23
5	11	3	173	171	13
6	11	3	54	29	-37
7	11	3	25	20	-97
8	11	3	27	34	-102
-10	12	3	84	37	-35
-9	12	3	65	30	-41
-8	12	3	25	5	-96
-7	12	3	45	12	-45
-6	12	3	23	49	-87
-5	12	3	111	116	18
-4	12	3	107	104	18
-3	12	3	70	44	-25
-2	12	3	137	139	15
-1	12	3	81	98	-29
0	12	3	151	143	12
1	12	3	92	98	14
2	12	3	135	145	14
3	12	3	21	31	-82
4	12	3	42	3	-45
5	12	3	131	138	17
6	12	3	50	50	-47
7	12	3	40	18	-64
8	12	3	27	17	-105
-9	13	3	77	42	-37
-8	13	3	69	13	-37
-7	13	3	25	18	-95
-6	13	3	49	51	-41
-5	13	3	111	121	18
-4	13	3	38	1	-48
-3	13	3	54	47	-33
-2	13	3	49	55	-37
-1	13	3	35	20	-39
0	13	3	103	99	22
1	13	3	112	110	11
2	13	3	32	66	-56
3	13	3	68	42	-27
4	13	3	67	30	-29
5	13	3	67	87	-35
6	13	3	25	2	-97
7	13	3	26	13	-101
-9	14	3	98	43	29
-8	14	3	27	31	-102

Table 57. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-7	14	3	40	16	-63
-6	14	3	25	7	-96
-5	14	3	72	38	-28
-4	14	3	37	80	-53
-3	14	3	55	42	-33
-2	14	3	118	112	16
-1	14	3	21	11	-58
0	14	3	115	117	12
1	14	3	76	80	19
2	14	3	83	80	23
3	14	3	38	51	-51
4	14	3	25	35	-95
5	14	3	39	69	-63
6	14	3	51	43	-51
7	14	3	59	27	-47
-8	15	3	27	11	-105
-7	15	3	70	72	-38
-6	15	3	25	1	-97
-5	15	3	57	13	-41
-4	15	3	23	38	-88
-3	15	3	66	65	-30
-2	15	3	22	45	-85
-1	15	3	65	51	20
0	15	3	92	82	16
1	15	3	22	6	-60
2	15	3	23	15	-86
3	15	3	93	100	26
4	15	3	25	22	-96
5	15	3	47	0	-55
6	15	3	50	46	-56
-7	16	3	40	2	-69
-6	16	3	43	37	-60
-5	16	3	49	7	-51
-4	16	3	39	20	-60
-3	16	3	78	79	-30
-2	16	3	24	51	-93
-1	16	3	46	16	-37
0	16	3	52	13	-29
1	16	3	54	52	-35
2	16	3	24	7	-92
3	16	3	56	17	-44
4	16	3	26	3	-99
5	16	3	27	7	-102
-6	17	3	27	33	-103
-5	17	3	37	2	-70
-4	17	3	26	14	-99
-3	17	3	26	28	-98
-2	17	3	50	19	-48
-1	17	3	37	18	-45
0	17	3	24	24	-65
1	17	3	39	8	-45
2	17	3	60	19	-41
3	17	3	94	102	29
4	17	3	27	28	-102
-5	18	3	27	12	-103
-4	18	3	27	39	-103
-3	18	3	68	47	-39
-2	18	3	43	10	-59
-1	18	3	71	47	-27
0	18	3	81	73	24
1	18	3	25	11	-67
2	18	3	26	5	-100
3	18	3	27	6	-103
-3	19	3	90	46	-31
-2	19	3	26	1	-101
-1	19	3	25	7	-69
0	19	3	33	49	-57
1	19	3	46	8	-45
-12	0	4	27	20	-102
-10	0	4	98	85	21
-8	0	4	371	358	9
-6	0	4	184	218	10
-4	0	4	83	123	13
-2	0	4	184	174	8
0	0	4	504	420	11
2	0	4	540	511	9
4	0	4	145	148	11
6	0	4	154	156	14
8	0	4	23	31	-88
10	0	4	27	16	-104
-12	1	4	60	32	-40
-11	1	4	35	45	-53
-10	1	4	50	18	-35
-9	1	4	59	44	-23
-8	1	4	333	336	17
-7	1	4	45	47	-27
-6	1	4	19	45	-52
-5	1	4	247	257	51
-4	1	4	195	216	11
-3	1	4	181	153	8
-2	1	4	594	551	8
-1	1	4	679	634	7

Table 57. (cont).
F(obs), F(calc), and σ_F

($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
0	1	4	358	274	5
1	1	4	78	75	7
2	1	4	211	215	7
3	1	4	45	33	-26
4	1	4	20	5	-53
5	1	4	168	162	16
6	1	4	173	174	17
7	1	4	97	113	16
8	1	4	53	72	-29
9	1	4	93	73	20
10	1	4	51	35	-45
-12	2	4	47	27	-58
-11	2	4	25	17	-97
-10	2	4	96	70	21
-9	2	4	59	30	-32
-8	2	4	142	145	14
-7	2	4	116	121	16
-6	2	4	103	115	15
-5	2	4	357	455	7
-4	2	4	25	115	-43
-3	2	4	26	45	-39
-2	2	4	282	240	7
-1	2	4	175	171	12
0	2	4	111	81	11
1	2	4	16	1	-44
2	2	4	265	294	7
3	2	4	31	3	-40
4	2	4	84	93	19
5	2	4	324	327	9
6	2	4	22	11	-85
7	2	4	22	53	-85
8	2	4	23	18	-88
9	2	4	72	42	-36
10	2	4	27	33	-104
-12	3	4	27	3	-103
-11	3	4	53	64	-48
-10	3	4	129	107	16
-9	3	4	74	71	-26
-8	3	4	140	152	15
-7	3	4	21	1	-79
-6	3	4	82	68	20
-5	3	4	91	89	15
-4	3	4	285	332	7
-3	3	4	325	365	7
-1	3	4	1072	974	7
0	3	4	307	365	13
1	3	4	230	206	5
2	3	4	71	65	18
3	3	4	32	25	-41
4	3	4	81	89	21
5	3	4	260	264	10
6	3	4	92	45	20
7	3	4	91	101	22
8	3	4	23	6	-89
9	3	4	120	123	23
10	3	4	27	29	-105
-12	4	4	64	9	-44
-11	4	4	25	5	-97
-10	4	4	23	32	-89
-9	4	4	54	49	-35
-8	4	4	140	144	14
-7	4	4	21	25	-80
-6	4	4	233	280	9
-5	4	4	481	591	8
-4	4	4	151	166	10
-3	4	4	433	401	7
-2	4	4	265	278	7
-1	4	4	219	173	16
0	4	4	170	192	6
1	4	4	385	384	5
2	4	4	657	641	10
3	4	4	213	215	9
4	4	4	259	290	9
5	4	4	193	158	11
6	4	4	90	93	21
7	4	4	100	120	21
8	4	4	39	20	-61
9	4	4	49	68	-55
10	4	4	82	55	-35
-12	5	4	27	17	-104
-11	5	4	83	10	-31
-10	5	4	102	114	21
-9	5	4	22	11	-85
-8	5	4	75	58	-26
-7	5	4	21	13	-82
-6	5	4	134	124	13
-5	5	4	117	133	14
-4	5	4	46	23	-26
-3	5	4	269	275	7
-2	5	4	104	119	11
-1	5	4	321	306	5
0	5	4	235	254	6

Table 57. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
1	5	4	282	278	5
2	5	4	307	267	7
3	5	4	49	49	-32
4	5	4	113	134	16
5	5	4	92	75	20
6	5	4	22	36	-84
7	5	4	129	133	17
8	5	4	78	65	-31
9	5	4	26	1	-100
10	5	4	28	50	-105
-12	6	4	28	22	-105
-11	6	4	26	8	-100
-10	6	4	52	41	-40
-9	6	4	58	2	-34
-8	6	4	114	116	18
-7	6	4	66	60	-28
-6	6	4	60	73	-28
-5	6	4	20	9	-76
-4	6	4	19	38	-71
-3	6	4	416	424	8
-2	6	4	55	12	-22
-1	6	4	44	19	-18
0	6	4	33	59	-27
1	6	4	159	172	9
2	6	4	531	504	9
3	6	4	181	196	11
4	6	4	149	135	13
5	6	4	39	5	-47
6	6	4	50	38	-38
7	6	4	49	41	-41
8	6	4	25	7	-96
9	6	4	27	7	-102
-12	7	4	28	10	-106
-11	7	4	27	60	-102
-10	7	4	60	36	-42
-9	7	4	33	2	-62
-8	7	4	80	69	24
-7	7	4	22	19	-83
-6	7	4	90	106	20
-5	7	4	67	102	-25
-4	7	4	283	295	8
-3	7	4	607	584	9
-2	7	4	71	61	18
-1	7	4	143	117	7
0	7	4	33	39	-30
1	7	4	240	240	13
2	7	4	41	34	-36
3	7	4	51	28	-32
4	7	4	40	10	-43
5	7	4	65	80	-29
6	7	4	53	54	-36
7	7	4	207	222	12
8	7	4	54	31	-45
9	7	4	83	58	-33
-11	8	4	27	6	-103
-10	8	4	26	21	-98
-9	8	4	44	25	-47
-8	8	4	22	32	-85
-7	8	4	104	103	18
-6	8	4	167	191	13
-5	8	4	50	37	-34
-4	8	4	20	12	-77
-3	8	4	224	227	10
-2	8	4	35	10	-40
-1	8	4	84	95	12
0	8	4	65	58	16
1	8	4	370	380	14
2	8	4	20	36	-78
3	8	4	277	284	9
4	8	4	219	223	11
5	8	4	22	50	-84
6	8	4	50	12	-39
7	8	4	25	37	-96
8	8	4	26	36	-99
9	8	4	41	9	-68
-11	9	4	27	10	-103
-10	9	4	107	100	25
-9	9	4	80	54	-26
-8	9	4	23	2	-86
-7	9	4	22	30	-84
-6	9	4	22	34	-85
-5	9	4	50	12	-35
-4	9	4	21	19	-79
-3	9	4	171	169	12
-2	9	4	29	14	-53
-1	9	4	58	41	-23
0	9	4	375	396	8
1	9	4	53	20	-29
2	9	4	38	1	-44
3	9	4	151	157	13
4	9	4	42	49	-43
5	9	4	22	23	-85

Table 57. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
6	9	4	23	8	-87
7	9	4	87	78	-28
8	9	4	26	15	-99
9	9	4	56	1	-51
-11	10	4	56	6	-51
-10	10	4	26	12	-101
-9	10	4	67	11	-37
-8	10	4	88	54	23
-7	10	4	22	1	-86
-6	10	4	247	247	10
-5	10	4	46	40	-40
-4	10	4	21	5	-81
-3	10	4	21	61	-80
-2	10	4	37	39	-44
-1	10	4	49	55	-24
0	10	4	217	224	7
1	10	4	78	73	15
2	10	4	55	48	-32
3	10	4	21	11	-81
4	10	4	264	279	10
5	10	4	22	43	-86
6	10	4	59	27	-35
7	10	4	51	6	-47
8	10	4	57	8	-49
-10	11	4	78	74	-36
-9	11	4	26	34	-98
-8	11	4	53	36	-39
-7	11	4	23	12	-87
-6	11	4	22	14	-85
-5	11	4	107	100	18
-4	11	4	102	104	18
-3	11	4	178	180	11
-2	11	4	48	35	-36
-1	11	4	97	85	13
0	11	4	299	296	7
1	11	4	163	176	9
2	11	4	32	0	-54
3	11	4	65	80	-27
4	11	4	102	99	19
5	11	4	47	19	-43
6	11	4	25	21	-95
7	11	4	71	96	-37
8	11	4	27	19	-103
-10	12	4	27	9	-105
-9	12	4	26	7	-100
-8	12	4	25	32	-97
-7	12	4	69	47	-30
-6	12	4	40	18	-49
-5	12	4	71	32	-26
-4	12	4	131	108	15
-3	12	4	201	184	11
-2	12	4	46	62	-38
-1	12	4	73	57	-27
0	12	4	91	101	14
1	12	4	93	85	25
2	12	4	38	74	-47
3	12	4	115	116	16
4	12	4	22	4	-86
5	12	4	61	76	-38
6	12	4	75	59	-33
7	12	4	62	4	-43
-9	13	4	27	13	-102
-8	13	4	60	57	-44
-7	13	4	56	52	-44
-6	13	4	23	15	-88
-5	13	4	68	45	-29
-4	13	4	22	25	-84
-3	13	4	171	168	12
-2	13	4	22	29	-84
-1	13	4	21	22	-58
0	13	4	21	11	-58
1	13	4	57	44	-28
2	13	4	34	31	-55
3	13	4	22	17	-85
4	13	4	23	49	-88
5	13	4	83	45	-29
6	13	4	50	5	-52
7	13	4	82	77	-34
-9	14	4	27	3	-104
-8	14	4	47	69	-58
-7	14	4	25	18	-97
-6	14	4	71	42	-34
-5	14	4	23	16	-88
-4	14	4	69	54	-28
-3	14	4	68	86	-28
-2	14	4	22	1	-84
-1	14	4	84	78	19
0	14	4	110	113	12
1	14	4	41	21	-32
2	14	4	120	125	17
3	14	4	54	33	-42
4	14	4	50	81	-48

Table 57. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
5	14	4	26	14	-99
6	14	4	66	28	-41
-8	15	4	27	10	-104
-7	15	4	42	56	-63
-6	15	4	26	7	-98
-5	15	4	25	3	-95
-4	15	4	38	42	-61
-3	15	4	22	13	-86
-2	15	4	23	38	-86
-1	15	4	121	113	12
0	15	4	41	31	-39
1	15	4	34	19	-44
2	15	4	70	45	-32
3	15	4	53	37	-44
4	15	4	25	2	-97
5	15	4	46	58	-58
-7	16	4	27	3	-103
-6	16	4	26	11	-100
-5	16	4	89	93	-29
-4	16	4	25	39	-96
-3	16	4	25	22	-94
-2	16	4	54	28	-41
-1	16	4	34	1	-46
0	16	4	24	24	-64
1	16	4	55	49	-32
2	16	4	61	28	-38
3	16	4	50	34	-50
4	16	4	26	26	-100
5	16	4	75	36	-37
-6	17	4	61	7	-46
-5	17	4	27	12	-102
-4	17	4	26	31	-99
-3	17	4	25	5	-97
-2	17	4	25	18	-95
-1	17	4	100	98	18
0	17	4	24	21	-66
1	17	4	53	16	-31
2	17	4	51	25	-50
3	17	4	45	15	-60
4	17	4	47	3	-60
-5	18	4	27	37	-104
-4	18	4	27	52	-103
-3	18	4	26	7	-101
-2	18	4	26	17	-99
-1	18	4	48	30	-41
0	18	4	32	13	-55
1	18	4	62	8	-34
2	18	4	91	71	-31
-2	19	4	92	50	-30
-1	19	4	43	8	-46
0	19	4	26	7	-70
-12	0	5	71	42	-38
-10	0	5	62	21	-31
-8	0	5	87	77	21
-6	0	5	45	72	-32
-4	0	5	108	104	11
-2	0	5	550	543	8
0	0	5	444	441	32
2	0	5	39	68	-31
4	0	5	153	77	12
6	0	5	22	29	-85
8	0	5	152	160	18
-13	1	5	28	9	-76
-12	1	5	43	7	-50
-11	1	5	76	8	-36
-10	1	5	23	36	-61
-9	1	5	22	35	-60
-8	1	5	106	118	13
-7	1	5	63	101	19
-6	1	5	378	422	97
-5	1	5	134	170	22
-4	1	5	332	362	31
-3	1	5	199	188	7
-2	1	5	236	220	11
-1	1	5	236	210	6
0	1	5	58	22	17
1	1	5	176	216	4
2	1	5	31	8	-28
3	1	5	106	105	11
4	1	5	617	606	5
5	1	5	74	94	17
6	1	5	22	5	-60
7	1	5	79	78	18
8	1	5	61	21	-37
9	1	5	27	11	-72
-12	2	5	51	10	-53
-11	2	5	121	93	21
-10	2	5	23	9	-86
-9	2	5	198	188	12
-8	2	5	45	43	-40
-7	2	5	21	60	-80
-6	2	5	156	188	11

Table 57. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-5	2	5	93	105	14
-4	2	5	112	118	11
-3	2	5	475	506	8
-2	2	5	261	253	7
-1	2	5	343	329	5
0	2	5	515	520	10
1	2	5	596	562	18
2	2	5	93	105	15
3	2	5	72	35	20
4	2	5	33	24	-52
5	2	5	46	64	-40
6	2	5	134	142	15
7	2	5	104	109	20
8	2	5	68	89	-36
9	2	5	82	78	-34
-12	3	5	27	11	-102
-11	3	5	65	43	-38
-10	3	5	47	7	-42
-9	3	5	22	39	-85
-8	3	5	48	26	-38
-7	3	5	54	62	-31
-6	3	5	20	3	-76
-5	3	5	228	291	8
-4	3	5	166	196	9
-3	3	5	496	500	8
-2	3	5	80	89	14
-1	3	5	132	95	8
0	3	5	111	107	13
1	3	5	680	576	20
2	3	5	224	247	8
3	3	5	88	101	18
4	3	5	56	15	-31
5	3	5	37	11	-50
6	3	5	89	120	22
7	3	5	72	49	-28
8	3	5	26	46	-98
9	3	5	40	15	-69
-12	4	5	67	21	-42
-11	4	5	26	21	-98
-10	4	5	49	19	-41
-9	4	5	161	168	13
-8	4	5	87	103	22
-7	4	5	144	156	14
-6	4	5	21	28	-80
-5	4	5	76	74	20
-4	4	5	255	282	8
-3	4	5	229	218	7
-2	4	5	288	258	7
-1	4	5	26	29	-33
0	4	5	170	190	6
1	4	5	430	439	7
2	4	5	78	77	19
3	4	5	33	52	-47
4	4	5	21	9	-81
5	4	5	35	54	-53
6	4	5	179	202	13
7	4	5	88	81	23
8	4	5	57	54	-44
9	4	5	27	6	-103
-12	5	5	63	19	-45
-11	5	5	91	68	29
-10	5	5	23	11	-89
-9	5	5	22	51	-86
-8	5	5	75	59	-25
-7	5	5	47	84	-38
-6	5	5	279	308	8
-5	5	5	145	187	12
-4	5	5	139	116	11
-3	5	5	392	373	8
-2	5	5	126	110	11
-1	5	5	145	139	9
0	5	5	36	11	-27
1	5	5	117	122	9
2	5	5	133	131	12
3	5	5	120	123	14
4	5	5	285	301	9
5	5	5	22	21	-84
6	5	5	217	223	11
7	5	5	23	14	-88
8	5	5	26	1	-98
9	5	5	27	38	-105
-12	6	5	41	20	-72
-11	6	5	107	85	26
-10	6	5	47	50	-45
-9	6	5	23	3	-86
-8	6	5	34	37	-54
-7	6	5	121	114	16
-6	6	5	101	106	17
-5	6	5	21	58	-79
-4	6	5	294	303	8
-3	6	5	87	59	16
-2	6	5	179	153	9

Table 57. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-1	6	5	497	504	11
0	6	5	27	14	-36
1	6	5	192	193	7
2	6	5	92	83	18
3	6	5	87	91	19
4	6	5	76	80	24
5	6	5	45	28	-41
6	6	5	60	57	-34
7	6	5	25	55	-95
8	6	5	99	63	26
9	6	5	104	90	29
-12	7	5	28	4	-106
-11	7	5	27	39	-102
-10	7	5	25	23	-97
-9	7	5	75	63	-27
-8	7	5	22	14	-85
-7	7	5	150	160	14
-6	7	5	47	33	-38
-5	7	5	70	82	-24
-4	7	5	167	167	11
-3	7	5	111	97	14
-2	7	5	102	105	15
-1	7	5	136	142	9
0	7	5	287	275	10
1	7	5	73	93	-30
2	7	5	20	23	-77
3	7	5	268	278	10
4	7	5	130	138	15
5	7	5	22	46	-84
6	7	5	33	25	-60
7	7	5	36	8	-65
8	7	5	26	18	-99
9	7	5	66	21	-44
-11	8	5	114	73	25
-10	8	5	26	32	-98
-9	8	5	77	34	-26
-8	8	5	47	36	-41
-7	8	5	22	25	-85
-6	8	5	94	75	20
-5	8	5	21	38	-81
-4	8	5	21	12	-79
-3	8	5	108	96	15
-2	8	5	66	43	-23
-1	8	5	477	448	6
0	8	5	66	61	16
1	8	5	59	69	-24
2	8	5	103	100	18
3	8	5	36	56	-49
4	8	5	22	27	-83
5	8	5	22	24	-85
6	8	5	113	98	19
7	8	5	25	42	-96
8	8	5	27	13	-102
-11	9	5	52	17	-55
-10	9	5	26	7	-98
-9	9	5	23	0	-89
-8	9	5	73	90	-28
-7	9	5	94	88	21
-6	9	5	123	124	16
-5	9	5	194	199	11
-4	9	5	362	395	9
-3	9	5	21	5	-79
-2	9	5	43	20	-37
-1	9	5	47	33	-24
0	9	5	87	81	14
1	9	5	42	51	-33
2	9	5	249	257	10
3	9	5	111	101	16
4	9	5	22	12	-83
5	9	5	23	16	-87
6	9	5	132	152	20
7	9	5	25	41	-97
8	9	5	27	31	-103
-11	10	5	65	7	-44
-10	10	5	43	0	-61
-9	10	5	52	52	-48
-8	10	5	74	90	-29
-7	10	5	85	70	23
-6	10	5	66	74	-29
-5	10	5	116	99	18
-4	10	5	66	86	-28
-3	10	5	30	4	-56
-2	10	5	21	42	-80
-1	10	5	141	123	9
0	10	5	152	161	9
1	10	5	63	30	-23
2	10	5	243	247	10
3	10	5	109	115	17
4	10	5	22	36	-85
5	10	5	44	50	-46
6	10	5	139	147	19
7	10	5	26	16	-99

Table 57. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
8	10	5	27	1	-104
-10	11	5	50	6	-55
-9	11	5	47	45	-53
-8	11	5	25	34	-97
-7	11	5	23	39	-87
-6	11	5	68	32	-28
-5	11	5	55	33	-34
-4	11	5	201	197	11
-3	11	5	42	48	-43
-2	11	5	63	47	-29
-1	11	5	96	107	13
0	11	5	41	38	-35
1	11	5	34	1	-40
2	11	5	113	126	17
3	11	5	123	118	16
4	11	5	33	28	-59
5	11	5	64	13	-36
6	11	5	58	76	-44
7	11	5	46	6	-57
-10	12	5	27	3	-104
-9	12	5	65	43	-40
-8	12	5	81	55	-31
-7	12	5	79	66	-27
-6	12	5	61	36	-32
-5	12	5	22	25	-85
-4	12	5	22	30	-84
-3	12	5	21	3	-82
-2	12	5	94	84	19
-1	12	5	293	304	15
0	12	5	29	27	-44
1	12	5	51	44	-31
2	12	5	85	104	23
3	12	5	39	65	-49
4	12	5	23	51	-88
5	12	5	74	39	-33
6	12	5	40	40	-64
7	12	5	27	5	-103
-9	13	5	53	46	-53
-8	13	5	26	31	-100
-7	13	5	25	22	-95
-6	13	5	70	58	-30
-5	13	5	39	38	-51
-4	13	5	45	48	-43
-3	13	5	22	18	-83
-2	13	5	82	65	23
-1	13	5	22	11	-58
0	13	5	37	6	-38
1	13	5	50	29	-27
2	13	5	79	68	24
3	13	5	76	88	-26
4	13	5	105	101	23
5	13	5	26	40	-98
6	13	5	27	22	-102
-9	14	5	27	26	-104
-8	14	5	27	3	-102
-7	14	5	25	5	-96
-6	14	5	25	36	-96
-5	14	5	23	25	-89
-4	14	5	38	24	-52
-3	14	5	38	40	-49
-2	14	5	98	101	20
-1	14	5	108	98	13
0	14	5	48	1	-34
1	14	5	32	40	-45
2	14	5	24	38	-91
3	14	5	25	17	-94
4	14	5	25	8	-97
5	14	5	26	17	-101
6	14	5	39	27	-73
-8	15	5	27	15	-104
-7	15	5	26	1	-100
-6	15	5	26	58	-99
-5	15	5	52	55	-47
-4	15	5	25	49	-95
-3	15	5	25	26	-94
-2	15	5	67	41	-30
-1	15	5	41	22	-38
0	15	5	55	17	-26
1	15	5	39	50	-39
2	15	5	56	42	-41
3	15	5	25	15	-97
4	15	5	26	56	-100
5	15	5	27	33	-103
-7	16	5	27	8	-104
-6	16	5	26	9	-101
-5	16	5	41	38	-63
-4	16	5	25	21	-96
-3	16	5	70	59	-35
-2	16	5	42	50	-55
-1	16	5	52	7	-36
0	16	5	24	21	-64
1	16	5	116	119	15

Table 57. (cont).
F(obs), F(calc), and σ_F

($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
2	16	5	25	18	-97
3	16	5	57	14	-46
4	16	5	88	13	-32
-6	17	5	50	28	-56
-5	17	5	27	28	-102
-4	17	5	46	11	-57
-3	17	5	88	56	-29
-2	17	5	80	84	-32
-1	17	5	45	10	-37
0	17	5	48	30	-40
1	17	5	79	61	23
2	17	5	26	8	-100
3	17	5	70	11	-39
-4	18	5	27	16	-104
-3	18	5	27	25	-102
-2	18	5	89	31	-30
-1	18	5	25	0	-69
0	18	5	82	28	-35
1	18	5	26	25	-70
-12	0	6	53	27	-51
-10	0	6	23	1	-87
-8	0	6	47	50	-37
-6	0	6	73	69	20
-2	0	6	44	21	-26
0	0	6	196	169	18
2	0	6	40	33	-38
4	0	6	21	26	-82
6	0	6	250	259	11
8	0	6	26	41	-98
-13	1	6	51	3	-48
-12	1	6	83	54	-35
-11	1	6	80	28	-28
-10	1	6	85	84	17
-9	1	6	84	80	18
-8	1	6	22	22	-58
-7	1	6	37	73	-32
-6	1	6	170	213	52
-5	1	6	55	36	-22
-4	1	6	51	76	-17
-3	1	6	45	35	-24
-2	1	6	109	113	8
-1	1	6	30	3	-24
0	1	6	937	847	21
1	1	6	177	169	5
2	1	6	112	109	10
3	1	6	235	243	7
4	1	6	21	7	-57
5	1	6	38	59	-39
6	1	6	90	84	28
7	1	6	30	23	-52
8	1	6	51	42	-42
9	1	6	69	25	-40
-13	2	6	64	9	-47
-12	2	6	27	14	-102
-11	2	6	25	25	-97
-10	2	6	23	7	-87
-9	2	6	62	70	-31
-8	2	6	22	6	-83
-7	2	6	181	219	11
-6	2	6	66	46	-24
-5	2	6	264	274	8
-4	2	6	438	460	7
-3	2	6	211	185	8
-2	2	6	136	157	10
-1	2	6	183	199	12
0	2	6	113	47	31
1	2	6	126	136	16
2	2	6	63	45	-24
3	2	6	531	557	10
4	2	6	108	128	18
5	2	6	35	51	-53
6	2	6	74	57	-27
7	2	6	98	92	25
8	2	6	64	13	-40
9	2	6	27	11	-105
-12	3	6	45	17	-61
-11	3	6	62	48	-41
-10	3	6	23	15	-87
-9	3	6	68	49	-27
-8	3	6	97	86	19
-7	3	6	214	263	10
-6	3	6	154	176	12
-5	3	6	31	33	-46
-4	3	6	102	110	14
-3	3	6	101	106	13
-2	3	6	329	349	7
-1	3	6	263	279	7
0	3	6	213	205	6
1	3	6	85	108	20
2	3	6	147	166	12
3	3	6	292	277	9
4	3	6	21	18	-82

Table 57. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
5	3	6	22	15	-84
6	3	6	59	2	-33
7	3	6	58	91	-42
8	3	6	75	85	-35
9	3	6	28	46	-106
-12	4	6	53	51	-54
-11	4	6	75	49	-34
-10	4	6	54	24	-38
-9	4	6	73	62	-26
-8	4	6	22	32	-84
-7	4	6	113	138	17
-6	4	6	171	196	11
-5	4	6	20	47	-76
-4	4	6	122	105	12
-3	4	6	18	13	-69
-2	4	6	305	292	7
-1	4	6	89	88	12
0	4	6	112	109	9
1	4	6	35	25	-29
2	4	6	57	79	-28
3	4	6	349	358	9
4	4	6	22	36	-82
5	4	6	57	30	-33
6	4	6	100	104	21
7	4	6	25	23	-95
8	4	6	66	49	-40
9	4	6	28	4	-105
-12	5	6	68	58	-42
-11	5	6	26	21	-99
-10	5	6	75	59	-28
-9	5	6	104	99	19
-8	5	6	43	3	-43
-7	5	6	88	99	21
-6	5	6	85	98	20
-5	5	6	48	79	-33
-4	5	6	74	91	21
-3	5	6	19	13	-71
-2	5	6	237	202	8
-1	5	6	92	65	26
0	5	6	343	356	7
1	5	6	140	149	9
2	5	6	112	112	15
3	5	6	60	73	-29
4	5	6	53	58	-34
5	5	6	22	19	-85
6	5	6	93	118	22
7	5	6	78	51	-32
8	5	6	49	95	-56
-12	6	6	27	20	-105
-11	6	6	26	35	-100
-10	6	6	44	33	-47
-9	6	6	46	31	-43
-8	6	6	40	57	-47
-7	6	6	120	134	16
-6	6	6	53	70	-33
-5	6	6	219	249	10
-4	6	6	262	266	9
-3	6	6	19	4	-74
-2	6	6	48	43	-29
-1	6	6	248	260	6
0	6	6	98	97	11
1	6	6	59	69	-29
2	6	6	73	86	23
3	6	6	21	57	-82
4	6	6	63	27	-28
5	6	6	288	317	10
6	6	6	73	84	-28
7	6	6	25	4	-96
8	6	6	27	37	-103
-12	7	6	75	16	-39
-11	7	6	26	19	-100
-10	7	6	43	20	-57
-9	7	6	145	143	15
-8	7	6	22	58	-86
-7	7	6	46	75	-42
-6	7	6	22	36	-83
-5	7	6	21	18	-81
-4	7	6	96	102	18
-3	7	6	21	21	-79
-2	7	6	59	47	-28
-1	7	6	135	122	9
0	7	6	20	18	-54
1	7	6	360	368	12
2	7	6	47	48	-35
3	7	6	40	35	-44
4	7	6	71	94	-26
5	7	6	51	1	-38
6	7	6	25	20	-95
7	7	6	25	1	-97
8	7	6	69	8	-40
-11	8	6	27	5	-102
-10	8	6	25	16	-97

Table 57. (cont).
F(obs), F(calc), and σ_F

($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-9	8	6	23	6	-89
-8	8	6	38	50	-51
-7	8	6	92	96	21
-6	8	6	22	31	-84
-5	8	6	189	189	11
-4	8	6	42	61	-41
-3	8	6	21	8	-78
-2	8	6	346	329	9
-1	8	6	52	41	-28
0	8	6	43	0	-26
1	8	6	101	109	13
2	8	6	21	4	-81
3	8	6	68	39	-26
4	8	6	108	115	18
5	8	6	184	191	12
6	8	6	25	2	-95
7	8	6	26	10	-99
8	8	6	76	27	-38
-11	9	6	42	17	-66
-10	9	6	26	68	-100
-9	9	6	62	53	-40
-8	9	6	60	73	-34
-7	9	6	75	6	-25
-6	9	6	81	75	23
-5	9	6	78	95	24
-4	9	6	150	122	13
-3	9	6	56	65	-31
-2	9	6	427	427	9
-1	9	6	57	15	-28
0	9	6	21	4	-56
1	9	6	143	150	11
2	9	6	175	185	12
3	9	6	44	56	-40
4	9	6	22	8	-85
5	9	6	93	64	22
6	9	6	25	2	-96
7	9	6	26	3	-100
-11	10	6	59	7	-49
-10	10	6	27	14	-101
-9	10	6	57	32	-44
-8	10	6	34	23	-60
-7	10	6	23	19	-86
-6	10	6	91	91	21
-5	10	6	70	47	-27
-4	10	6	50	7	-36
-3	10	6	71	67	-25
-2	10	6	274	251	10
-1	10	6	72	80	17
0	10	6	75	77	19
1	10	6	67	62	19
2	10	6	85	80	22
3	10	6	78	63	23
4	10	6	93	91	21
5	10	6	25	39	-96
6	10	6	81	54	-31
7	10	6	53	33	-51
-10	11	6	27	15	-103
-9	11	6	56	55	-46
-8	11	6	25	13	-96
-7	11	6	23	26	-88
-6	11	6	23	50	-86
-5	11	6	89	77	22
-4	11	6	22	39	-84
-3	11	6	21	3	-82
-2	11	6	269	259	10
-1	11	6	66	58	-26
0	11	6	88	75	15
1	11	6	179	198	9
2	11	6	22	32	-83
3	11	6	22	20	-84
4	11	6	25	25	-94
5	11	6	75	11	-33
6	11	6	65	31	-41
7	11	6	27	14	-103
-10	12	6	27	24	-104
-9	12	6	26	19	-101
-8	12	6	26	17	-98
-7	12	6	25	44	-95
-6	12	6	86	33	24
-5	12	6	149	137	14
-4	12	6	39	52	-49
-3	12	6	58	14	-31
-2	12	6	102	87	19
-1	12	6	22	13	-83
0	12	6	39	24	-32
1	12	6	65	93	-21
2	12	6	22	30	-85
3	12	6	61	58	-32
4	12	6	25	46	-95
5	12	6	87	108	-30
6	12	6	27	15	-102
-9	13	6	39	56	-71

Table 57. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
-8	13	6	26	13	-100	-3	16	6	71	69	-35
-7	13	6	25	2	-96	-2	16	6	25	46	-96
-6	13	6	100	76	25	-1	16	6	43	3	-42
-5	13	6	23	27	-88	0	16	6	73	55	-28
-4	13	6	23	26	-86	1	16	6	37	16	-49
-3	13	6	69	52	-27	2	16	6	25	17	-97
-2	13	6	22	42	-85	3	16	6	76	67	-37
-1	13	6	47	19	-34	-6	17	6	87	44	-33
0	13	6	91	109	15	-5	17	6	72	16	-39
1	13	6	130	137	11	-4	17	6	26	14	-101
2	13	6	62	36	-31	-3	17	6	26	23	-99
3	13	6	25	3	-95	-2	17	6	26	1	-98
4	13	6	44	55	-56	-1	17	6	25	53	-68
5	13	6	26	3	-100	0	17	6	73	49	-26
-9	14	6	28	19	-105	1	17	6	25	1	-69
-8	14	6	27	22	-103	2	17	6	27	13	-102
-7	14	6	26	5	-98	-3	18	6	26	8	-101
-6	14	6	25	27	-97	-2	18	6	27	3	-102
-5	14	6	52	25	-45	-1	18	6	41	32	-44
-4	14	6	78	89	-27	0	18	6	44	27	-46
-3	14	6	96	98	21	-12	0	7	56	3	-49
-2	14	6	59	48	-34	-10	0	7	98	90	21
-1	14	6	48	15	-31	-8	0	7	200	242	11
0	14	6	45	11	-36	-6	0	7	54	55	-29
1	14	6	23	20	-63	-4	0	7	105	122	14
2	14	6	24	12	-92	-2	0	7	159	155	9
3	14	6	80	38	-31	0	0	7	273	309	7
4	14	6	45	23	-57	2	0	7	673	665	3
5	14	6	51	45	-54	4	0	7	55	41	-33
-8	15	6	28	5	-105	6	0	7	23	20	-88
-7	15	6	52	62	-53	8	0	7	105	104	27
-6	15	6	39	26	-66	-13	1	7	51	29	-49
-5	15	6	57	11	-44	-12	1	7	109	69	22
-4	15	6	25	1	-95	-11	1	7	25	7	-68
-3	15	6	38	36	-61	-10	1	7	79	77	19
-2	15	6	36	12	-63	-9	1	7	22	6	-59
-1	15	6	45	39	-33	-8	1	7	58	48	-31
0	15	6	96	80	16	-7	1	7	82	99	-27
1	15	6	47	51	-39	-6	1	7	83	86	15
2	15	6	71	8	-33	-5	1	7	255	273	66
3	15	6	80	62	-32	-4	1	7	97	92	10
4	15	6	40	4	-68	-3	1	7	41	42	-27
-7	16	6	49	45	-58	-2	1	7	164	179	11
-6	16	6	27	0	-102	-1	1	7	296	253	9
-5	16	6	50	2	-52	0	1	7	36	10	-22
-4	16	6	65	13	-39	1	1	7	46	14	-21

Table 57. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
2	1	7	271	247	8
3	1	7	45	18	-27
4	1	7	45	13	-34
5	1	7	223	230	18
6	1	7	33	49	-47
7	1	7	25	54	-69
8	1	7	47	55	-48
-12	2	7	27	19	-102
-11	2	7	25	27	-97
-10	2	7	45	11	-44
-9	2	7	22	12	-84
-8	2	7	121	133	16
-7	2	7	85	116	21
-6	2	7	83	117	21
-5	2	7	131	173	13
-4	2	7	19	42	-74
-3	2	7	176	182	9
-2	2	7	82	62	17
-1	2	7	361	356	5
0	2	7	19	18	-51
1	2	7	141	138	8
2	2	7	268	295	9
3	2	7	21	20	-81
4	2	7	22	1	-82
5	2	7	73	40	-27
6	2	7	23	38	-88
7	2	7	25	51	-97
8	2	7	27	62	-103
-12	3	7	27	26	-103
-11	3	7	25	1	-97
-10	3	7	97	87	22
-9	3	7	40	12	-48
-8	3	7	47	13	-39
-7	3	7	75	105	24
-6	3	7	21	42	-80
-5	3	7	367	407	8
-4	3	7	19	17	-73
-3	3	7	88	79	16
-2	3	7	162	163	10
-1	3	7	281	274	10
0	3	7	52	43	-27
1	3	7	51	32	-21
2	3	7	56	27	-29
3	3	7	21	6	-82
4	3	7	45	51	-40
5	3	7	283	292	10
6	3	7	23	21	-88
7	3	7	61	68	-41
8	3	7	69	3	-40
-12	4	7	27	34	-104
-11	4	7	51	19	-49
-10	4	7	124	109	18
-9	4	7	40	27	-48
-8	4	7	108	122	18
-7	4	7	96	78	19
-6	4	7	104	120	18
-5	4	7	198	231	10
-4	4	7	74	91	20
-3	4	7	19	6	-73
-2	4	7	265	250	8
-1	4	7	318	306	15
0	4	7	228	244	7
1	4	7	128	136	13
2	4	7	188	193	11
3	4	7	60	95	-30
4	4	7	49	63	-37
5	4	7	69	32	-28
6	4	7	25	8	-94
7	4	7	49	9	-52
8	4	7	27	25	-104
-12	5	7	61	27	-47
-11	5	7	45	28	-56
-10	5	7	58	42	-37
-9	5	7	23	43	-87
-8	5	7	22	37	-85
-7	5	7	48	70	-38
-6	5	7	92	88	19
-5	5	7	85	74	21
-4	5	7	105	101	16
-3	5	7	403	402	8
-2	5	7	187	182	10
-1	5	7	177	148	12
0	5	7	98	90	16
1	5	7	110	106	11
2	5	7	90	48	19
3	5	7	114	117	16
4	5	7	155	168	13
5	5	7	77	95	-27
6	5	7	70	6	-34
7	5	7	52	58	-50
8	5	7	27	33	-104
-12	6	7	28	15	-106

Table 57. (cont).
F(obs), F(calc), and σ_F

($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-11	6	7	43	17	-61
-10	6	7	58	56	-43
-9	6	7	23	1	-87
-8	6	7	139	139	15
-7	6	7	96	98	20
-6	6	7	46	21	-39
-5	6	7	131	123	15
-4	6	7	37	42	-43
-3	6	7	21	26	-79
-2	6	7	113	112	15
-1	6	7	55	20	-20
0	6	7	138	130	15
1	6	7	127	130	10
2	6	7	156	157	13
3	6	7	136	156	14
4	6	7	22	15	-84
5	6	7	23	11	-87
6	6	7	25	30	-96
7	6	7	50	53	-53
8	6	7	87	29	-33
-12	7	7	28	25	-106
-11	7	7	52	40	-51
-10	7	7	25	30	-97
-9	7	7	23	8	-87
-8	7	7	22	28	-86
-7	7	7	62	65	-30
-6	7	7	22	21	-84
-5	7	7	121	110	16
-4	7	7	68	34	-25
-3	7	7	527	539	5
-2	7	7	231	230	9
-1	7	7	74	88	-30
0	7	7	35	41	-37
1	7	7	74	62	-26
2	7	7	21	19	-82
3	7	7	166	179	13
4	7	7	70	34	-27
5	7	7	23	43	-88
6	7	7	25	21	-97
7	7	7	122	129	23
-11	8	7	27	11	-103
-10	8	7	26	44	-98
-9	8	7	42	10	-49
-8	8	7	23	5	-86
-7	8	7	126	122	16
-6	8	7	118	118	17
-5	8	7	22	28	-84
-4	8	7	21	18	-82
-3	8	7	247	232	10
-2	8	7	88	82	20
-1	8	7	100	92	12
0	8	7	274	286	7
1	8	7	78	80	18
2	8	7	22	21	-82
3	8	7	144	139	14
4	8	7	156	162	14
5	8	7	25	19	-94
6	8	7	26	25	-98
7	8	7	55	49	-50
-11	9	7	27	2	-104
-10	9	7	46	54	-57
-9	9	7	25	31	-97
-8	9	7	69	44	-29
-7	9	7	56	6	-35
-6	9	7	121	132	17
-5	9	7	22	43	-84
-4	9	7	22	17	-83
-3	9	7	78	79	23
-2	9	7	40	36	-44
-1	9	7	45	24	-29
0	9	7	89	79	14
1	9	7	44	26	-28
2	9	7	21	57	-82
3	9	7	22	10	-84
4	9	7	103	116	20
5	9	7	25	17	-96
6	9	7	65	32	-40
7	9	7	27	40	-104
-11	10	7	41	15	-72
-10	10	7	102	65	27
-9	10	7	25	7	-97
-8	10	7	58	7	-35
-7	10	7	43	24	-46
-6	10	7	58	75	-34
-5	10	7	22	22	-84
-4	10	7	49	7	-37
-3	10	7	22	70	-82
-2	10	7	22	1	-83
-1	10	7	35	52	-38
0	10	7	363	372	10
1	10	7	62	66	-29
2	10	7	22	22	-83

Table 57. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
3	10	7	22	29	-85
4	10	7	66	78	-35
5	10	7	81	1	-30
6	10	7	27	23	-102
-10	11	7	43	42	-65
-9	11	7	26	21	-99
-8	11	7	25	19	-96
-7	11	7	73	44	-28
-6	11	7	87	81	23
-5	11	7	96	85	21
-4	11	7	22	47	-84
-3	11	7	151	140	13
-2	11	7	22	10	-82
-1	11	7	68	67	18
0	11	7	22	45	-59
1	11	7	45	9	-34
2	11	7	22	10	-85
3	11	7	95	94	21
4	11	7	93	67	26
5	11	7	26	59	-99
6	11	7	63	42	-44
-10	12	7	41	11	-70
-9	12	7	26	12	-101
-8	12	7	52	55	-49
-7	12	7	95	74	26
-6	12	7	23	21	-88
-5	12	7	23	9	-86
-4	12	7	102	88	19
-3	12	7	22	8	-84
-2	12	7	55	26	-34
-1	12	7	52	46	-25
0	12	7	43	59	-36
1	12	7	60	34	-23
2	12	7	86	69	24
3	12	7	25	38	-95
4	12	7	25	0	-97
5	12	7	43	33	-63
-9	13	7	74	8	-38
-8	13	7	27	3	-101
-7	13	7	25	9	-97
-6	13	7	25	18	-96
-5	13	7	23	33	-88
-4	13	7	46	31	-43
-3	13	7	144	133	15
-2	13	7	71	62	-28
-1	13	7	66	49	-25
0	13	7	62	16	-31
1	13	7	23	37	-63
2	13	7	64	35	-35
3	13	7	71	76	-35
4	13	7	26	6	-99
5	13	7	27	6	-103
-8	14	7	79	70	-36
-7	14	7	26	47	-100
-6	14	7	26	21	-98
-5	14	7	46	54	-52
-4	14	7	55	39	-43
-3	14	7	25	40	-95
-2	14	7	24	21	-92
-1	14	7	23	15	-63
0	14	7	44	48	-35
1	14	7	54	10	-28
2	14	7	87	90	-28
3	14	7	26	56	-99
4	14	7	27	25	-102
-8	15	7	28	27	-108
-7	15	7	27	25	-103
-6	15	7	49	19	-54
-5	15	7	41	53	-61
-4	15	7	25	15	-96
-3	15	7	40	25	-60
-2	15	7	25	46	-95
-1	15	7	117	104	16
0	15	7	24	37	-65
1	15	7	55	31	-37
2	15	7	26	23	-98
3	15	7	26	4	-101
-6	16	7	27	10	-104
-5	16	7	56	40	-48
-4	16	7	76	33	-34
-3	16	7	26	3	-98
-2	16	7	25	9	-97
-1	16	7	77	60	-31
0	16	7	60	28	-37
1	16	7	25	25	-68
2	16	7	26	10	-100
-5	17	7	82	56	-35
-4	17	7	27	32	-103
-3	17	7	27	11	-102
-2	17	7	26	4	-100
-1	17	7	54	30	-39
0	17	7	26	28	-69

Table 57. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-12	0	8	27	5	-101
-10	0	8	55	33	-37
-8	0	8	37	52	-48
-6	0	8	185	231	11
-4	0	8	57	79	-26
-2	0	8	315	325	8
0	0	8	97	92	14
2	0	8	73	75	-24
4	0	8	406	395	9
6	0	8	25	51	-96
-12	1	8	48	15	-46
-11	1	8	50	49	-38
-10	1	8	23	4	-62
-9	1	8	62	56	-23
-8	1	8	112	101	24
-7	1	8	31	11	-43
-6	1	8	186	215	45
-5	1	8	40	26	-33
-4	1	8	134	146	12
-3	1	8	20	35	-53
-2	1	8	58	51	19
-1	1	8	106	115	8
0	1	8	180	201	6
1	1	8	286	300	8
2	1	8	110	103	13
3	1	8	46	40	-34
4	1	8	288	289	8
5	1	8	32	23	-46
6	1	8	47	0	-42
7	1	8	50	30	-38
-12	2	8	27	11	-102
-11	2	8	26	35	-99
-10	2	8	23	29	-88
-9	2	8	36	54	-53
-8	2	8	63	32	-29
-7	2	8	22	33	-82
-6	2	8	21	52	-81
-5	2	8	20	40	-78
-4	2	8	73	75	21
-3	2	8	430	448	8
-2	2	8	119	135	14
-1	2	8	80	81	16
0	2	8	71	83	16
1	2	8	98	77	21
2	2	8	54	53	-33
3	2	8	35	18	-51
4	2	8	181	174	12
5	2	8	38	6	-52
6	2	8	25	22	-96
7	2	8	119	125	24
-12	3	8	27	11	-103
-11	3	8	96	63	27
-10	3	8	23	16	-88
-9	3	8	136	129	15
-8	3	8	67	83	-28
-7	3	8	22	33	-83
-6	3	8	35	49	-49
-5	3	8	41	1	-40
-4	3	8	132	144	13
-3	3	8	95	88	18
-2	3	8	20	53	-76
-1	3	8	86	87	15
0	3	8	55	58	-29
1	3	8	329	312	19
2	3	8	167	164	12
3	3	8	66	52	-27
4	3	8	22	3	-85
5	3	8	23	27	-88
6	3	8	47	8	-50
7	3	8	44	37	-62
-12	4	8	27	19	-104
-11	4	8	26	21	-99
-10	4	8	23	4	-89
-9	4	8	76	59	-26
-8	4	8	46	28	-40
-7	4	8	51	53	-37
-6	4	8	104	107	19
-5	4	8	40	49	-42
-4	4	8	260	290	9
-3	4	8	282	295	9
-2	4	8	43	4	-36
-1	4	8	97	74	15
0	4	8	20	32	-55
1	4	8	106	95	14
2	4	8	55	62	-33
3	4	8	79	75	23
4	4	8	75	78	-26
5	4	8	23	3	-88
6	4	8	120	114	21
7	4	8	77	97	-37
-12	5	8	56	2	-52
-11	5	8	26	11	-100

Table 57. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-10	5	8	55	55	-44
-9	5	8	23	29	-87
-8	5	8	129	123	15
-7	5	8	143	143	14
-6	5	8	206	203	11
-5	5	8	96	82	19
-4	5	8	21	49	-81
-3	5	8	104	98	17
-2	5	8	20	17	-78
-1	5	8	121	119	11
0	5	8	101	108	19
1	5	8	58	31	-25
2	5	8	268	290	9
3	5	8	22	61	-83
4	5	8	46	64	-42
5	5	8	55	23	-42
6	5	8	25	23	-97
7	5	8	27	7	-102
-12	6	8	28	10	-106
-11	6	8	27	80	-102
-10	6	8	25	26	-97
-9	6	8	42	22	-48
-8	6	8	22	16	-85
-7	6	8	71	32	-26
-6	6	8	49	58	-39
-5	6	8	78	65	23
-4	6	8	178	179	11
-3	6	8	21	18	-80
-2	6	8	21	1	-80
-1	6	8	354	357	25
0	6	8	122	129	14
1	6	8	30	27	-43
2	6	8	37	4	-49
3	6	8	22	9	-84
4	6	8	94	89	21
5	6	8	25	69	-95
6	6	8	26	49	-99
7	6	8	59	10	-47
-12	7	8	60	8	-49
-11	7	8	27	29	-104
-10	7	8	25	8	-97
-9	7	8	59	32	-35
-8	7	8	22	5	-86
-7	7	8	93	104	21
-6	7	8	121	135	16
-5	7	8	131	123	15
-4	7	8	145	158	14
-3	7	8	79	92	23
-2	7	8	111	127	17
-1	7	8	304	298	16
0	7	8	55	70	-22
1	7	8	81	62	16
2	7	8	82	58	22
3	7	8	99	112	20
4	7	8	60	65	-33
5	7	8	25	17	-96
6	7	8	42	10	-63
7	7	8	27	6	-104
-11	8	8	27	52	-105
-10	8	8	59	19	-43
-9	8	8	25	1	-95
-8	8	8	45	59	-45
-7	8	8	51	26	-37
-6	8	8	59	72	-32
-5	8	8	65	52	-28
-4	8	8	142	142	15
-3	8	8	90	94	21
-2	8	8	48	3	-37
-1	8	8	233	230	10
0	8	8	126	127	12
1	8	8	21	20	-58
2	8	8	111	97	17
3	8	8	22	19	-85
4	8	8	58	8	-40
5	8	8	58	53	-42
6	8	8	89	87	-31
-11	9	8	27	24	-105
-10	9	8	26	18	-101
-9	9	8	64	27	-38
-8	9	8	90	90	24
-7	9	8	23	5	-87
-6	9	8	22	7	-85
-5	9	8	59	52	-32
-4	9	8	118	105	16
-3	9	8	22	42	-83
-2	9	8	40	36	-46
-1	9	8	124	127	11
0	9	8	56	61	-24
1	9	8	47	26	-32
2	9	8	227	249	11
3	9	8	69	57	-27
4	9	8	74	22	-32

Table 57. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
5	9	8	26	22	-98
6	9	8	27	8	-103
-11	10	8	45	6	-65
-10	10	8	27	14	-102
-9	10	8	39	14	-66
-8	10	8	25	23	-97
-7	10	8	47	30	-44
-6	10	8	75	60	-27
-5	10	8	22	51	-85
-4	10	8	172	161	12
-3	10	8	38	30	-46
-2	10	8	22	18	-83
-1	10	8	44	57	-30
0	10	8	22	39	-58
1	10	8	22	25	-59
2	10	8	35	31	-56
3	10	8	25	11	-94
4	10	8	25	24	-96
5	10	8	39	12	-67
-10	11	8	27	16	-104
-9	11	8	45	54	-60
-8	11	8	79	52	-32
-7	11	8	25	26	-95
-6	11	8	46	29	-44
-5	11	8	23	42	-87
-4	11	8	22	14	-86
-3	11	8	32	42	-57
-2	11	8	53	61	-36
-1	11	8	118	116	12
0	11	8	22	20	-59
1	11	8	72	69	21
2	11	8	143	146	16
3	11	8	57	62	-42
4	11	8	26	13	-98
5	11	8	27	9	-101
-9	12	8	27	1	-103
-8	12	8	26	44	-100
-7	12	8	25	3	-96
-6	12	8	25	14	-95
-5	12	8	67	65	-31
-4	12	8	23	32	-88
-3	12	8	56	48	-34
-2	12	8	63	88	-32
-1	12	8	135	132	20
0	12	8	55	14	-33
1	12	8	51	0	-35
2	12	8	24	5	-93
3	12	8	25	17	-97
4	12	8	26	37	-101
-9	13	8	27	27	-105
-8	13	8	27	13	-103
-7	13	8	55	3	-46
-6	13	8	93	88	27
-5	13	8	81	59	-30
-4	13	8	25	17	-94
-3	13	8	23	8	-88
-2	13	8	75	53	-27
-1	13	8	61	53	-33
0	13	8	24	35	-64
1	13	8	24	9	-64
2	13	8	25	20	-94
3	13	8	45	35	-57
4	13	8	51	62	-54
-8	14	8	28	22	-106
-7	14	8	26	8	-101
-6	14	8	42	57	-62
-5	14	8	45	28	-56
-4	14	8	55	13	-43
-3	14	8	68	43	-35
-2	14	8	25	44	-95
-1	14	8	79	75	24
0	14	8	24	19	-65
1	14	8	65	42	-35
2	14	8	65	20	-38
3	14	8	27	31	-102
-7	15	8	27	3	-103
-6	15	8	73	33	-37
-5	15	8	48	59	-55
-4	15	8	48	57	-54
-3	15	8	26	7	-98
-2	15	8	25	26	-96
-1	15	8	24	5	-66
0	15	8	48	24	-41
1	15	8	81	68	23
2	15	8	26	50	-101
-6	16	8	45	34	-64
-5	16	8	27	4	-103
-4	16	8	59	7	-46
-3	16	8	61	74	-45
-2	16	8	50	33	-51
-1	16	8	49	6	-42
0	16	8	25	19	-69

Table 57. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
1	16	8	64	38	-31
-3	17	8	27	9	-103
-2	17	8	27	14	-102
-12	0	9	27	12	-102
-10	0	9	23	15	-88
-8	0	9	22	34	-84
-6	0	9	21	20	-81
-4	0	9	351	377	9
-2	0	9	158	163	12
0	0	9	270	254	15
2	0	9	87	91	21
4	0	9	22	17	-86
6	0	9	26	60	-100
-12	1	9	41	30	-52
-11	1	9	41	30	-48
-10	1	9	60	42	-24
-9	1	9	22	20	-61
-8	1	9	86	76	25
-7	1	9	45	14	-34
-6	1	9	51	46	-24
-5	1	9	46	48	-29
-4	1	9	382	372	6
-3	1	9	40	32	-29
-2	1	9	128	120	10
-1	1	9	134	143	10
0	1	9	171	153	8
1	1	9	44	12	-27
2	1	9	21	1	-58
3	1	9	79	64	17
4	1	9	22	4	-61
5	1	9	43	26	-45
6	1	9	135	144	15
7	1	9	54	13	-45
-12	2	9	27	3	-104
-11	2	9	58	9	-43
-10	2	9	23	8	-89
-9	2	9	91	95	23
-8	2	9	56	46	-33
-7	2	9	168	205	13
-6	2	9	39	26	-46
-5	2	9	21	26	-81
-4	2	9	172	169	11
-3	2	9	37	34	-44
-2	2	9	103	106	17
-1	2	9	157	163	9
0	2	9	58	23	-24
1	2	9	86	71	16
2	2	9	51	45	-35
3	2	9	309	332	10
4	2	9	32	6	-61
5	2	9	25	24	-95
6	2	9	67	29	-39
7	2	9	27	9	-104
-12	3	9	27	33	-105
-11	3	9	73	56	-35
-10	3	9	74	1	-31
-9	3	9	35	8	-57
-8	3	9	82	84	24
-7	3	9	22	2	-85
-6	3	9	22	4	-83
-5	3	9	93	131	20
-4	3	9	36	67	-48
-3	3	9	55	46	-31
-2	3	9	333	326	9
-1	3	9	261	274	7
0	3	9	21	7	-57
1	3	9	73	28	-33
2	3	9	40	65	-45
3	3	9	87	43	22
4	3	9	23	42	-87
5	3	9	25	11	-96
6	3	9	26	8	-100
-12	4	9	69	10	-42
-11	4	9	26	7	-99
-10	4	9	37	18	-64
-9	4	9	40	37	-51
-8	4	9	22	22	-85
-7	4	9	124	126	16
-6	4	9	141	136	14
-5	4	9	22	16	-83
-4	4	9	21	23	-82
-3	4	9	48	13	-35
-2	4	9	21	30	-81
-1	4	9	21	39	-57
0	4	9	100	100	13
1	4	9	43	12	-29
2	4	9	37	21	-48
3	4	9	181	185	12
4	4	9	72	95	-28
5	4	9	25	19	-96
6	4	9	27	16	-101
-12	5	9	54	50	-56

Table 57. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-11	5	9	77	27	-34
-10	5	9	52	19	-47
-9	5	9	64	75	-33
-8	5	9	23	8	-86
-7	5	9	22	51	-84
-6	5	9	95	87	20
-5	5	9	40	37	-47
-4	5	9	200	187	11
-3	5	9	77	68	23
-2	5	9	308	312	9
-1	5	9	136	137	15
0	5	9	115	124	13
1	5	9	143	141	15
2	5	9	22	13	-83
3	5	9	22	3	-85
4	5	9	24	49	-94
5	5	9	54	53	-46
6	5	9	101	104	28
-12	6	9	28	21	-107
-11	6	9	74	34	-37
-10	6	9	26	5	-98
-9	6	9	77	66	-27
-8	6	9	23	6	-86
-7	6	9	33	19	-58
-6	6	9	36	40	-52
-5	6	9	207	197	11
-4	6	9	128	123	15
-3	6	9	37	52	-49
-2	6	9	100	82	18
-1	6	9	21	37	-57
0	6	9	47	30	-26
1	6	9	282	317	8
2	6	9	22	40	-84
3	6	9	61	32	-32
4	6	9	78	72	-30
5	6	9	65	80	-40
6	6	9	48	31	-56
-11	7	9	27	20	-103
-10	7	9	26	6	-98
-9	7	9	56	58	-44
-8	7	9	67	42	-30
-7	7	9	22	16	-86
-6	7	9	22	24	-85
-5	7	9	98	87	20
-4	7	9	125	124	15
-3	7	9	22	25	-82
-2	7	9	58	44	-32
-1	7	9	21	10	-58
0	7	9	67	4	-30
1	7	9	124	139	11
2	7	9	22	17	-85
3	7	9	53	30	-37
4	7	9	25	25	-96
5	7	9	84	84	-32
6	7	9	61	23	-46
-11	8	9	62	23	-46
-10	8	9	26	25	-100
-9	8	9	51	66	-50
-8	8	9	23	6	-88
-7	8	9	49	47	-41
-6	8	9	109	108	18
-5	8	9	22	13	-84
-4	8	9	102	103	18
-3	8	9	36	8	-50
-2	8	9	56	28	-33
-1	8	9	35	11	-40
0	8	9	21	13	-58
1	8	9	217	231	14
2	8	9	98	114	21
3	8	9	24	44	-93
4	8	9	25	42	-96
5	8	9	26	35	-101
-11	9	9	70	22	-42
-10	9	9	46	20	-58
-9	9	9	26	23	-99
-8	9	9	79	25	-30
-7	9	9	23	2	-88
-6	9	9	44	24	-45
-5	9	9	60	42	-32
-4	9	9	22	1	-84
-3	9	9	38	1	-47
-2	9	9	293	265	10
-1	9	9	63	59	-24
0	9	9	44	2	-35
1	9	9	75	57	18
2	9	9	23	15	-87
3	9	9	25	18	-95
4	9	9	26	74	-98
5	9	9	27	30	-102
-10	10	9	27	15	-103
-9	10	9	26	23	-101
-8	10	9	26	20	-98

Table 57. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-7	10	9	46	47	-51
-6	10	9	131	110	16
-5	10	9	23	59	-86
-4	10	9	41	2	-46
-3	10	9	36	40	-52
-2	10	9	34	27	-56
-1	10	9	22	22	-59
0	10	9	43	41	-37
1	10	9	56	19	-33
2	10	9	45	34	-49
3	10	9	25	36	-96
4	10	9	61	73	-43
5	10	9	75	33	-38
-10	11	9	45	11	-65
-9	11	9	77	29	-36
-8	11	9	40	4	-64
-7	11	9	25	17	-96
-6	11	9	46	19	-51
-5	11	9	42	1	-49
-4	11	9	46	19	-43
-3	11	9	22	18	-85
-2	11	9	137	125	15
-1	11	9	22	10	-60
0	11	9	64	53	-28
1	11	9	54	60	-35
2	11	9	25	33	-94
3	11	9	50	11	-50
4	11	9	27	31	-102
-9	12	9	57	36	-50
-8	12	9	27	17	-101
-7	12	9	92	64	28
-6	12	9	91	72	27
-5	12	9	56	42	-43
-4	12	9	67	67	-36
-3	12	9	57	1	-34
-2	12	9	38	10	-59
-1	12	9	65	33	-22
0	12	9	36	11	-47
1	12	9	94	100	18
2	12	9	25	21	-96
3	12	9	73	38	-36
-8	13	9	27	7	-104
-7	13	9	26	39	-101
-6	13	9	44	35	-58
-5	13	9	45	10	-54
-4	13	9	104	92	24
-3	13	9	25	31	-96
-2	13	9	25	16	-94
-1	13	9	50	8	-31
0	13	9	89	73	24
1	13	9	69	69	-29
2	13	9	26	37	-99
3	13	9	27	6	-103
-7	14	9	41	25	-67
-6	14	9	38	9	-70
-5	14	9	26	24	-100
-4	14	9	26	37	-98
-3	14	9	114	73	23
-2	14	9	25	13	-96
-1	14	9	47	8	-41
0	14	9	25	22	-67
1	14	9	64	48	-36
2	14	9	47	3	-56
-6	15	9	27	10	-104
-5	15	9	27	9	-103
-4	15	9	27	58	-102
-3	15	9	26	43	-100
-2	15	9	26	39	-98
-1	15	9	25	38	-68
0	15	9	57	19	-31
1	15	9	37	37	-52
-4	16	9	27	9	-103
-3	16	9	27	23	-103
-2	16	9	26	16	-101
-1	16	9	34	22	-57
-12	0	10	76	47	-38
-10	0	10	25	30	-96
-8	0	10	23	94	-86
-6	0	10	37	3	-49
-4	0	10	35	47	-50
-2	0	10	347	364	9
0	0	10	21	5	-57
2	0	10	112	84	18
4	0	10	25	2	-94
6	0	10	70	23	-40
-12	1	10	52	38	-39
-11	1	10	26	2	-70
-10	1	10	58	53	-30
-9	1	10	23	13	-61
-8	1	10	70	80	20
-7	1	10	55	50	-32
-6	1	10	38	19	-38

Table 57. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-5	1	10	184	186	31
-4	1	10	86	86	15
-3	1	10	36	3	-38
-2	1	10	95	77	14
-1	1	10	67	65	15
0	1	10	52	42	-19
1	1	10	126	133	8
2	1	10	195	198	11
3	1	10	23	26	-61
4	1	10	37	26	-49
5	1	10	63	69	-30
6	1	10	73	11	-38
-12	2	10	28	24	-106
-11	2	10	26	3	-99
-10	2	10	25	33	-96
-9	2	10	23	24	-88
-8	2	10	55	73	-36
-7	2	10	61	30	-30
-6	2	10	95	51	20
-5	2	10	107	110	18
-4	2	10	55	41	-32
-3	2	10	122	109	16
-2	2	10	161	156	13
-1	2	10	132	128	10
0	2	10	116	135	11
1	2	10	74	75	18
2	2	10	53	30	-35
3	2	10	23	7	-86
4	2	10	41	9	-59
5	2	10	109	97	24
6	2	10	46	44	-61
-12	3	10	46	19	-62
-11	3	10	26	5	-100
-10	3	10	25	15	-96
-9	3	10	46	5	-44
-8	3	10	23	35	-86
-7	3	10	83	78	24
-6	3	10	71	39	-26
-5	3	10	286	304	9
-4	3	10	21	37	-82
-3	3	10	63	66	-28
-2	3	10	114	116	17
-1	3	10	35	1	-38
0	3	10	21	5	-57
1	3	10	89	106	19
2	3	10	66	76	-29
3	3	10	71	50	-27
4	3	10	25	47	-95
5	3	10	138	130	20
6	3	10	27	20	-103
-12	4	10	58	23	-50
-11	4	10	27	11	-102
-10	4	10	54	68	-46
-9	4	10	68	41	-30
-8	4	10	32	1	-61
-7	4	10	92	78	21
-6	4	10	31	11	-59
-5	4	10	38	17	-49
-4	4	10	55	17	-33
-3	4	10	21	27	-82
-2	4	10	156	133	13
-1	4	10	98	76	21
0	4	10	203	211	17
1	4	10	125	119	11
2	4	10	78	51	24
3	4	10	24	13	-93
4	4	10	55	8	-44
5	4	10	27	63	-101
-12	5	10	28	0	-107
-11	5	10	27	4	-102
-10	5	10	69	35	-37
-9	5	10	48	19	-43
-8	5	10	82	62	25
-7	5	10	57	68	-34
-6	5	10	62	57	-30
-5	5	10	168	177	13
-4	5	10	22	13	-83
-3	5	10	207	193	11
-2	5	10	47	17	-38
-1	5	10	49	15	-25
0	5	10	189	214	8
1	5	10	50	64	-27
2	5	10	102	109	20
3	5	10	95	101	25
4	5	10	38	27	-64
5	5	10	55	28	-49
-11	6	10	27	21	-103
-10	6	10	26	16	-98
-9	6	10	25	13	-96
-8	6	10	23	18	-89
-7	6	10	52	67	-39
-6	6	10	69	57	-28

Table 57. (cont).
F(obs), F(calc), and σ_F

($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-5	6	10	73	67	-26
-4	6	10	22	36	-83
-3	6	10	198	178	11
-2	6	10	151	156	13
-1	6	10	21	6	-57
0	6	10	73	81	18
1	6	10	66	67	-22
2	6	10	60	67	-33
3	6	10	25	6	-95
4	6	10	25	20	-97
5	6	10	27	31	-102
-11	7	10	27	2	-104
-10	7	10	44	20	-60
-9	7	10	65	36	-39
-8	7	10	23	17	-89
-7	7	10	145	148	15
-6	7	10	68	41	-28
-5	7	10	22	25	-85
-4	7	10	22	52	-84
-3	7	10	129	130	15
-2	7	10	40	49	-46
-1	7	10	51	14	-33
0	7	10	46	12	-30
1	7	10	42	46	-33
2	7	10	82	59	-27
3	7	10	167	180	16
4	7	10	26	53	-99
5	7	10	70	36	-40
-11	8	10	28	5	-106
-10	8	10	56	65	-50
-9	8	10	51	31	-49
-8	8	10	25	10	-96
-7	8	10	42	24	-50
-6	8	10	53	25	-36
-5	8	10	57	14	-33
-4	8	10	67	59	-29
-3	8	10	164	151	13
-2	8	10	61	43	-31
-1	8	10	62	22	-29
0	8	10	152	156	21
1	8	10	22	5	-61
2	8	10	24	16	-93
3	8	10	63	24	-39
4	8	10	26	5	-101
-10	9	10	42	5	-68
-9	9	10	26	12	-101
-8	9	10	50	36	-50
-7	9	10	25	40	-95
-6	9	10	58	33	-35
-5	9	10	23	2	-87
-4	9	10	89	50	22
-3	9	10	50	12	-39
-2	9	10	64	25	-30
-1	9	10	36	37	-42
0	9	10	55	56	-28
1	9	10	23	12	-64
2	9	10	24	29	-93
3	9	10	61	65	-41
4	9	10	75	74	-37
-10	10	10	76	63	-39
-9	10	10	27	18	-102
-8	10	10	26	1	-99
-7	10	10	25	5	-96
-6	10	10	25	10	-95
-5	10	10	23	32	-89
-4	10	10	60	52	-34
-3	10	10	23	23	-86
-2	10	10	62	8	-32
-1	10	10	23	31	-61
0	10	10	166	177	15
1	10	10	24	27	-65
2	10	10	25	23	-95
3	10	10	26	32	-100
4	10	10	27	25	-103
-9	11	10	63	12	-45
-8	11	10	26	1	-101
-7	11	10	25	31	-97
-6	11	10	25	19	-97
-5	11	10	93	76	27
-4	11	10	70	87	-34
-3	11	10	25	58	-95
-2	11	10	39	13	-56
-1	11	10	49	14	-38
0	11	10	24	16	-65
1	11	10	53	22	-37
2	11	10	77	10	-33
3	11	10	40	48	-68
-9	12	10	63	3	-46
-8	12	10	58	34	-50
-7	12	10	26	30	-100
-6	12	10	26	2	-98
-5	12	10	65	70	-39

Table 57. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-4	12	10	72	1	-34
-3	12	10	81	51	-30
-2	12	10	25	37	-94
-1	12	10	59	7	-36
0	12	10	51	39	-38
1	12	10	25	5	-67
2	12	10	105	38	24
-8	13	10	28	42	-106
-7	13	10	86	46	-33
-6	13	10	26	13	-101
-5	13	10	60	1	-44
-4	13	10	47	51	-55
-3	13	10	72	53	-36
-2	13	10	25	0	-96
-1	13	10	24	10	-66
0	13	10	25	14	-68
1	13	10	25	16	-69
-7	14	10	47	42	-61
-6	14	10	27	7	-103
-5	14	10	63	29	-43
-4	14	10	26	9	-101
-3	14	10	26	10	-100
-2	14	10	73	67	-36
-1	14	10	66	48	-27
0	14	10	25	33	-69
-5	15	10	51	56	-57
-4	15	10	27	22	-103
-3	15	10	52	6	-53
-2	15	10	27	2	-101
-1	15	10	47	15	-44
-12	0	11	28	8	-105
-10	0	11	25	11	-97
-8	0	11	61	78	-34
-6	0	11	228	247	11
-4	0	11	42	38	-43
-2	0	11	22	28	-83
0	0	11	97	100	14
2	0	11	22	17	-86
4	0	11	166	167	17
-12	1	11	46	13	-49
-11	1	11	26	22	-71
-10	1	11	48	35	-42
-9	1	11	32	26	-48
-8	1	11	33	5	-45
-7	1	11	22	8	-60
-6	1	11	78	89	-36
-5	1	11	22	15	-59
-4	1	11	67	34	20
-3	1	11	133	119	25
-2	1	11	22	43	-59
-1	1	11	89	93	10
0	1	11	262	272	5
1	1	11	71	65	15
2	1	11	60	38	-32
3	1	11	36	8	-50
4	1	11	34	10	-56
5	1	11	64	16	-40
-12	2	11	28	9	-106
-11	2	11	27	16	-102
-10	2	11	25	1	-97
-9	2	11	25	17	-95
-8	2	11	43	41	-47
-7	2	11	58	22	-33
-6	2	11	75	77	-26
-5	2	11	69	33	-27
-4	2	11	55	42	-33
-3	2	11	170	164	12
-2	2	11	41	50	-45
-1	2	11	22	18	-58
0	2	11	57	40	-25
1	2	11	98	99	14
2	2	11	40	32	-50
3	2	11	25	33	-95
4	2	11	55	79	-48
5	2	11	50	25	-55
-12	3	11	28	4	-107
-11	3	11	64	32	-43
-10	3	11	25	6	-97
-9	3	11	25	43	-96
-8	3	11	72	66	-29
-7	3	11	22	18	-86
-6	3	11	59	72	-32
-5	3	11	45	43	-41
-4	3	11	22	25	-84
-3	3	11	211	186	11
-2	3	11	22	8	-84
-1	3	11	98	97	13
0	3	11	99	98	13
1	3	11	106	105	16
2	3	11	86	86	25
3	3	11	25	22	-95
4	3	11	26	3	-100

Table 57. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
5	3	11	49	11	-58
-11	4	11	27	34	-103
-10	4	11	44	6	-57
-9	4	11	25	6	-96
-8	4	11	81	75	-27
-7	4	11	23	2	-86
-6	4	11	44	42	-44
-5	4	11	53	17	-36
-4	4	11	104	95	18
-3	4	11	221	213	10
-2	4	11	22	11	-83
-1	4	11	124	119	11
0	4	11	57	43	-28
1	4	11	48	12	-34
2	4	11	114	131	21
3	4	11	43	56	-56
4	4	11	98	83	28
-11	5	11	99	31	28
-10	5	11	41	43	-64
-9	5	11	25	13	-97
-8	5	11	54	43	-39
-7	5	11	74	58	-28
-6	5	11	40	4	-48
-5	5	11	48	25	-40
-4	5	11	92	103	21
-3	5	11	41	17	-45
-2	5	11	22	2	-84
-1	5	11	100	100	13
0	5	11	83	64	16
1	5	11	56	7	-32
2	5	11	75	83	-31
3	5	11	67	44	-37
4	5	11	26	21	-101
-11	6	11	28	31	-106
-10	6	11	44	14	-60
-9	6	11	25	16	-97
-8	6	11	25	59	-96
-7	6	11	23	25	-88
-6	6	11	66	44	-30
-5	6	11	142	139	15
-4	6	11	49	19	-38
-3	6	11	71	67	-27
-2	6	11	61	38	-31
-1	6	11	49	40	-35
0	6	11	22	1	-60
1	6	11	24	4	-64
2	6	11	47	66	-50
3	6	11	63	43	-40
4	6	11	52	87	-53
-11	7	11	73	54	-42
-10	7	11	48	25	-57
-9	7	11	46	11	-56
-8	7	11	66	42	-37
-7	7	11	23	9	-88
-6	7	11	23	39	-88
-5	7	11	23	15	-88
-4	7	11	65	72	-31
-3	7	11	66	58	-29
-2	7	11	53	17	-36
-1	7	11	181	168	15
0	7	11	64	67	-25
1	7	11	79	36	-36
2	7	11	47	22	-50
3	7	11	26	15	-99
4	7	11	27	6	-102
-10	8	11	27	21	-103
-9	8	11	40	11	-67
-8	8	11	66	28	-38
-7	8	11	25	29	-95
-6	8	11	49	36	-43
-5	8	11	105	96	20
-4	8	11	90	99	23
-3	8	11	23	4	-87
-2	8	11	23	9	-87
-1	8	11	37	14	-38
0	8	11	24	2	-64
1	8	11	24	25	-64
2	8	11	75	74	-33
3	8	11	48	24	-55
-10	9	11	27	13	-105
-9	9	11	79	16	-35
-8	9	11	83	75	-32
-7	9	11	25	28	-96
-6	9	11	44	25	-56
-5	9	11	35	13	-66
-4	9	11	23	2	-88
-3	9	11	23	13	-87
-2	9	11	83	61	-27
-1	9	11	53	44	-31
0	9	11	44	25	-40
1	9	11	24	4	-65
2	9	11	26	87	-99

Table 57. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
3	9	11	89	30	-30
-9	10	11	27	2	-104
-8	10	11	27	28	-102
-7	10	11	61	21	-42
-6	10	11	56	62	-45
-5	10	11	25	7	-96
-4	10	11	25	61	-95
-3	10	11	25	23	-95
-2	10	11	25	54	-95
-1	10	11	46	11	-41
0	10	11	66	25	-35
1	10	11	25	11	-66
2	10	11	54	93	-49
-9	11	11	68	33	-44
-8	11	11	84	60	-34
-7	11	11	26	11	-100
-6	11	11	48	36	-54
-5	11	11	26	28	-98
-4	11	11	40	5	-61
-3	11	11	44	40	-54
-2	11	11	25	57	-96
-1	11	11	86	97	27
0	11	11	25	10	-67
1	11	11	37	18	-50
2	11	11	86	69	-31
-8	12	11	28	10	-106
-7	12	11	27	2	-103
-6	12	11	55	37	-49
-5	12	11	79	51	-33
-4	12	11	26	3	-98
-3	12	11	25	12	-97
-2	12	11	26	44	-98
-1	12	11	25	29	-67
0	12	11	25	21	-68
1	12	11	26	12	-69
-7	13	11	27	5	-104
-6	13	11	27	17	-103
-5	13	11	27	10	-103
-4	13	11	26	3	-101
-3	13	11	49	30	-55
-2	13	11	26	34	-100
-1	13	11	71	64	-26
0	13	11	36	27	-54
-5	14	11	28	54	-106
-4	14	11	50	23	-55
-3	14	11	27	24	-103
-2	14	11	64	10	-42
-10	0	12	71	11	-35
-8	0	12	36	43	-59
-6	0	12	63	82	-32
-4	0	12	22	25	-86
-2	0	12	62	66	-31
0	0	12	99	93	14
2	0	12	73	103	-32
4	0	12	27	12	-102
-11	1	12	44	10	-45
-10	1	12	26	5	-70
-9	1	12	47	20	-43
-8	1	12	41	19	-40
-7	1	12	23	38	-62
-6	1	12	42	29	-33
-5	1	12	56	25	-25
-4	1	12	270	242	11
-3	1	12	30	24	-47
-2	1	12	22	18	-60
-1	1	12	39	8	-28
0	1	12	32	0	-34
1	1	12	31	22	-38
2	1	12	43	45	-43
3	1	12	26	57	-71
4	1	12	27	32	-73
-11	2	12	63	32	-46
-10	2	12	26	5	-100
-9	2	12	40	51	-64
-8	2	12	62	44	-38
-7	2	12	51	40	-40
-6	2	12	107	100	19
-5	2	12	22	2	-86
-4	2	12	60	42	-32
-3	2	12	22	20	-84
-2	2	12	22	17	-85
-1	2	12	181	177	8
0	2	12	22	28	-60
1	2	12	24	53	-64
2	2	12	84	67	-27
3	2	12	68	66	-39
4	2	12	27	6	-103
-11	3	12	28	31	-105
-10	3	12	47	7	-55
-9	3	12	79	52	-32
-8	3	12	25	18	-96
-7	3	12	42	37	-49

Table 57. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-6	3	12	86	57	24
-5	3	12	23	28	-87
-4	3	12	88	66	22
-3	3	12	22	31	-85
-2	3	12	76	81	-27
-1	3	12	123	112	12
0	3	12	59	27	-23
1	3	12	73	58	-35
2	3	12	24	2	-93
3	3	12	122	123	22
4	3	12	82	46	-33
-11	4	12	27	23	-105
-10	4	12	26	2	-100
-9	4	12	26	7	-99
-8	4	12	42	9	-58
-7	4	12	58	41	-36
-6	4	12	88	78	23
-5	4	12	23	41	-88
-4	4	12	79	64	25
-3	4	12	22	17	-86
-2	4	12	94	86	21
-1	4	12	134	131	11
0	4	12	23	33	-63
1	4	12	49	33	-32
2	4	12	25	17	-95
3	4	12	87	39	-30
-11	5	12	28	25	-106
-10	5	12	47	5	-57
-9	5	12	74	30	-35
-8	5	12	61	2	-40
-7	5	12	43	26	-57
-6	5	12	93	89	23
-5	5	12	23	32	-88
-4	5	12	107	92	19
-3	5	12	71	64	-28
-2	5	12	23	7	-87
-1	5	12	109	102	14
0	5	12	37	7	-45
1	5	12	58	2	-30
2	5	12	68	24	-36
3	5	12	50	35	-54
-10	6	12	27	6	-103
-9	6	12	83	72	-33
-8	6	12	61	55	-41
-7	6	12	25	17	-95
-6	6	12	23	4	-89
-5	6	12	64	20	-32
-4	6	12	23	7	-88
-3	6	12	33	33	-60
-2	6	12	53	56	-38
-1	6	12	23	10	-63
0	6	12	56	31	-35
1	6	12	131	147	13
2	6	12	84	32	-30
3	6	12	26	1	-101
-10	7	12	27	6	-104
-9	7	12	27	4	-103
-8	7	12	42	0	-60
-7	7	12	25	39	-97
-6	7	12	25	21	-96
-5	7	12	25	27	-94
-4	7	12	49	35	-42
-3	7	12	49	67	-42
-2	7	12	47	58	-48
-1	7	12	24	26	-64
0	7	12	24	19	-65
1	7	12	67	41	-25
2	7	12	25	4	-98
3	7	12	27	17	-103
-10	8	12	28	21	-106
-9	8	12	96	52	30
-8	8	12	53	35	-50
-7	8	12	26	20	-98
-6	8	12	59	34	-42
-5	8	12	76	28	-32
-4	8	12	25	35	-96
-3	8	12	25	42	-95
-2	8	12	87	65	27
-1	8	12	55	32	-32
0	8	12	24	8	-66
1	8	12	100	99	-40
2	8	12	63	37	-41
-9	9	12	49	1	-59
-8	9	12	27	16	-101
-7	9	12	62	8	-42
-6	9	12	78	81	-34
-5	9	12	53	21	-47
-4	9	12	25	28	-96
-3	9	12	100	64	24
-2	9	12	94	100	27
-1	9	12	53	10	-36
0	9	12	25	6	-67

Table 57. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
1	9	12	25	9	-69
2	9	12	27	7	-101
-8	10	12	27	6	-104
-7	10	12	86	22	-31
-6	10	12	27	56	-101
-5	10	12	26	30	-99
-4	10	12	26	44	-98
-3	10	12	25	7	-97
-2	10	12	97	67	26
-1	10	12	25	16	-67
0	10	12	51	32	-40
1	10	12	26	24	-69
-8	11	12	28	15	-105
-7	11	12	90	40	-31
-6	11	12	52	56	-53
-5	11	12	26	26	-101
-4	11	12	39	9	-67
-3	11	12	26	12	-99
-2	11	12	62	37	-41
-1	11	12	42	15	-46
0	11	12	37	7	-51
-7	12	12	27	5	-105
-6	12	12	27	42	-105
-5	12	12	96	22	29
-4	12	12	67	18	-41
-3	12	12	71	6	-38
-2	12	12	26	14	-100
-1	12	12	26	26	-69
-4	13	12	77	44	-37
-3	13	12	77	42	-37
-10	0	13	27	18	-102
-8	0	13	56	31	-44
-6	0	13	39	5	-52
-4	0	13	53	34	-37
-2	0	13	156	140	14
0	0	13	24	14	-64
2	0	13	26	33	-98
-11	1	13	64	6	-41
-10	1	13	70	30	-29
-9	1	13	26	26	-71
-8	1	13	44	17	-45
-7	1	13	25	17	-68
-6	1	13	23	2	-62
-5	1	13	45	22	-39
-4	1	13	77	63	24
-3	1	13	23	12	-62
-2	1	13	101	81	17
-1	1	13	55	19	-25
0	1	13	51	38	-23
1	1	13	65	55	19
2	1	13	78	94	24
-11	2	13	60	7	-49
-10	2	13	27	31	-102
-9	2	13	26	14	-100
-8	2	13	26	7	-98
-7	2	13	70	67	-35
-6	2	13	49	1	-48
-5	2	13	114	98	19
-4	2	13	23	42	-88
-3	2	13	61	39	-33
-2	2	13	103	113	22
-1	2	13	40	19	-43
0	2	13	24	21	-64
1	2	13	25	1	-66
2	2	13	25	27	-97
-10	3	13	27	22	-104
-9	3	13	71	45	-38
-8	3	13	25	16	-98
-7	3	13	25	10	-96
-6	3	13	58	15	-41
-5	3	13	36	63	-58
-4	3	13	23	52	-89
-3	3	13	23	38	-88
-2	3	13	24	26	-92
-1	3	13	24	24	-64
0	3	13	47	58	-39
1	3	13	104	100	24
2	3	13	26	11	-98
-10	4	13	27	23	-104
-9	4	13	26	36	-101
-8	4	13	50	4	-51
-7	4	13	26	49	-98
-6	4	13	25	7	-95
-5	4	13	75	78	-32
-4	4	13	44	76	-54
-3	4	13	75	71	-31
-2	4	13	24	40	-93
-1	4	13	35	50	-49
0	4	13	46	8	-41
1	4	13	63	15	-31
2	4	13	26	14	-99
-10	5	13	27	38	-105

Table 57. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-9	5	13	41	30	-66
-8	5	13	49	23	-52
-7	5	13	113	86	23
-6	5	13	25	31	-96
-5	5	13	53	56	-45
-4	5	13	25	2	-95
-3	5	13	25	11	-96
-2	5	13	25	52	-94
-1	5	13	41	27	-44
0	5	13	85	74	-27
1	5	13	57	53	-31
2	5	13	26	36	-100
-10	6	13	55	1	-53
-9	6	13	77	28	-36
-8	6	13	26	5	-100
-7	6	13	26	18	-98
-6	6	13	58	18	-43
-5	6	13	25	35	-96
-4	6	13	38	38	-63
-3	6	13	81	81	-30
-2	6	13	55	79	-44
-1	6	13	40	26	-44
0	6	13	25	28	-66
1	6	13	50	43	-37
-9	7	13	27	13	-104
-8	7	13	26	0	-101
-7	7	13	128	93	21
-6	7	13	59	51	-43
-5	7	13	25	10	-97
-4	7	13	25	6	-97
-3	7	13	25	28	-97
-2	7	13	25	6	-96
-1	7	13	47	38	-35
0	7	13	48	31	-42
1	7	13	26	7	-69
-9	8	13	28	11	-106
-8	8	13	58	8	-48
-7	8	13	26	26	-101
-6	8	13	26	14	-99
-5	8	13	26	27	-99
-4	8	13	26	24	-98
-3	8	13	26	48	-99
-2	8	13	77	17	-32
-1	8	13	25	44	-67
0	8	13	52	55	-34
1	8	13	74	15	-36
-8	9	13	27	26	-104
-7	9	13	80	37	-35
-6	9	13	55	26	-48
-5	9	13	26	6	-100
-4	9	13	26	9	-100
-3	9	13	26	29	-100
-2	9	13	73	47	-36
-1	9	13	53	29	-39
0	9	13	96	100	20
-7	10	13	82	4	-34
-6	10	13	27	6	-103
-5	10	13	27	25	-102
-4	10	13	64	68	-42
-3	10	13	77	28	-35
-2	10	13	26	12	-101
-1	10	13	53	24	-41
-6	11	13	27	5	-104
-5	11	13	27	2	-104
-4	11	13	27	28	-104
-3	11	13	27	8	-104
-2	11	13	43	24	-64
-10	0	14	28	14	-105
-8	0	14	71	30	-38
-6	0	14	25	44	-97
-4	0	14	25	28	-96
-2	0	14	25	24	-94
0	0	14	104	107	17
-10	1	14	60	36	-42
-9	1	14	46	3	-48
-8	1	14	51	43	-43
-7	1	14	26	2	-69
-6	1	14	45	39	-44
-5	1	14	54	46	-39
-4	1	14	64	6	-31
-3	1	14	46	57	-44
-2	1	14	38	51	-48
-1	1	14	25	12	-47
0	1	14	78	65	17
1	1	14	61	25	-25
-10	2	14	28	0	-105
-9	2	14	27	6	-104
-8	2	14	26	15	-101
-7	2	14	26	33	-99
-6	2	14	25	23	-97
-5	2	14	25	1	-97
-4	2	14	25	41	-97

Table 57. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-3	2	14	25	7	-97
-2	2	14	25	20	-95
-1	2	14	25	39	-66
0	2	14	37	46	-50
1	2	14	43	41	-48
-10	3	14	67	19	-44
-9	3	14	80	4	-35
-8	3	14	47	23	-57
-7	3	14	26	4	-99
-6	3	14	25	2	-97
-5	3	14	26	45	-98
-4	3	14	25	41	-97
-3	3	14	130	114	20
-2	3	14	44	63	-54
-1	3	14	25	6	-67
0	3	14	25	15	-68
1	3	14	61	10	-38
-9	4	14	27	6	-104
-8	4	14	72	65	-39
-7	4	14	52	52	-51
-6	4	14	50	32	-51
-5	4	14	43	44	-59
-4	4	14	46	15	-53
-3	4	14	26	26	-98
-2	4	14	54	6	-44
-1	4	14	44	15	-44
0	4	14	50	43	-41
1	4	14	26	28	-70
-9	5	14	27	1	-105
-8	5	14	27	13	-103
-7	5	14	46	18	-58
-6	5	14	26	14	-100
-5	5	14	67	11	-38
-4	5	14	58	11	-43
-3	5	14	26	29	-98
-2	5	14	58	43	-43
-1	5	14	72	64	-30
0	5	14	49	15	-42
-9	6	14	27	6	-105
-8	6	14	27	32	-104
-7	6	14	48	28	-56
-6	6	14	60	37	-44
-5	6	14	84	60	-32
-4	6	14	26	28	-99
-3	6	14	26	30	-99
-2	6	14	26	14	-98

APPENDIX J

TABLE 58

Table 58. Mixed Trichlorobenzene/Trimethylbenzene Thiourea Host/Guest Adduct

F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
2	0	0	470	463	4	3	5	0	131	139	7
4	0	0	181	152	6	4	5	0	289	305	6
6	0	0	201	206	8	5	5	0	331	321	7
8	0	0	72	74	18	6	5	0	42	9	-25
10	0	0	126	123	15	7	5	0	17	6	-71
1	1	0	89	70	3	8	5	0	82	86	17
2	1	0	301	281	4	9	5	0	36	27	-37
3	1	0	612	529	4	10	5	0	31	47	-50
4	1	0	210	209	6	0	6	0	48	34	13
5	1	0	167	188	8	1	6	0	119	141	7
6	1	0	151	144	9	2	6	0	222	221	6
7	1	0	168	158	10	3	6	0	41	51	-18
8	1	0	77	69	17	4	6	0	163	161	8
9	1	0	18	13	-74	5	6	0	183	184	9
10	1	0	41	18	-36	6	6	0	62	32	18
0	2	0	85	299	-4	7	6	0	59	53	-23
1	2	0	23	19	-13	8	6	0	50	36	-27
2	2	0	79	63	7	9	6	0	94	87	17
3	2	0	584	499	5	10	6	0	75	64	22
4	2	0	31	12	-22	1	7	0	53	75	14
5	2	0	43	52	-19	2	7	0	40	71	-19
6	2	0	15	3	-65	3	7	0	78	76	11
7	2	0	283	271	8	4	7	0	104	94	11
8	2	0	17	13	-71	5	7	0	493	482	7
9	2	0	46	34	-29	6	7	0	68	65	17
10	2	0	19	34	-80	7	7	0	93	102	15
1	3	0	48	50	9	8	7	0	52	82	-26
2	3	0	361	313	4	9	7	0	18	9	-78
3	3	0	803	730	5	10	7	0	19	39	-80
4	3	0	62	44	12	1	8	0	33	42	-24
5	3	0	110	101	10	3	8	0	66	72	15
6	3	0	15	23	-65	4	8	0	170	183	9
7	3	0	232	227	9	5	8	0	16	16	-68
8	3	0	42	2	-29	6	8	0	48	30	-24
9	3	0	38	22	-34	7	8	0	65	65	20
10	3	0	34	2	-42	8	8	0	106	103	15
3	4	0	145	146	7	9	8	0	26	45	-55
4	4	0	46	39	-16	1	9	0	57	60	16
5	4	0	31	18	-28	3	9	0	15	31	-62
6	4	0	15	15	-65	4	9	0	16	38	-65
7	4	0	186	191	10	5	9	0	118	131	13
8	4	0	168	162	11	6	9	0	31	23	-37
9	4	0	18	20	-74	7	9	0	17	6	-72
10	4	0	80	86	21	8	9	0	55	20	-23
1	5	0	162	149	6	9	9	0	19	24	-79

Table 58. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
0	10	0	168	164	9	6	15	0	19	22	-79
1	10	0	84	84	13	0	16	0	17	9	-73
2	10	0	313	324	8	1	16	0	17	10	-73
3	10	0	15	8	-65	2	16	0	41	7	-31
4	10	0	16	6	-68	3	16	0	33	34	-43
5	10	0	17	26	-72	4	16	0	18	13	-75
6	10	0	25	6	-46	5	16	0	19	5	-79
7	10	0	18	12	-74	1	17	0	18	4	-75
8	10	0	76	74	21	2	17	0	18	24	-77
9	10	0	19	5	-79	3	17	0	45	43	-34
1	11	0	106	123	12	0	18	0	72	61	24
2	11	0	157	175	11	1	18	0	18	13	-78
3	11	0	77	82	16	-10	0	1	18	6	-76
4	11	0	62	52	20	-8	0	1	50	15	-27
5	11	0	189	204	11	-6	0	1	92	90	12
6	11	0	43	19	-28	-4	0	1	860	839	5
7	11	0	31	17	-44	-2	0	1	171	180	4
8	11	0	19	25	-80	0	0	1	36	23	9
0	12	0	209	233	10	2	0	1	837	709	4
1	12	0	96	89	14	4	0	1	451	432	5
2	12	0	46	42	-24	6	0	1	336	318	7
3	12	0	17	43	-70	8	0	1	41	14	-30
4	12	0	16	10	-69	10	0	1	18	18	-77
5	12	0	17	12	-71	-11	1	1	19	31	-81
6	12	0	90	81	18	-10	1	1	56	28	-24
7	12	0	36	23	-39	-9	1	1	59	35	-22
8	12	0	19	16	-78	-8	1	1	361	363	9
1	13	0	16	2	-68	-7	1	1	16	12	-67
2	13	0	16	9	-68	-6	1	1	257	246	7
3	13	0	39	14	-28	-5	1	1	174	157	7
4	13	0	33	23	-38	-4	1	1	113	102	8
5	13	0	108	110	16	-3	1	1	242	243	5
6	13	0	30	6	-44	-2	1	1	43	52	10
7	13	0	18	3	-77	-1	1	1	92	296	-4
0	14	0	134	123	13	0	1	1	19	4	-9
1	14	0	90	74	15	1	1	1	132	128	4
2	14	0	50	64	-26	2	1	1	1253	1184	4
3	14	0	47	14	-25	3	1	1	33	30	-20
4	14	0	47	17	-26	4	1	1	199	191	6
5	14	0	32	42	-42	5	1	1	187	132	7
6	14	0	18	8	-77	6	1	1	63	66	18
1	15	0	26	28	-46	7	1	1	42	9	-27
2	15	0	18	37	-74	8	1	1	49	57	-26
3	15	0	109	98	15	9	1	1	97	95	16
4	15	0	18	29	-76	10	1	1	18	24	-76
5	15	0	18	15	-77	-11	2	1	63	61	-27

Table 58. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-10	2	1	39	33	-36
-9	2	1	18	3	-74
-8	2	1	38	17	-35
-7	2	1	52	33	-22
-6	2	1	66	67	16
-5	2	1	382	380	6
-4	2	1	421	405	5
-3	2	1	315	316	5
0	2	1	22	10	-8
1	2	1	97	108	5
2	2	1	332	337	4
3	2	1	412	379	5
4	2	1	136	101	7
5	2	1	452	432	6
6	2	1	52	56	-21
7	2	1	148	134	11
8	2	1	29	23	-42
9	2	1	45	54	-33
10	2	1	18	28	-77
-10	3	1	64	48	-23
-9	3	1	74	84	19
-8	3	1	17	29	-73
-7	3	1	81	85	15
-6	3	1	353	351	7
-5	3	1	63	72	14
-4	3	1	125	125	7
-3	3	1	334	328	5
-2	3	1	662	686	3
0	3	1	130	105	6
1	3	1	160	147	5
2	3	1	24	73	-27
3	3	1	232	218	6
4	3	1	153	134	7
5	3	1	112	57	10
6	3	1	34	5	-31
7	3	1	34	18	-35
8	3	1	48	56	-26
9	3	1	164	169	12
10	3	1	19	42	-79
-10	4	1	19	44	-80
-9	4	1	29	49	-45
-8	4	1	81	79	17
-7	4	1	16	20	-68
-6	4	1	241	241	8
-5	4	1	142	142	8
-4	4	1	205	197	6
-3	4	1	191	193	6
1	4	1	119	117	7
2	4	1	248	229	5
3	4	1	212	247	6
4	4	1	271	303	6
5	4	1	335	324	7
6	4	1	235	236	8
7	4	1	52	41	-24
8	4	1	17	2	-71
9	4	1	18	12	-76
10	4	1	34	24	-44
-10	5	1	80	78	20
-9	5	1	17	19	-73
-8	5	1	157	158	12
-7	5	1	31	37	-38
-6	5	1	275	288	8
-5	5	1	75	74	13
-4	5	1	55	49	15
-3	5	1	50	49	14
-2	5	1	62	57	11
3	5	1	60	68	13
4	5	1	30	36	-27
5	5	1	76	60	14
6	5	1	16	21	-68
7	5	1	161	156	11
8	5	1	43	38	-30
9	5	1	18	36	-77
10	5	1	63	30	-25
-10	6	1	19	6	-78
-9	6	1	75	61	19
-8	6	1	37	23	-35
-7	6	1	28	28	-42
-6	6	1	153	173	10
-5	6	1	159	164	9
-4	6	1	154	134	8
-2	6	1	80	103	10
-1	6	1	94	77	8
1	6	1	66	66	11
2	6	1	163	127	7
3	6	1	303	304	6
4	6	1	97	88	11
5	6	1	54	49	19
6	6	1	131	129	11
7	6	1	187	191	10
8	6	1	44	3	-28
9	6	1	19	45	-79

Table 58. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-10	7	1	19	4	-79
-9	7	1	71	68	21
-8	7	1	85	109	18
-7	7	1	17	9	-70
-6	7	1	128	158	12
-5	7	1	15	25	-64
-4	7	1	41	24	-21
-3	7	1	303	318	7
-2	7	1	175	146	7
-1	7	1	67	68	11
2	7	1	92	65	10
3	7	1	29	76	-30
4	7	1	15	17	-63
5	7	1	50	33	-22
6	7	1	115	135	12
7	7	1	139	146	12
8	7	1	18	10	-74
9	7	1	49	62	-30
-10	8	1	31	26	-49
-9	8	1	18	13	-76
-8	8	1	29	54	-46
-7	8	1	17	18	-71
-6	8	1	132	144	12
-5	8	1	37	56	-30
-4	8	1	34	15	-27
-2	8	1	226	220	7
-1	8	1	37	44	-20
0	8	1	206	212	9
1	8	1	139	128	8
2	8	1	42	29	-19
3	8	1	129	132	9
4	8	1	309	323	8
5	8	1	68	56	17
6	8	1	24	13	-48
7	8	1	178	181	11
8	8	1	18	41	-76
9	8	1	19	11	-78
-9	9	1	18	10	-78
-8	9	1	30	20	-44
-7	9	1	16	7	-69
-6	9	1	201	204	11
-5	9	1	113	117	12
-4	9	1	15	15	-64
-3	9	1	15	32	-63
-2	9	1	79	71	13
-1	9	1	51	54	17
1	9	1	48	49	-19
2	9	1	74	78	14
3	9	1	111	107	11
4	9	1	216	231	9
5	9	1	68	54	18
6	9	1	17	1	-70
7	9	1	18	31	-75
8	9	1	18	10	-76
9	9	1	19	11	-78
-9	10	1	44	30	-33
-8	10	1	35	12	-38
-7	10	1	50	46	-26
-6	10	1	197	188	11
-5	10	1	36	16	-32
-4	10	1	16	10	-66
-3	10	1	63	74	18
-2	10	1	36	52	-28
-1	10	1	94	87	12
0	10	1	21	14	-33
1	10	1	112	116	11
2	10	1	15	12	-63
3	10	1	83	85	15
4	10	1	318	308	9
5	10	1	62	63	19
6	10	1	17	21	-72
7	10	1	18	7	-74
8	10	1	35	17	-41
-8	11	1	45	23	-32
-7	11	1	17	12	-72
-6	11	1	85	91	17
-5	11	1	17	12	-70
-4	11	1	73	77	17
-3	11	1	34	11	-32
-2	11	1	71	72	16
-1	11	1	119	132	12
0	11	1	108	130	9
1	11	1	197	197	9
2	11	1	33	43	-33
3	11	1	16	13	-68
4	11	1	86	71	16
5	11	1	45	27	-26
6	11	1	17	4	-72
7	11	1	37	65	-41
8	11	1	38	29	-39
-8	12	1	40	10	-36
-7	12	1	18	9	-74

Table 58. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-6	12	1	42	30	-30
-5	12	1	42	50	-30
-4	12	1	30	62	-40
-3	12	1	228	236	10
-2	12	1	16	6	-67
-1	12	1	30	28	-35
0	12	1	62	71	13
1	12	1	40	32	-26
2	12	1	57	37	-20
3	12	1	17	7	-70
4	12	1	58	55	-21
5	12	1	35	34	-36
6	12	1	45	26	-30
7	12	1	52	55	-28
-7	13	1	19	40	-80
-6	13	1	30	9	-43
-5	13	1	43	9	-28
-4	13	1	57	51	-21
-3	13	1	16	6	-68
-2	13	1	72	74	18
-1	13	1	24	18	-46
0	13	1	36	15	-27
1	13	1	147	156	11
2	13	1	118	118	13
3	13	1	17	35	-72
4	13	1	49	63	-29
5	13	1	62	74	-23
6	13	1	18	31	-77
7	13	1	62	61	-25
-7	14	1	34	34	-45
-6	14	1	28	10	-48
-5	14	1	33	32	-40
-4	14	1	74	56	19
-3	14	1	93	86	15
-2	14	1	24	8	-48
-1	14	1	73	84	20
0	14	1	24	12	-37
1	14	1	61	37	19
2	14	1	36	30	-35
3	14	1	38	11	-31
4	14	1	66	57	21
5	14	1	39	27	-34
6	14	1	46	33	-31
-6	15	1	50	44	-30
-5	15	1	27	23	-52
-4	15	1	40	19	-32
-3	15	1	18	35	-74
-2	15	1	60	36	-22
-1	15	1	88	82	18
0	15	1	51	70	-19
1	15	1	17	10	-72
2	15	1	82	67	18
3	15	1	52	43	-26
4	15	1	45	1	-29
5	15	1	68	36	21
-5	16	1	55	44	-29
-4	16	1	32	2	-43
-3	16	1	18	4	-75
-2	16	1	18	21	-74
-1	16	1	73	73	21
0	16	1	38	15	-29
1	16	1	42	27	-32
2	16	1	30	40	-46
3	16	1	36	6	-37
4	16	1	19	27	-78
-4	17	1	41	36	-37
-3	17	1	19	9	-78
-2	17	1	18	14	-75
-1	17	1	67	56	22
0	17	1	18	9	-53
1	17	1	18	3	-77
2	17	1	18	23	-77
3	17	1	19	19	-78
-1	18	1	38	13	-37
0	18	1	30	9	-37
-10	0	2	32	19	-42
-8	0	2	68	89	19
-6	0	2	359	374	7
-4	0	2	38	15	-18
0	0	2	126	86	8
2	0	2	243	193	5
4	0	2	526	427	6
6	0	2	103	99	12
8	0	2	201	193	11
10	0	2	19	13	-79
-11	1	2	66	40	23
-10	1	2	18	14	-74
-9	1	2	48	62	-30
-8	1	2	17	36	-72
-7	1	2	78	73	15
-6	1	2	226	217	8
-5	1	2	187	173	7

Table 58. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-4	1	2	100	97	9
-1	1	2	42	51	8
0	1	2	162	170	3
1	1	2	261	155	4
2	1	2	134	161	6
3	1	2	78	74	10
4	1	2	776	713	6
5	1	2	119	133	10
6	1	2	16	46	-68
7	1	2	65	40	19
8	1	2	169	179	11
9	1	2	18	14	-76
10	1	2	50	9	-30
-11	2	2	19	41	-80
-10	2	2	18	32	-74
-9	2	2	207	206	11
-8	2	2	93	88	15
-7	2	2	101	105	13
-6	2	2	194	185	8
-5	2	2	178	153	7
-4	2	2	343	352	6
-1	2	2	163	179	4
1	2	2	1489	1399	4
2	2	2	728	726	4
3	2	2	460	432	5
4	2	2	377	393	6
5	2	2	15	20	-63
6	2	2	34	9	-32
7	2	2	40	27	-29
8	2	2	132	136	13
9	2	2	62	78	-24
10	2	2	19	37	-81
-11	3	2	19	45	-80
-10	3	2	18	51	-75
-9	3	2	123	138	14
-8	3	2	43	20	-27
-7	3	2	136	137	11
-6	3	2	193	188	8
-5	3	2	165	164	7
-4	3	2	368	356	6
-1	3	2	11	32	-47
0	3	2	181	197	4
1	3	2	194	203	5
2	3	2	303	259	5
3	3	2	132	125	7
4	3	2	132	122	9
5	3	2	149	162	9
6	3	2	215	240	9
7	3	2	71	63	19
8	3	2	18	25	-75
9	3	2	19	68	-79
10	3	2	19	0	-81
-11	4	2	38	25	-41
-10	4	2	54	1	-25
-9	4	2	93	108	17
-8	4	2	62	56	20
-7	4	2	57	84	-22
-6	4	2	187	204	9
-5	4	2	207	199	7
-4	4	2	217	204	7
-1	4	2	51	41	12
0	4	2	28	37	-19
2	4	2	379	369	5
3	4	2	25	37	-29
4	4	2	205	212	7
5	4	2	22	17	-45
6	4	2	38	20	-29
7	4	2	31	1	-36
8	4	2	18	21	-76
9	4	2	44	18	-32
-10	5	2	30	22	-47
-9	5	2	98	96	16
-8	5	2	32	3	-37
-7	5	2	105	107	14
-6	5	2	173	190	10
-5	5	2	24	17	-36
-3	5	2	247	259	6
-2	5	2	64	21	11
0	5	2	56	54	9
1	5	2	135	127	7
2	5	2	44	93	-16
3	5	2	91	77	10
4	5	2	185	180	8
5	5	2	38	20	-26
6	5	2	245	223	9
7	5	2	36	17	-33
8	5	2	83	85	19
9	5	2	31	12	-45
-10	6	2	26	17	-54
-9	6	2	17	23	-73
-8	6	2	49	20	-24
-7	6	2	310	301	9

Table 58. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-6	6	2	244	235	8
-5	6	2	15	21	-62
-4	6	2	45	12	-19
-3	6	2	77	61	11
-2	6	2	56	54	13
0	6	2	141	163	5
1	6	2	103	107	8
2	6	2	88	81	10
3	6	2	173	186	8
4	6	2	179	163	8
5	6	2	187	181	9
6	6	2	55	80	-24
7	6	2	17	1	-70
8	6	2	68	84	22
9	6	2	28	55	-55
-10	7	2	41	36	-35
-9	7	2	18	2	-74
-8	7	2	34	16	-35
-7	7	2	29	24	-42
-6	7	2	16	20	-69
-5	7	2	53	37	-19
-4	7	2	14	13	-60
-3	7	2	79	79	12
1	7	2	62	55	13
2	7	2	79	81	11
3	7	2	232	229	7
4	7	2	70	63	16
5	7	2	60	48	19
6	7	2	90	89	16
7	7	2	17	17	-70
8	7	2	18	3	-75
9	7	2	41	35	-39
-10	8	2	19	0	-78
-9	8	2	34	35	-42
-8	8	2	101	81	15
-7	8	2	166	179	11
-6	8	2	30	27	-38
-5	8	2	37	38	-28
-4	8	2	129	138	10
-3	8	2	40	1	-22
-2	8	2	82	77	12
0	8	2	207	214	5
1	8	2	128	126	9
2	8	2	34	20	-25
3	8	2	270	301	8
4	8	2	15	13	-64
5	8	2	40	28	-28
6	8	2	53	62	-25
7	8	2	17	16	-73
8	8	2	18	20	-76
9	8	2	40	39	-38
-9	9	2	18	8	-75
-8	9	2	18	14	-75
-7	9	2	75	91	18
-6	9	2	37	42	-34
-5	9	2	16	3	-67
-4	9	2	367	381	8
-3	9	2	15	14	-62
-2	9	2	62	70	15
-1	9	2	243	247	8
0	9	2	193	208	12
1	9	2	78	82	13
2	9	2	54	48	18
3	9	2	67	61	17
4	9	2	51	20	-23
5	9	2	24	9	-47
6	9	2	270	269	10
7	9	2	17	7	-72
8	9	2	64	50	-23
-9	10	2	54	55	-27
-8	10	2	62	50	-24
-7	10	2	34	32	-37
-6	10	2	17	12	-71
-5	10	2	56	54	-21
-4	10	2	164	171	10
-3	10	2	34	35	-29
-2	10	2	191	188	9
-1	10	2	157	148	9
0	10	2	185	182	8
1	10	2	52	58	-19
2	10	2	259	277	8
3	10	2	125	135	12
4	10	2	81	71	16
5	10	2	28	47	-42
6	10	2	17	7	-73
7	10	2	30	33	-47
8	10	2	30	3	-47
-9	11	2	37	13	-43
-8	11	2	45	39	-32
-7	11	2	18	21	-74
-6	11	2	32	8	-38
-5	11	2	16	11	-68

Table 58. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-4	11	2	166	164	11
-3	11	2	16	4	-68
-2	11	2	35	39	-30
-1	11	2	74	80	16
0	11	2	26	18	-27
1	11	2	86	79	14
2	11	2	23	30	-47
3	11	2	87	93	16
4	11	2	58	48	-21
5	11	2	33	1	-37
6	11	2	125	139	15
7	11	2	18	8	-77
-8	12	2	18	19	-76
-7	12	2	59	67	-25
-6	12	2	48	55	-28
-5	12	2	17	13	-70
-4	12	2	16	10	-69
-3	12	2	27	14	-44
-2	12	2	16	16	-68
-1	12	2	176	180	10
0	12	2	78	76	12
1	12	2	16	41	-69
2	12	2	49	23	-23
3	12	2	203	203	10
4	12	2	24	15	-49
5	12	2	59	12	-21
6	12	2	18	25	-77
7	12	2	18	4	-77
-8	13	2	38	40	-42
-7	13	2	18	21	-76
-6	13	2	18	36	-75
-5	13	2	39	13	-32
-4	13	2	57	52	-22
-3	13	2	17	16	-70
-2	13	2	157	145	12
-1	13	2	133	133	13
0	13	2	89	88	11
1	13	2	16	26	-68
2	13	2	52	53	-23
3	13	2	71	83	20
4	13	2	76	75	19
5	13	2	28	7	-47
6	13	2	19	24	-78
-7	14	2	34	22	-45
-6	14	2	19	53	-79
-5	14	2	62	67	-24
-4	14	2	39	19	-31
-3	14	2	36	54	-35
-2	14	2	36	15	-32
-1	14	2	50	45	-24
0	14	2	17	3	-49
1	14	2	79	77	18
2	14	2	43	18	-29
3	14	2	17	3	-72
4	14	2	48	72	-32
5	14	2	18	2	-74
6	14	2	51	7	-29
-6	15	2	18	26	-77
-5	15	2	18	9	-76
-4	15	2	31	46	-43
-3	15	2	74	50	18
-2	15	2	17	20	-71
-1	15	2	46	26	-27
0	15	2	17	25	-51
1	15	2	17	10	-73
2	15	2	29	2	-43
3	15	2	59	46	-23
4	15	2	18	4	-75
5	15	2	35	22	-42
-5	16	2	49	38	-30
-4	16	2	40	27	-35
-3	16	2	18	10	-74
-2	16	2	62	43	22
-1	16	2	18	26	-75
0	16	2	24	6	-41
1	16	2	103	119	18
2	16	2	18	6	-76
3	16	2	41	1	-34
4	16	2	60	38	-26
-4	17	2	19	1	-78
-3	17	2	18	31	-77
-2	17	2	32	46	-46
-1	17	2	18	11	-75
0	17	2	18	9	-53
1	17	2	18	17	-77
2	17	2	19	19	-78
-10	0	3	157	161	13
-8	0	3	35	3	-34
-6	0	3	95	79	11
0	0	3	1085	1102	14
2	0	3	107	72	7
4	0	3	204	180	7

Table 58. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
6	0	3	212	195	9
8	0	3	122	133	14
-11	1	3	18	13	-76
-10	1	3	49	39	-29
-9	1	3	60	39	-21
-8	1	3	84	65	16
-7	1	3	275	272	8
-6	1	3	63	40	15
-5	1	3	317	342	6
-2	1	3	80	74	9
0	1	3	1093	975	16
1	1	3	200	217	5
2	1	3	17	28	-35
3	1	3	313	329	6
4	1	3	157	157	8
5	1	3	109	85	11
6	1	3	76	68	17
7	1	3	18	34	-75
8	1	3	45	36	-30
9	1	3	18	23	-75
-11	2	3	37	16	-41
-10	2	3	56	61	-27
-9	2	3	17	36	-73
-8	2	3	45	31	-28
-7	2	3	28	29	-42
-6	2	3	22	8	-41
-5	2	3	171	172	8
-3	2	3	137	154	7
-1	2	3	42	59	14
0	2	3	555	457	1
1	2	3	34	42	-18
2	2	3	131	119	6
3	2	3	262	198	6
4	2	3	129	134	9
5	2	3	127	106	10
6	2	3	45	40	-26
7	2	3	214	232	10
8	2	3	18	23	-76
9	2	3	19	10	-78
-11	3	3	19	10	-78
-10	3	3	60	43	-24
-9	3	3	61	61	-23
-8	3	3	58	54	-22
-7	3	3	459	458	8
-6	3	3	49	31	-20
-5	3	3	14	25	-60
-3	3	3	141	158	7
-1	3	3	12	25	-50
0	3	3	86	66	10
1	3	3	75	59	9
2	3	3	437	455	5
3	3	3	946	872	1
4	3	3	85	98	12
5	3	3	50	77	-22
6	3	3	17	32	-70
7	3	3	51	58	-27
8	3	3	61	53	-22
9	3	3	57	31	-26
-11	4	3	37	31	-41
-10	4	3	18	41	-77
-9	4	3	28	36	-45
-8	4	3	52	68	-25
-7	4	3	69	92	18
-6	4	3	74	61	14
-5	4	3	263	271	7
-4	4	3	164	214	7
-1	4	3	12	17	-50
1	4	3	85	36	8
2	4	3	83	83	10
3	4	3	92	50	11
4	4	3	74	84	13
5	4	3	75	67	15
6	4	3	127	135	12
7	4	3	158	160	11
8	4	3	111	96	15
9	4	3	19	17	-80
-11	5	3	43	26	-36
-10	5	3	38	33	-36
-9	5	3	39	46	-33
-8	5	3	153	165	12
-7	5	3	141	135	11
-6	5	3	58	53	19
-5	5	3	307	325	7
-4	5	3	191	228	7
-3	5	3	170	106	7
-1	5	3	73	71	10
1	5	3	43	45	-15
2	5	3	133	149	8
3	5	3	118	112	9
4	5	3	15	6	-63
5	5	3	82	68	14
6	5	3	27	25	-43

Table 58. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
7	5	3	85	90	17
8	5	3	18	10	-77
9	5	3	35	29	-43
-10	6	3	47	52	-31
-9	6	3	103	100	17
-8	6	3	75	75	18
-7	6	3	143	142	11
-6	6	3	74	75	16
-5	6	3	197	196	8
-4	6	3	150	119	8
-1	6	3	47	23	15
1	6	3	147	188	7
2	6	3	39	56	-21
3	6	3	72	35	14
4	6	3	15	68	-65
5	6	3	309	328	8
6	6	3	96	94	14
7	6	3	17	5	-72
8	6	3	70	70	22
9	6	3	38	34	-40
-10	7	3	36	20	-40
-9	7	3	73	94	22
-8	7	3	32	35	-38
-7	7	3	82	79	16
-6	7	3	34	13	-32
-5	7	3	289	303	8
-4	7	3	97	97	11
-2	7	3	13	3	-56
-1	7	3	120	112	8
0	7	3	157	163	6
2	7	3	14	4	-61
3	7	3	157	166	9
4	7	3	152	165	10
5	7	3	165	178	11
6	7	3	16	8	-69
7	7	3	17	19	-73
8	7	3	48	59	-31
-10	8	3	19	18	-78
-9	8	3	66	52	22
-8	8	3	98	95	15
-7	8	3	17	16	-70
-6	8	3	26	23	-42
-5	8	3	163	166	10
-4	8	3	55	53	19
-3	8	3	41	47	-23
-1	8	3	80	78	12
0	8	3	51	57	12
1	8	3	209	197	8
2	8	3	50	8	-19
3	8	3	60	68	18
4	8	3	95	87	14
5	8	3	189	207	10
6	8	3	17	7	-71
7	8	3	18	3	-75
8	8	3	58	50	-27
-10	9	3	32	47	-50
-9	9	3	44	1	-33
-8	9	3	28	32	-47
-7	9	3	33	10	-37
-6	9	3	45	65	-27
-5	9	3	79	76	15
-4	9	3	52	48	-21
-3	9	3	156	155	10
-2	9	3	15	20	-63
-1	9	3	110	117	11
0	9	3	43	39	15
1	9	3	74	82	15
2	9	3	354	368	8
3	9	3	28	46	-40
4	9	3	16	34	-69
5	9	3	54	30	-23
6	9	3	17	2	-71
7	9	3	18	13	-75
8	9	3	52	59	-30
-9	10	3	19	13	-78
-8	10	3	18	19	-74
-7	10	3	17	14	-71
-6	10	3	17	7	-70
-5	10	3	60	45	20
-4	10	3	16	22	-67
-3	10	3	23	17	-44
-1	10	3	58	65	19
0	10	3	58	58	13
1	10	3	70	60	16
2	10	3	31	28	-35
3	10	3	16	20	-68
4	10	3	16	22	-68
5	10	3	51	37	-26
6	10	3	18	3	-74
7	10	3	18	30	-76
-9	11	3	55	46	-28
-8	11	3	18	10	-75

Table 58. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-7	11	3	68	70	22
-6	11	3	91	85	16
-5	11	3	164	165	11
-4	11	3	16	29	-69
-3	11	3	38	26	-28
-2	11	3	68	76	18
-1	11	3	64	59	17
0	11	3	55	56	15
1	11	3	194	189	10
2	11	3	179	178	10
3	11	3	16	1	-68
4	11	3	60	58	21
5	11	3	129	133	14
6	11	3	50	23	-27
7	11	3	19	7	-78
-8	12	3	18	5	-75
-7	12	3	35	12	-38
-6	12	3	35	37	-37
-5	12	3	86	78	16
-4	12	3	94	105	16
-3	12	3	17	25	-70
-2	12	3	96	103	14
-1	12	3	43	61	-28
0	12	3	133	139	8
1	12	3	73	60	17
2	12	3	123	111	13
3	12	3	17	2	-70
4	12	3	17	3	-70
5	12	3	116	115	15
6	12	3	49	37	-29
-8	13	3	48	4	-32
-7	13	3	18	7	-77
-6	13	3	43	32	-32
-5	13	3	103	99	15
-4	13	3	17	0	-71
-3	13	3	81	60	17
-2	13	3	17	36	-70
-1	13	3	16	25	-68
0	13	3	91	92	12
1	13	3	64	69	20
2	13	3	83	59	16
3	13	3	35	17	-34
4	13	3	40	21	-31
5	13	3	67	47	21
6	13	3	18	1	-77
-7	14	3	46	23	-31
-6	14	3	18	3	-75
-5	14	3	43	20	-31
-4	14	3	44	47	-31
-3	14	3	61	48	21
-2	14	3	96	87	16
-1	14	3	45	1	-26
0	14	3	79	72	19
1	14	3	66	58	21
2	14	3	58	38	-23
3	14	3	18	44	-74
4	14	3	17	22	-73
5	14	3	64	48	-24
-6	15	3	19	7	-79
-5	15	3	18	9	-74
-4	15	3	18	40	-75
-3	15	3	58	49	-23
-2	15	3	18	26	-74
-1	15	3	40	38	-34
0	15	3	63	48	16
1	15	3	17	3	-72
2	15	3	37	9	-36
3	15	3	75	75	21
4	15	3	18	18	-76
-5	16	3	18	10	-76
-4	16	3	18	11	-76
-3	16	3	75	55	20
-2	16	3	44	33	-33
-1	16	3	18	7	-74
0	16	3	18	4	-53
1	16	3	18	30	-76
2	16	3	52	8	-26
3	16	3	19	13	-79
-3	17	3	35	13	-40
-2	17	3	19	17	-78
-1	17	3	18	8	-76
0	17	3	54	20	-22
1	17	3	29	1	-47
2	17	3	19	11	-78
-10	0	4	81	76	19
-8	0	4	326	325	9
-6	0	4	246	218	8
-2	0	4	199	216	6
0	0	4	590	437	16
2	0	4	528	497	5
4	0	4	135	186	9
6	0	4	121	129	12

Table 58. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
8	0	4	44	18	-30	1	3	4	205	192	6
-11	1	4	32	36	-45	2	3	4	78	58	11
-10	1	4	17	2	-74	3	3	4	47	10	-18
-9	1	4	53	54	-24	4	3	4	79	81	14
-8	1	4	324	330	9	5	3	4	248	231	8
-7	1	4	48	43	-23	6	3	4	54	44	-23
-6	1	4	65	73	16	7	3	4	66	75	23
-4	1	4	158	175	7	8	3	4	28	5	-50
0	1	4	390	393	4	9	3	4	86	91	20
1	1	4	81	54	9	-11	4	4	53	24	-26
2	1	4	171	144	7	-10	4	4	46	22	-30
3	1	4	60	53	15	-9	4	4	45	41	-28
4	1	4	22	9	-43	-8	4	4	135	136	12
5	1	4	164	182	10	-7	4	4	50	23	-22
6	1	4	177	176	10	-6	4	4	256	260	8
7	1	4	78	74	19	-4	4	4	212	193	7
8	1	4	50	43	-29	-2	4	4	227	253	6
9	1	4	62	63	-27	-1	4	4	218	165	6
-11	2	4	19	0	-79	0	4	4	174	191	5
-10	2	4	73	51	20	1	4	4	367	340	6
-9	2	4	17	29	-72	2	4	4	641	657	6
-8	2	4	116	104	13	3	4	4	194	186	7
-7	2	4	132	123	11	4	4	4	224	239	8
-6	2	4	142	129	9	5	4	4	140	158	11
-4	2	4	167	146	7	6	4	4	62	70	21
-3	2	4	28	38	-23	7	4	4	93	107	16
-1	2	4	182	175	6	8	4	4	40	8	-33
0	2	4	157	97	4	-11	5	4	46	13	-33
1	2	4	12	28	-51	-10	5	4	119	103	15
2	2	4	234	269	6	-9	5	4	42	16	-29
3	2	4	35	32	-23	-8	5	4	88	82	16
4	2	4	74	108	14	-7	5	4	31	25	-37
5	2	4	273	240	8	-6	5	4	111	106	11
6	2	4	17	19	-72	-5	5	4	164	130	9
7	2	4	18	21	-74	-4	5	4	34	36	-24
8	2	4	18	28	-74	-2	5	4	114	89	8
9	2	4	48	36	-34	0	5	4	146	137	7
-11	3	4	19	46	-79	1	5	4	268	270	6
-10	3	4	92	103	18	2	5	4	262	245	7
-9	3	4	31	41	-41	3	5	4	67	67	15
-8	3	4	148	147	12	4	5	4	126	132	10
-7	3	4	16	3	-68	5	5	4	60	69	20
-6	3	4	92	97	13	6	5	4	43	29	-29
-5	3	4	78	77	13	7	5	4	105	115	15
-2	3	4	59	38	11	8	5	4	53	33	-28
0	3	4	392	453	4	-11	6	4	28	6	-54

Table 58. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-10	6	4	19	31	-79
-9	6	4	18	15	-74
-8	6	4	93	98	16
-7	6	4	73	73	18
-6	6	4	37	48	-29
-5	6	4	15	4	-63
-4	6	4	57	28	16
-2	6	4	51	48	16
-1	6	4	53	24	14
0	6	4	34	34	-21
1	6	4	164	166	8
2	6	4	500	430	6
3	6	4	142	153	9
4	6	4	106	91	12
5	6	4	16	33	-68
6	6	4	25	20	-45
7	6	4	18	29	-76
8	6	4	36	12	-39
-10	7	4	42	42	-34
-9	7	4	38	9	-36
-8	7	4	42	52	-30
-7	7	4	17	2	-70
-6	7	4	105	102	13
-5	7	4	40	72	-26
-4	7	4	287	279	8
-2	7	4	37	31	-22
-1	7	4	108	108	10
0	7	4	14	28	-40
1	7	4	197	215	8
2	7	4	33	26	-29
3	7	4	15	9	-64
4	7	4	16	0	-69
5	7	4	17	60	-72
6	7	4	17	30	-73
7	7	4	158	172	13
8	7	4	31	19	-47
-10	8	4	19	10	-79
-9	8	4	30	20	-42
-8	8	4	66	46	19
-7	8	4	101	102	14
-6	8	4	164	179	11
-5	8	4	30	28	-35
-4	8	4	78	60	15
-3	8	4	206	207	8
-2	8	4	46	22	-19
-1	8	4	81	55	12
0	8	4	50	76	15
1	8	4	324	345	7
2	8	4	33	26	-30
3	8	4	232	248	9
4	8	4	198	188	10
5	8	4	17	18	-70
6	8	4	17	8	-73
7	8	4	18	15	-76
8	8	4	19	22	-79
-10	9	4	70	86	-26
-9	9	4	18	44	-77
-8	9	4	17	4	-73
-7	9	4	47	30	-26
-6	9	4	56	53	-22
-5	9	4	16	23	-67
-4	9	4	15	14	-65
-3	9	4	126	139	11
-2	9	4	35	7	-28
-1	9	4	47	43	-21
0	9	4	310	334	8
1	9	4	16	10	-66
2	9	4	23	4	-44
3	9	4	123	123	12
4	9	4	68	61	19
5	9	4	16	23	-69
6	9	4	18	17	-74
7	9	4	19	42	-78
-9	10	4	19	16	-78
-8	10	4	43	49	-34
-7	10	4	36	7	-35
-6	10	4	196	207	11
-5	10	4	74	49	17
-4	10	4	16	20	-67
-3	10	4	71	87	16
-2	10	4	34	38	-30
-1	10	4	54	44	-20
0	10	4	193	205	14
1	10	4	36	37	-30
2	10	4	61	61	19
3	10	4	16	8	-68
4	10	4	212	221	10
5	10	4	44	35	-29
6	10	4	18	21	-75
7	10	4	51	13	-29
-9	11	4	19	27	-80
-8	11	4	36	35	-37

Table 58. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-7	11	4	29	6	-42
-6	11	4	17	10	-71
-5	11	4	83	77	16
-4	11	4	87	80	15
-3	11	4	179	174	10
-2	11	4	28	22	-40
-1	11	4	43	50	-28
0	11	4	251	238	10
1	11	4	140	139	12
2	11	4	33	11	-33
3	11	4	56	61	-22
4	11	4	70	84	21
5	11	4	26	11	-49
6	11	4	18	22	-76
-8	12	4	38	29	-38
-7	12	4	26	43	-54
-6	12	4	17	3	-73
-5	12	4	17	43	-72
-4	12	4	100	96	15
-3	12	4	184	163	11
-2	12	4	44	48	-28
-1	12	4	61	31	20
0	12	4	90	87	15
1	12	4	63	77	20
2	12	4	85	59	16
3	12	4	76	92	19
4	12	4	17	14	-72
5	12	4	58	42	-23
6	12	4	19	37	-79
-8	13	4	48	49	-34
-7	13	4	59	42	-24
-6	13	4	51	11	-26
-5	13	4	18	44	-74
-4	13	4	29	7	-41
-3	13	4	113	126	15
-2	13	4	32	31	-37
-1	13	4	46	26	-26
0	13	4	37	28	-25
1	13	4	38	16	-31
2	13	4	18	29	-74
3	13	4	17	9	-73
4	13	4	18	28	-75
5	13	4	18	43	-77
-7	14	4	45	9	-32
-6	14	4	56	33	-25
-5	14	4	36	27	-37
-4	14	4	18	38	-75
-3	14	4	64	58	21
-2	14	4	32	8	-37
-1	14	4	58	56	-23
0	14	4	101	81	12
1	14	4	33	9	-37
2	14	4	108	92	15
3	14	4	38	14	-34
4	14	4	63	57	-24
5	14	4	19	10	-78
-6	15	4	18	7	-76
-5	15	4	18	6	-77
-4	15	4	18	25	-77
-3	15	4	18	12	-75
-2	15	4	18	23	-75
-1	15	4	97	106	17
0	15	4	35	23	-32
1	15	4	17	23	-73
2	15	4	44	27	-31
3	15	4	40	24	-34
4	15	4	33	6	-43
-5	16	4	96	63	18
-4	16	4	60	34	-24
-3	16	4	29	16	-46
-2	16	4	46	26	-30
-1	16	4	18	12	-76
0	16	4	18	10	-52
1	16	4	35	33	-41
2	16	4	19	1	-78
-3	17	4	18	2	-77
-2	17	4	18	14	-77
-1	17	4	49	58	-34
0	17	4	36	15	-34
1	17	4	19	11	-79
-10	0	5	35	5	-38
-8	0	5	92	90	16
-6	0	5	92	96	13
-4	0	5	67	98	13
0	0	5	463	410	4
2	0	5	28	30	-31
4	0	5	146	40	11
6	0	5	24	27	-50
8	0	5	132	138	15
-11	1	5	31	3	-46
-10	1	5	41	25	-32
-9	1	5	35	16	-38

Table 58. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
-8	1	5	114	114	13	4	3	5	51	49	-23
-7	1	5	81	87	15	5	3	5	31	13	-38
-5	1	5	191	199	8	6	3	5	82	91	17
-2	1	5	212	228	6	7	3	5	42	6	-31
-1	1	5	254	335	6	8	3	5	46	37	-31
0	1	5	37	24	-14	-11	4	5	38	16	-41
1	1	5	187	168	7	-10	4	5	46	20	-31
2	1	5	14	0	-59	-9	4	5	147	146	13
3	1	5	108	105	10	-8	4	5	132	120	12
4	1	5	535	527	7	-7	4	5	160	171	10
5	1	5	84	92	15	-6	4	5	24	38	-43
6	1	5	36	15	-33	-5	4	5	168	146	9
7	1	5	55	65	-25	-4	4	5	260	251	7
8	1	5	19	20	-79	-3	4	5	198	193	7
-11	2	5	96	84	18	-2	4	5	276	270	6
-10	2	5	18	15	-75	-1	4	5	40	31	-18
-9	2	5	187	181	11	0	4	5	159	157	8
-8	2	5	35	52	-36	1	4	5	372	354	6
-7	2	5	37	62	-30	2	4	5	68	76	14
-6	2	5	189	206	9	3	4	5	15	2	-63
-5	2	5	156	138	9	4	4	5	47	39	-25
-4	2	5	134	117	8	5	4	5	65	55	19
-1	2	5	273	266	6	6	4	5	158	170	12
0	2	5	526	530	4	7	4	5	18	62	-77
1	2	5	576	572	5	8	4	5	56	46	-26
2	2	5	69	84	12	-11	5	5	78	64	22
3	2	5	32	7	-28	-10	5	5	18	12	-76
4	2	5	87	83	15	-9	5	5	30	58	-43
5	2	5	42	35	-29	-8	5	5	62	73	-22
6	2	5	130	127	12	-7	5	5	54	58	-22
7	2	5	78	81	19	-6	5	5	291	287	8
8	2	5	75	72	21	-5	5	5	188	177	9
-11	3	5	38	33	-40	-4	5	5	158	153	8
-10	3	5	39	8	-34	-2	5	5	131	95	8
-9	3	5	18	36	-74	-1	5	5	115	113	9
-8	3	5	50	27	-23	0	5	5	38	32	-21
-7	3	5	56	49	-22	1	5	5	83	114	12
-6	3	5	15	4	-64	2	5	5	109	96	10
-5	3	5	273	290	7	3	5	5	116	119	11
-4	3	5	196	207	7	4	5	5	246	248	8
-2	3	5	77	82	10	5	5	5	40	45	-29
-1	3	5	128	155	7	6	5	5	156	162	12
0	3	5	122	106	6	7	5	5	18	14	-75
1	3	5	686	617	6	8	5	5	19	14	-80
2	3	5	214	264	7	-11	6	5	87	81	20
3	3	5	75	81	13	-10	6	5	18	49	-77

Table 58. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-9	6	5	18	11	-74
-8	6	5	41	29	-30
-7	6	5	128	123	12
-6	6	5	101	124	13
-5	6	5	44	38	-23
-4	6	5	295	303	8
-3	6	5	76	71	13
-2	6	5	146	151	8
0	6	5	14	9	-41
1	6	5	179	176	8
2	6	5	80	89	13
3	6	5	49	78	-22
4	6	5	81	91	16
5	6	5	16	20	-69
6	6	5	46	39	-31
7	6	5	18	43	-75
8	6	5	30	42	-50
-10	7	5	19	37	-79
-9	7	5	49	52	-30
-8	7	5	17	8	-70
-7	7	5	136	140	12
-6	7	5	40	12	-29
-5	7	5	59	85	19
-4	7	5	207	206	9
-3	7	5	86	76	12
-2	7	5	92	97	11
-1	7	5	116	136	10
0	7	5	249	243	6
1	7	5	72	104	14
2	7	5	15	14	-65
3	7	5	229	240	8
4	7	5	99	111	14
5	7	5	17	46	-71
6	7	5	18	17	-77
7	7	5	18	2	-77
-10	8	5	18	28	-78
-9	8	5	18	34	-78
-8	8	5	46	47	-29
-7	8	5	17	10	-71
-6	8	5	71	40	18
-5	8	5	39	39	-28
-4	8	5	16	36	-65
-3	8	5	67	78	17
-2	8	5	15	25	-63
0	8	5	51	68	17
1	8	5	43	40	-24
2	8	5	96	84	13
3	8	5	16	29	-68
4	8	5	24	11	-48
5	8	5	17	19	-70
6	8	5	83	91	19
7	8	5	18	23	-77
-10	9	5	19	13	-79
-9	9	5	18	7	-77
-8	9	5	55	70	-27
-7	9	5	58	55	-22
-6	9	5	133	137	13
-5	9	5	198	175	10
-4	9	5	332	351	9
-3	9	5	16	15	-65
-2	9	5	16	38	-65
-1	9	5	40	8	-26
0	9	5	61	54	14
1	9	5	43	58	-24
2	9	5	222	224	9
3	9	5	75	76	18
4	9	5	16	2	-69
5	9	5	17	17	-73
6	9	5	98	118	17
7	9	5	19	31	-78
-9	10	5	40	48	-38
-8	10	5	111	87	15
-7	10	5	55	64	-25
-6	10	5	48	77	-27
-5	10	5	152	115	11
-4	10	5	58	71	-22
-3	10	5	23	14	-47
-2	10	5	16	31	-68
-1	10	5	163	167	10
0	10	5	116	118	11
1	10	5	24	29	-45
2	10	5	190	179	10
3	10	5	86	94	16
4	10	5	32	41	-36
5	10	5	18	36	-74
6	10	5	103	115	18
-9	11	5	19	32	-80
-8	11	5	18	17	-76
-7	11	5	31	36	-43
-6	11	5	17	8	-73
-5	11	5	47	38	-27
-4	11	5	142	147	12

Table 58. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-3	11	5	57	46	-22
-2	11	5	62	61	20
-1	11	5	79	81	17
0	11	5	45	54	-23
1	11	5	27	5	-41
2	11	5	101	103	13
3	11	5	118	112	14
4	11	5	17	35	-71
5	11	5	44	16	-31
6	11	5	19	36	-81
-8	12	5	44	45	-34
-7	12	5	55	52	-26
-6	12	5	42	23	-32
-5	12	5	49	30	-27
-4	12	5	17	20	-72
-3	12	5	16	8	-69
-2	12	5	88	84	15
-1	12	5	227	241	11
0	12	5	17	36	-50
1	12	5	16	24	-68
2	12	5	75	68	18
3	12	5	38	37	-35
4	12	5	18	34	-74
5	12	5	18	23	-77
-8	13	5	19	28	-79
-7	13	5	18	21	-74
-6	13	5	49	49	-30
-5	13	5	42	32	-30
-4	13	5	41	45	-32
-3	13	5	17	12	-71
-2	13	5	67	49	19
-1	13	5	17	17	-71
0	13	5	25	1	-36
1	13	5	40	4	-31
2	13	5	80	59	17
3	13	5	49	59	-29
4	13	5	81	70	19
5	13	5	39	27	-37
-7	14	5	19	3	-78
-6	14	5	48	32	-29
-5	14	5	18	23	-76
-4	14	5	18	16	-74
-3	14	5	48	30	-28
-2	14	5	69	68	22
-1	14	5	64	79	22
0	14	5	17	5	-51
1	14	5	62	42	-22
2	14	5	18	25	-74
3	14	5	18	23	-76
4	14	5	19	6	-78
-6	15	5	66	38	23
-5	15	5	66	38	22
-4	15	5	18	40	-77
-3	15	5	18	28	-75
-2	15	5	18	39	-77
-1	15	5	32	18	-42
0	15	5	18	12	-52
1	15	5	43	37	-34
2	15	5	18	22	-77
3	15	5	28	3	-51
-5	16	5	19	23	-81
-4	16	5	36	15	-40
-3	16	5	39	37	-38
-2	16	5	40	25	-36
-1	16	5	36	5	-38
0	16	5	30	12	-38
1	16	5	74	84	22
-2	17	5	52	54	-32
-1	17	5	38	3	-39
-10	0	6	18	2	-76
-8	0	6	60	36	21
-6	0	6	16	33	-66
-2	0	6	32	90	-23
0	0	6	177	98	6
2	0	6	54	71	18
4	0	6	31	1	-38
6	0	6	211	201	10
8	0	6	34	19	-45
-11	1	6	35	21	-42
-10	1	6	84	75	18
-9	1	6	76	93	19
-8	1	6	38	11	-32
-7	1	6	93	79	13
-6	1	6	218	206	9
-5	1	6	24	60	-40
-4	1	6	68	53	14
-3	1	6	33	46	-24
-2	1	6	122	123	8
-1	1	6	14	71	-57
0	1	6	923	865	4
1	1	6	190	146	7
2	1	6	105	95	11

Table 58. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
3	1	6	175	140	10	-7	4	6	107	105	13
4	1	6	17	8	-70	-6	4	6	194	209	9
5	1	6	45	58	-26	-5	4	6	36	25	-26
6	1	6	79	87	19	-4	4	6	131	136	9
7	1	6	31	23	-44	-3	4	6	51	27	16
8	1	6	19	20	-79	-2	4	6	278	296	7
-11	2	6	19	26	-78	-1	4	6	94	77	10
-10	2	6	18	10	-74	0	4	6	120	139	9
-9	2	6	77	67	18	1	4	6	14	8	-61
-8	2	6	29	3	-40	2	4	6	72	65	15
-7	2	6	219	217	9	3	4	6	315	297	8
-6	2	6	64	50	17	4	4	6	38	24	-30
-5	2	6	303	292	7	5	4	6	32	12	-39
-3	2	6	217	202	7	6	4	6	66	79	22
-2	2	6	181	210	7	7	4	6	18	1	-76
-1	2	6	163	164	7	-11	5	6	19	12	-78
0	2	6	102	45	7	-10	5	6	44	53	-34
1	2	6	122	122	9	-9	5	6	100	101	16
2	2	6	53	55	18	-8	5	6	17	18	-71
3	2	6	497	523	7	-7	5	6	59	78	-23
4	2	6	121	127	12	-6	5	6	98	95	14
5	2	6	54	18	-22	-5	5	6	77	87	15
6	2	6	18	10	-75	-4	5	6	89	98	12
7	2	6	62	84	-25	-3	5	6	14	5	-60
-11	3	6	35	48	-45	-2	5	6	180	208	8
-10	3	6	18	14	-75	-1	5	6	73	77	13
-9	3	6	57	57	-24	0	5	6	316	313	13
-8	3	6	107	101	14	1	5	6	146	125	9
-7	3	6	266	271	9	2	5	6	105	92	11
-6	3	6	150	172	10	3	5	6	62	47	18
-5	3	6	36	65	-27	4	5	6	60	43	19
-4	3	6	119	105	10	5	5	6	35	26	-37
-3	3	6	109	105	9	6	5	6	91	95	17
-1	3	6	251	258	7	7	5	6	18	34	-77
0	3	6	188	148	15	-11	6	6	38	29	-41
1	3	6	66	95	14	-10	6	6	28	31	-50
2	3	6	138	173	9	-9	6	6	50	40	-29
3	3	6	235	241	8	-8	6	6	27	50	-48
4	3	6	23	10	-48	-7	6	6	129	149	13
5	3	6	27	18	-46	-6	6	6	43	60	-26
6	3	6	18	12	-75	-5	6	6	205	223	9
7	3	6	71	75	21	-4	6	6	239	248	8
-11	4	6	19	60	-80	-3	6	6	15	3	-62
-10	4	6	18	28	-77	-2	6	6	30	38	-30
-9	4	6	72	67	20	-1	6	6	209	229	8
-8	4	6	17	26	-71	0	6	6	96	62	9

Table 58. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
1	6	6	61	69	16
2	6	6	75	75	15
3	6	6	16	43	-68
4	6	6	17	9	-71
5	6	6	239	279	10
6	6	6	40	46	-33
7	6	6	19	3	-79
-10	7	6	27	17	-51
-9	7	6	144	135	14
-8	7	6	63	62	20
-7	7	6	75	73	19
-6	7	6	16	35	-69
-5	7	6	31	1	-35
-4	7	6	98	108	12
-3	7	6	31	14	-32
-2	7	6	63	70	17
-1	7	6	110	92	11
0	7	6	26	12	-30
1	7	6	311	334	8
2	7	6	53	49	-20
3	7	6	17	48	-70
4	7	6	61	82	-21
5	7	6	39	30	-34
6	7	6	29	32	-47
7	7	6	18	7	-78
-10	8	6	19	11	-79
-9	8	6	39	11	-37
-8	8	6	59	49	-23
-7	8	6	82	80	17
-6	8	6	47	41	-26
-5	8	6	160	152	11
-4	8	6	16	37	-67
-3	8	6	16	33	-66
-2	8	6	282	298	8
-1	8	6	50	65	-22
0	8	6	22	15	-34
1	8	6	99	97	13
2	8	6	16	30	-69
3	8	6	53	28	-22
4	8	6	87	83	16
5	8	6	131	131	14
6	8	6	32	1	-43
-10	9	6	65	57	-25
-9	9	6	58	46	-25
-8	9	6	61	64	-24
-7	9	6	45	17	-27
-6	9	6	98	79	15
-5	9	6	68	77	20
-4	9	6	115	109	13
-3	9	6	59	60	20
-2	9	6	360	395	9
-1	9	6	16	6	-68
0	9	6	16	21	-48
1	9	6	103	111	13
2	9	6	150	142	11
3	9	6	16	17	-69
4	9	6	17	12	-72
5	9	6	43	54	-34
6	9	6	34	4	-42
-9	10	6	40	21	-35
-8	10	6	18	19	-75
-7	10	6	31	14	-41
-6	10	6	81	77	18
-5	10	6	59	66	-22
-4	10	6	17	15	-69
-3	10	6	83	58	15
-2	10	6	233	231	10
-1	10	6	56	62	-21
0	10	6	68	70	14
1	10	6	70	65	19
2	10	6	47	86	-28
3	10	6	41	53	-30
4	10	6	62	71	-23
5	10	6	18	35	-77
6	10	6	49	34	-30
-9	11	6	66	48	-24
-8	11	6	35	12	-40
-7	11	6	18	30	-74
-6	11	6	40	46	-34
-5	11	6	58	71	-24
-4	11	6	31	35	-40
-3	11	6	16	8	-69
-2	11	6	211	203	10
-1	11	6	43	40	-28
0	11	6	84	69	22
1	11	6	167	167	11
2	11	6	17	12	-70
3	11	6	17	7	-71
4	11	6	18	26	-75
5	11	6	27	4	-54
-8	12	6	34	19	-42
-7	12	6	39	40	-36

Table 58. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-6	12	6	48	31	-28
-5	12	6	128	124	14
-4	12	6	66	59	20
-3	12	6	31	13	-37
-2	12	6	66	65	20
-1	12	6	17	12	-71
0	12	6	17	35	-50
1	12	6	62	80	-22
2	12	6	45	21	-28
3	12	6	33	33	-40
4	12	6	18	33	-77
-7	13	6	19	20	-78
-6	13	6	63	55	-25
-5	13	6	18	19	-75
-4	13	6	25	13	-51
-3	13	6	42	46	-30
-2	13	6	73	47	18
-1	13	6	29	20	-43
0	13	6	90	96	12
1	13	6	119	98	14
2	13	6	18	36	-75
3	13	6	28	1	-48
4	13	6	58	36	-26
-7	14	6	19	2	-78
-6	14	6	28	25	-52
-5	14	6	18	18	-76
-4	14	6	66	67	22
-3	14	6	66	76	-24
-2	14	6	37	41	-38
-1	14	6	17	11	-73
0	14	6	25	16	-39
1	14	6	56	16	-24
2	14	6	18	15	-76
3	14	6	19	37	-79
-6	15	6	19	24	-80
-5	15	6	47	3	-31
-4	15	6	18	2	-76
-3	15	6	41	22	-34
-2	15	6	18	7	-75
-1	15	6	18	27	-75
0	15	6	64	47	17
1	15	6	35	29	-39
2	15	6	18	8	-78
-4	16	6	43	3	-33
-3	16	6	63	41	-25
-2	16	6	19	28	-79
-1	16	6	19	2	-78
0	16	6	60	37	20
-10	0	7	114	104	16
-8	0	7	231	230	10
-6	0	7	54	43	-20
-4	0	7	103	125	11
-2	0	7	149	168	9
0	0	7	275	307	6
2	0	7	617	608	7
4	0	7	37	20	-33
6	0	7	18	9	-74
-11	1	7	18	12	-78
-10	1	7	47	64	-31
-9	1	7	17	3	-72
-8	1	7	18	35	-74
-7	1	7	82	99	16
-6	1	7	78	80	15
-5	1	7	279	300	8
-4	1	7	100	107	11
-3	1	7	77	62	13
-2	1	7	158	174	8
-1	1	7	292	270	7
0	1	7	15	5	-44
1	1	7	15	9	-64
2	1	7	253	238	8
3	1	7	17	12	-69
4	1	7	16	1	-69
5	1	7	194	197	11
6	1	7	49	40	-29
7	1	7	18	27	-77
-11	2	7	18	15	-77
-10	2	7	18	1	-75
-9	2	7	52	4	-24
-8	2	7	129	117	13
-7	2	7	120	130	12
-6	2	7	84	86	15
-5	2	7	186	176	9
-4	2	7	50	42	-20
-3	2	7	183	221	8
-2	2	7	77	87	13
-1	2	7	369	338	7
0	2	7	22	22	-31
1	2	7	119	127	10
2	2	7	234	217	8
3	2	7	16	2	-68
4	2	7	17	12	-69

Table 58. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
5	2	7	53	11	-28	-5	5	7	41	49	-28
6	2	7	18	31	-75	-4	5	7	112	115	11
7	2	7	19	38	-79	-2	5	7	177	196	9
-11	3	7	19	5	-79	-1	5	7	146	137	10
-10	3	7	95	92	18	0	5	7	89	86	15
-9	3	7	17	16	-73	1	5	7	93	80	13
-8	3	7	17	28	-70	2	5	7	91	93	14
-7	3	7	118	99	13	3	5	7	118	99	12
-6	3	7	16	30	-68	4	5	7	141	148	11
-4	3	7	15	47	-62	5	5	7	82	64	17
-3	3	7	87	98	12	6	5	7	18	2	-75
-2	3	7	175	132	8	-10	6	7	75	50	20
-1	3	7	248	244	7	-9	6	7	18	3	-75
0	3	7	30	28	-22	-8	6	7	144	156	13
1	3	7	15	8	-64	-7	6	7	126	115	13
2	3	7	16	9	-69	-6	6	7	34	60	-35
3	3	7	34	8	-33	-5	6	7	116	100	12
4	3	7	51	56	-24	-4	6	7	16	20	-67
5	3	7	233	240	10	-3	6	7	16	1	-68
6	3	7	42	39	-31	-2	6	7	87	96	13
7	3	7	19	39	-79	-1	6	7	34	24	-30
-11	4	7	19	14	-78	0	6	7	105	101	8
-10	4	7	96	105	18	1	6	7	115	123	11
-9	4	7	39	40	-32	2	6	7	137	123	11
-8	4	7	113	127	14	3	6	7	111	125	13
-7	4	7	76	77	18	4	6	7	17	10	-72
-6	4	7	127	124	11	5	6	7	17	9	-73
-5	4	7	202	231	9	6	6	7	42	24	-32
-4	4	7	102	102	11	-10	7	7	29	32	-52
-3	4	7	15	17	-63	-9	7	7	18	12	-77
-2	4	7	260	261	8	-8	7	7	41	26	-32
-1	4	7	302	314	7	-7	7	7	93	79	15
0	4	7	225	241	10	-6	7	7	26	23	-45
1	4	7	138	146	10	-5	7	7	114	127	13
2	4	7	173	166	9	-4	7	7	16	25	-68
3	4	7	46	85	-25	-2	7	7	193	188	9
4	4	7	53	36	-22	-1	7	7	77	73	15
5	4	7	67	59	21	0	7	7	53	60	-26
6	4	7	18	3	-74	1	7	7	31	58	-35
7	4	7	19	16	-78	2	7	7	34	4	-32
-11	5	7	19	15	-80	3	7	7	130	150	12
-10	5	7	53	47	-29	4	7	7	18	23	-75
-9	5	7	57	63	-25	5	7	7	18	20	-74
-8	5	7	25	17	-52	6	7	7	31	5	-44
-7	5	7	59	67	-22	-10	8	7	33	40	-45
-6	5	7	88	80	15	-9	8	7	31	6	-44

Table 58. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-8	8	7	36	22	-35
-7	8	7	126	121	13
-6	8	7	140	136	13
-5	8	7	41	32	-29
-4	8	7	16	30	-66
-3	8	7	200	208	10
-2	8	7	85	88	15
-1	8	7	90	79	14
0	8	7	257	260	17
1	8	7	68	60	18
2	8	7	17	6	-70
3	8	7	118	110	13
4	8	7	116	118	14
5	8	7	40	11	-32
6	8	7	19	17	-78
-10	9	7	49	49	-35
-9	9	7	42	27	-33
-8	9	7	48	50	-29
-7	9	7	17	11	-73
-6	9	7	107	116	15
-5	9	7	17	30	-70
-4	9	7	38	11	-31
-3	9	7	45	40	-28
-2	9	7	17	24	-71
-1	9	7	53	32	-22
0	9	7	68	65	16
1	9	7	43	36	-28
2	9	7	59	40	20
3	9	7	26	4	-49
4	9	7	109	104	15
5	9	7	18	14	-75
-9	10	7	18	4	-75
-8	10	7	18	5	-76
-7	10	7	55	20	-24
-6	10	7	52	68	-27
-5	10	7	36	16	-33
-4	10	7	17	2	-70
-3	10	7	28	43	-44
-2	10	7	16	4	-69
-1	10	7	36	63	-35
0	10	7	313	308	7
1	10	7	55	60	-23
2	10	7	16	15	-69
3	10	7	17	18	-73
4	10	7	64	50	22
5	10	7	60	4	-23
-9	11	7	19	13	-79
-8	11	7	18	21	-75
-7	11	7	71	35	19
-6	11	7	54	62	-27
-5	11	7	71	75	21
-4	11	7	64	47	20
-3	11	7	137	133	12
-2	11	7	17	15	-70
-1	11	7	33	52	-39
0	11	7	41	33	-24
1	11	7	17	1	-71
2	11	7	17	8	-72
3	11	7	61	78	-25
4	11	7	48	43	-30
-8	12	7	84	53	19
-7	12	7	87	64	19
-6	12	7	17	15	-73
-5	12	7	17	11	-73
-4	12	7	88	81	17
-3	12	7	17	11	-72
-2	12	7	40	25	-32
-1	12	7	50	24	-25
0	12	7	35	28	-30
1	12	7	17	34	-73
2	12	7	62	62	-23
3	12	7	56	24	-25
4	12	7	42	15	-35
-7	13	7	52	18	-29
-6	13	7	18	11	-76
-5	13	7	31	18	-44
-4	13	7	17	20	-73
-3	13	7	102	104	16
-2	13	7	41	54	-33
-1	13	7	58	43	-23
0	13	7	41	22	-29
1	13	7	17	34	-73
2	13	7	47	26	-28
3	13	7	47	56	-32
-6	14	7	18	15	-78
-5	14	7	66	49	23
-4	14	7	18	21	-76
-3	14	7	44	20	-31
-2	14	7	18	11	-74
-1	14	7	18	4	-75
0	14	7	44	43	-24
1	14	7	18	1	-76

Table 58. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
2	14	7	84	53	19	2	2	8	57	65	-21
-5	15	7	61	49	-25	3	2	8	38	4	-30
-4	15	7	61	20	-23	4	2	8	139	137	13
-3	15	7	27	14	-52	5	2	8	17	5	-73
-2	15	7	31	31	-47	6	2	8	18	19	-75
-1	15	7	73	73	23	-11	3	8	65	59	-26
0	15	7	24	22	-45	-10	3	8	41	17	-33
1	15	7	18	19	-77	-9	3	8	116	125	15
-10	0	8	31	41	-45	-8	3	8	105	103	15
-8	0	8	54	44	-25	-7	3	8	45	65	-28
-6	0	8	222	219	10	-6	3	8	30	55	-39
-4	0	8	88	62	13	-5	3	8	16	13	-68
0	0	8	96	88	9	-4	3	8	180	191	9
2	0	8	66	93	19	-3	3	8	77	83	15
4	0	8	383	395	9	-2	3	8	27	10	-36
6	0	8	36	19	-39	-1	3	8	83	74	14
-11	1	8	57	47	-27	0	3	8	64	72	21
-10	1	8	18	8	-75	1	3	8	319	296	8
-9	1	8	58	50	-24	2	3	8	131	143	12
-8	1	8	114	113	14	3	3	8	43	72	-27
-7	1	8	40	23	-30	4	3	8	18	6	-75
-6	1	8	224	220	10	5	3	8	17	32	-72
-5	1	8	47	17	-23	6	3	8	18	4	-77
-4	1	8	120	122	11	-11	4	8	19	18	-80
-3	1	8	15	12	-65	-10	4	8	18	5	-77
-2	1	8	73	65	15	-9	4	8	88	63	17
-1	1	8	94	106	12	-8	4	8	27	18	-46
0	1	8	181	193	6	-7	4	8	70	69	19
1	1	8	284	288	8	-6	4	8	109	122	14
2	1	8	100	90	14	-5	4	8	61	41	19
3	1	8	40	56	-30	-4	4	8	276	291	9
4	1	8	224	228	10	-3	4	8	248	253	9
5	1	8	17	26	-73	-2	4	8	15	2	-64
6	1	8	18	12	-77	-1	4	8	97	77	13
-11	2	8	44	50	-36	0	4	8	35	15	-27
-10	2	8	42	50	-35	1	4	8	88	87	15
-9	2	8	74	67	20	2	4	8	51	65	-24
-8	2	8	66	48	19	3	4	8	76	78	17
-7	2	8	24	29	-49	4	4	8	72	62	19
-6	2	8	64	57	18	5	4	8	33	14	-41
-5	2	8	76	61	16	6	4	8	73	83	22
-4	2	8	58	63	19	-11	5	8	27	9	-56
-2	2	8	110	105	11	-10	5	8	80	51	19
-1	2	8	86	73	13	-9	5	8	18	12	-75
0	2	8	69	80	12	-8	5	8	116	135	15
1	2	8	51	13	-25	-7	5	8	149	158	12

Table 58. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-6	5	8	210	216	10
-5	5	8	86	79	15
-4	5	8	17	20	-70
-3	5	8	110	118	12
-2	5	8	16	4	-66
-1	5	8	102	128	13
0	5	8	101	95	12
1	5	8	27	20	-41
2	5	8	239	231	9
3	5	8	52	60	-23
4	5	8	51	41	-27
5	5	8	33	35	-39
6	5	8	19	14	-79
-10	6	8	19	29	-79
-9	6	8	18	29	-75
-8	6	8	37	17	-36
-7	6	8	49	32	-25
-6	6	8	56	50	-23
-5	6	8	79	69	17
-4	6	8	143	151	11
-3	6	8	16	5	-68
-2	6	8	16	27	-67
-1	6	8	318	339	8
0	6	8	112	114	10
1	6	8	42	15	-26
2	6	8	30	2	-42
3	6	8	29	21	-39
4	6	8	75	73	18
5	6	8	31	44	-43
-10	7	8	28	2	-51
-9	7	8	18	31	-77
-8	7	8	34	0	-37
-7	7	8	95	100	15
-6	7	8	104	122	15
-5	7	8	113	122	14
-4	7	8	137	147	12
-3	7	8	67	83	19
-2	7	8	102	117	13
-1	7	8	272	284	9
0	7	8	51	55	17
1	7	8	70	52	18
2	7	8	75	62	18
3	7	8	84	86	16
4	7	8	44	36	-30
5	7	8	41	15	-34
-10	8	8	19	12	-79
-9	8	8	18	1	-77
-8	8	8	66	52	22
-7	8	8	26	17	-47
-6	8	8	62	73	22
-5	8	8	28	56	-44
-4	8	8	139	152	12
-3	8	8	96	113	15
-2	8	8	17	0	-70
-1	8	8	172	193	11
0	8	8	98	109	12
1	8	8	34	22	-35
2	8	8	86	94	16
3	8	8	41	14	-30
4	8	8	18	19	-74
5	8	8	38	38	-37
-9	9	8	18	20	-78
-8	9	8	69	78	24
-7	9	8	37	7	-34
-6	9	8	17	7	-73
-5	9	8	47	48	-28
-4	9	8	90	89	16
-3	9	8	25	29	-48
-2	9	8	55	6	-21
-1	9	8	89	92	15
0	9	8	47	47	-26
1	9	8	17	7	-71
2	9	8	208	198	11
3	9	8	18	49	-74
4	9	8	37	11	-37
-9	10	8	27	17	-53
-8	10	8	18	28	-77
-7	10	8	18	31	-76
-6	10	8	53	57	-27
-5	10	8	35	46	-36
-4	10	8	142	148	13
-3	10	8	17	24	-71
-2	10	8	17	9	-70
-1	10	8	60	67	-22
0	10	8	28	22	-34
1	10	8	17	18	-71
2	10	8	30	30	-44
3	10	8	17	1	-72
4	10	8	33	9	-41
-8	11	8	62	40	-24
-7	11	8	18	17	-75
-6	11	8	51	41	-27

Table 58. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-5	11	8	18	20	-74
-4	11	8	35	5	-37
-3	11	8	48	42	-26
-2	11	8	53	49	-24
-1	11	8	114	112	14
0	11	8	44	15	-20
1	11	8	65	51	21
2	11	8	101	112	16
3	11	8	61	45	-24
-8	12	8	19	33	-82
-7	12	8	19	5	-80
-6	12	8	18	14	-77
-5	12	8	70	53	21
-4	12	8	18	20	-75
-3	12	8	18	35	-75
-2	12	8	73	72	21
-1	12	8	102	102	17
0	12	8	17	11	-52
1	12	8	18	5	-74
2	12	8	57	7	-24
3	12	8	18	20	-75
-7	13	8	19	2	-79
-6	13	8	90	76	19
-5	13	8	76	54	20
-4	13	8	18	19	-74
-3	13	8	18	10	-76
-2	13	8	69	35	20
-1	13	8	18	44	-76
0	13	8	41	17	-29
1	13	8	18	3	-76
2	13	8	42	0	-36
-5	14	8	31	16	-46
-4	14	8	18	11	-77
-3	14	8	19	46	-79
-2	14	8	26	28	-54
-1	14	8	40	49	-39
0	14	8	58	18	-28
1	14	8	30	29	-51
-3	15	8	41	4	-37
-2	15	8	19	26	-81
-10	0	9	61	9	-23
-8	0	9	53	46	-25
-6	0	9	29	3	-40
-2	0	9	145	137	11
0	0	9	261	246	6
2	0	9	73	52	17
4	0	9	18	12	-74
-11	1	9	29	33	-54
-10	1	9	63	46	-23
-9	1	9	18	25	-75
-8	1	9	84	97	18
-7	1	9	17	15	-71
-6	1	9	78	67	17
-5	1	9	80	62	16
-3	1	9	16	10	-67
-2	1	9	126	118	11
-1	1	9	116	125	12
0	1	9	157	150	10
1	1	9	17	4	-72
2	1	9	36	17	-32
3	1	9	78	65	21
4	1	9	17	10	-72
5	1	9	18	14	-74
-11	2	9	33	5	-46
-10	2	9	18	4	-75
-9	2	9	105	112	16
-8	2	9	47	48	-27
-7	2	9	216	220	11
-6	2	9	17	27	-71
-5	2	9	17	29	-71
-4	2	9	166	170	11
-3	2	9	48	24	-24
-2	2	9	84	86	15
-1	2	9	160	148	10
0	2	9	48	58	-17
1	2	9	76	72	18
2	2	9	45	30	-28
3	2	9	282	288	10
4	2	9	32	11	-39
5	2	9	18	7	-76
-11	3	9	73	57	23
-10	3	9	18	12	-77
-9	3	9	18	20	-75
-8	3	9	80	97	18
-7	3	9	18	18	-74
-6	3	9	17	6	-71
-5	3	9	106	107	13
-4	3	9	76	73	17
-3	3	9	60	61	19
-2	3	9	319	319	8
-1	3	9	248	244	9
0	3	9	17	11	-49

Table 58. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
1	3	9	37	22	-34
2	3	9	42	68	-30
3	3	9	77	64	19
4	3	9	45	21	-29
5	3	9	18	10	-75
-10	4	9	18	13	-77
-9	4	9	67	38	21
-8	4	9	17	20	-73
-7	4	9	121	126	13
-6	4	9	147	155	12
-5	4	9	33	11	-36
-4	4	9	17	8	-70
-3	4	9	16	6	-69
-2	4	9	29	16	-41
-1	4	9	17	33	-69
0	4	9	90	97	12
1	4	9	17	22	-73
2	4	9	17	38	-71
3	4	9	159	146	12
4	4	9	37	61	-37
5	4	9	45	15	-31
-10	5	9	57	24	-25
-9	5	9	88	76	18
-8	5	9	18	20	-75
-7	5	9	48	51	-27
-6	5	9	93	89	16
-5	5	9	31	15	-40
-4	5	9	205	219	10
-3	5	9	57	50	-22
-2	5	9	277	281	9
-1	5	9	109	116	13
0	5	9	116	90	9
1	5	9	130	114	12
2	5	9	25	19	-48
3	5	9	18	3	-74
4	5	9	54	44	-25
5	5	9	34	38	-43
-10	6	9	19	8	-79
-9	6	9	67	57	23
-8	6	9	18	3	-74
-7	6	9	29	31	-42
-6	6	9	17	35	-74
-5	6	9	217	209	10
-4	6	9	132	143	12
-3	6	9	55	37	-22
-2	6	9	80	78	17
-1	6	9	44	60	-27
0	6	9	60	48	14
1	6	9	266	279	9
2	6	9	17	29	-71
3	6	9	39	26	-33
4	6	9	67	61	21
5	6	9	50	63	-31
-10	7	9	55	6	-26
-9	7	9	37	56	-43
-8	7	9	55	46	-27
-7	7	9	18	26	-75
-6	7	9	34	29	-36
-5	7	9	71	83	19
-4	7	9	92	104	16
-3	7	9	17	5	-70
-2	7	9	57	85	-24
-1	7	9	17	19	-71
0	7	9	17	7	-49
1	7	9	105	106	15
2	7	9	50	4	-25
3	7	9	18	13	-74
4	7	9	38	28	-37
-9	8	9	63	55	-25
-8	8	9	18	6	-76
-7	8	9	52	47	-27
-6	8	9	107	104	15
-5	8	9	17	5	-71
-4	8	9	101	89	14
-3	8	9	16	2	-69
-2	8	9	17	20	-73
-1	8	9	17	7	-71
0	8	9	25	0	-36
1	8	9	175	197	12
2	8	9	70	97	22
3	8	9	18	22	-74
4	8	9	31	27	-47
-9	9	9	19	9	-79
-8	9	9	18	17	-77
-7	9	9	25	2	-52
-6	9	9	36	24	-37
-5	9	9	60	42	-22
-4	9	9	35	4	-33
-3	9	9	17	8	-70
-2	9	9	233	250	11
-1	9	9	51	47	-25
0	9	9	40	4	-27

Table 58. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
1	9	9	46	31	-31
2	9	9	25	10	-51
3	9	9	18	9	-77
-8	10	9	19	19	-78
-7	10	9	48	48	-31
-6	10	9	113	100	16
-5	10	9	48	51	-28
-4	10	9	17	12	-71
-3	10	9	30	35	-43
-2	10	9	18	41	-75
-1	10	9	17	18	-73
0	10	9	37	14	-30
1	10	9	51	28	-26
2	10	9	18	28	-74
3	10	9	19	27	-78
-8	11	9	19	8	-79
-7	11	9	30	12	-47
-6	11	9	18	23	-76
-5	11	9	36	0	-36
-4	11	9	17	23	-71
-3	11	9	17	16	-72
-2	11	9	106	101	15
-1	11	9	17	0	-73
0	11	9	54	48	-22
1	11	9	19	44	-79
2	11	9	58	21	-24
-7	12	9	58	46	-28
-6	12	9	48	57	-30
-5	12	9	41	35	-34
-4	12	9	56	62	-27
-3	12	9	18	5	-75
-2	12	9	18	2	-74
-1	12	9	18	14	-74
0	12	9	26	14	-40
1	12	9	89	78	19
-6	13	9	19	30	-80
-5	13	9	35	9	-41
-4	13	9	94	77	18
-3	13	9	18	31	-77
-2	13	9	18	21	-76
-1	13	9	35	11	-38
0	13	9	59	52	20
-4	14	9	38	33	-40
-3	14	9	55	58	-31
-2	14	9	18	9	-76
-10	0	10	66	51	-24
-8	0	10	105	106	15
-6	0	10	50	12	-24
-4	0	10	47	48	-26
-2	0	10	319	354	9
0	0	10	50	27	-26
2	0	10	65	37	-23
4	0	10	18	1	-77
-10	1	10	39	52	-42
-9	1	10	18	16	-74
-8	1	10	60	82	-25
-7	1	10	78	78	18
-6	1	10	33	6	-38
-5	1	10	203	209	10
-4	1	10	96	78	14
-3	1	10	17	1	-69
-2	1	10	32	57	-40
-1	1	10	62	80	21
0	1	10	42	29	-22
1	1	10	123	145	13
2	1	10	193	183	11
3	1	10	18	10	-75
4	1	10	27	16	-52
-10	2	10	55	27	-27
-9	2	10	46	26	-30
-8	2	10	73	76	21
-7	2	10	44	31	-28
-6	2	10	75	70	19
-5	2	10	115	118	15
-4	2	10	69	50	19
-3	2	10	101	100	14
-2	2	10	133	133	12
-1	2	10	134	130	12
0	2	10	119	129	12
1	2	10	64	58	21
2	2	10	45	37	-31
3	2	10	18	2	-75
4	2	10	18	3	-77
-10	3	10	18	12	-77
-9	3	10	18	9	-77
-8	3	10	66	35	20
-7	3	10	101	101	15
-6	3	10	72	56	18
-5	3	10	301	304	10
-4	3	10	29	41	-43
-3	3	10	64	65	21
-2	3	10	103	101	14

Table 58. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-1	3	10	35	6	-35
0	3	10	17	9	-52
1	3	10	89	90	16
2	3	10	56	79	-25
3	3	10	18	31	-76
4	3	10	18	30	-76
-10	4	10	69	70	-25
-9	4	10	60	48	-25
-8	4	10	38	3	-35
-7	4	10	72	79	20
-6	4	10	34	17	-35
-5	4	10	18	12	-74
-4	4	10	44	18	-28
-3	4	10	38	0	-33
-2	4	10	144	145	11
-1	4	10	85	76	16
0	4	10	185	189	7
1	4	10	115	95	13
2	4	10	43	46	-33
3	4	10	18	1	-76
4	4	10	32	8	-45
-10	5	10	66	43	-24
-9	5	10	43	22	-34
-8	5	10	69	68	22
-7	5	10	59	64	-25
-6	5	10	62	52	21
-5	5	10	163	169	12
-4	5	10	39	28	-30
-3	5	10	212	187	10
-2	5	10	17	5	-70
-1	5	10	17	15	-70
0	5	10	185	204	11
1	5	10	18	61	-75
2	5	10	87	80	18
3	5	10	86	80	17
4	5	10	18	22	-77
-10	6	10	19	7	-81
-9	6	10	18	6	-77
-8	6	10	18	30	-76
-7	6	10	76	70	20
-6	6	10	66	50	20
-5	6	10	69	71	20
-4	6	10	51	49	-24
-3	6	10	184	193	11
-2	6	10	140	140	12
-1	6	10	17	1	-72
0	6	10	71	61	15
1	6	10	30	62	-42
2	6	10	41	46	-34
3	6	10	32	10	-45
4	6	10	19	12	-78
-9	7	10	52	36	-27
-8	7	10	42	13	-31
-7	7	10	141	135	14
-6	7	10	50	46	-27
-5	7	10	17	21	-72
-4	7	10	40	50	-32
-3	7	10	117	115	14
-2	7	10	17	45	-73
-1	7	10	17	12	-72
0	7	10	17	2	-52
1	7	10	18	27	-74
2	7	10	18	36	-75
3	7	10	128	142	15
-9	8	10	19	32	-82
-8	8	10	18	9	-75
-7	8	10	18	27	-78
-6	8	10	35	27	-38
-5	8	10	41	11	-31
-4	8	10	68	56	20
-3	8	10	132	146	14
-2	8	10	37	26	-33
-1	8	10	41	24	-31
0	8	10	132	127	10
1	8	10	18	10	-75
2	8	10	18	7	-75
3	8	10	29	8	-51
-8	9	10	54	33	-27
-7	9	10	43	30	-33
-6	9	10	18	29	-76
-5	9	10	26	8	-50
-4	9	10	18	51	-77
-3	9	10	17	30	-72
-2	9	10	35	23	-36
-1	9	10	35	37	-37
0	9	10	69	58	18
1	9	10	18	15	-76
2	9	10	27	22	-53
-8	10	10	19	7	-78
-7	10	10	46	1	-30
-6	10	10	18	6	-77
-5	10	10	19	32	-78

Table 58. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-4	10	10	35	40	-39
-3	10	10	18	30	-75
-2	10	10	18	12	-74
-1	10	10	18	18	-77
0	10	10	139	141	12
1	10	10	18	17	-77
2	10	10	18	22	-77
-7	11	10	42	38	-36
-6	11	10	33	23	-43
-5	11	10	71	78	24
-4	11	10	61	70	-26
-3	11	10	48	56	-30
-2	11	10	30	10	-45
-1	11	10	29	14	-43
0	11	10	55	26	-29
1	11	10	18	3	-77
-6	12	10	31	1	-47
-5	12	10	46	56	-35
-4	12	10	19	14	-78
-3	12	10	40	44	-40
-2	12	10	37	30	-40
-1	12	10	18	12	-75
0	12	10	42	13	-27
-4	13	10	19	40	-82
-3	13	10	60	37	-25
-2	13	10	44	10	-33
-10	0	11	52	10	-30
-8	0	11	102	93	16
-6	0	11	235	245	11
-4	0	11	38	22	-33
-2	0	11	27	1	-44
0	0	11	96	106	13
2	0	11	32	16	-41
-10	1	11	33	41	-45
-9	1	11	18	29	-76
-8	1	11	18	12	-76
-7	1	11	18	8	-74
-6	1	11	86	93	18
-5	1	11	33	12	-39
-4	1	11	49	39	-26
-3	1	11	128	133	13
-2	1	11	51	26	-23
-1	1	11	111	93	13
0	1	11	236	234	8
1	1	11	51	56	-28
2	1	11	46	35	-30
3	1	11	32	1	-45
-10	2	11	19	1	-79
-9	2	11	18	9	-77
-8	2	11	18	41	-75
-7	2	11	45	23	-30
-6	2	11	71	90	21
-5	2	11	49	57	-27
-4	2	11	47	56	-26
-3	2	11	152	159	12
-2	2	11	46	42	-27
-1	2	11	17	15	-72
0	2	11	57	29	-28
1	2	11	104	94	15
2	2	11	44	34	-32
3	2	11	32	31	-45
-10	3	11	19	6	-78
-9	3	11	45	54	-33
-8	3	11	70	68	22
-7	3	11	44	24	-30
-6	3	11	79	83	19
-5	3	11	57	60	-22
-4	3	11	17	16	-72
-3	3	11	176	198	12
-2	3	11	17	6	-70
-1	3	11	79	81	18
0	3	11	78	87	14
1	3	11	83	76	18
2	3	11	91	73	17
3	3	11	18	4	-77
-10	4	11	19	6	-79
-9	4	11	18	9	-77
-8	4	11	85	83	19
-7	4	11	30	13	-44
-6	4	11	19	54	-78
-5	4	11	38	25	-32
-4	4	11	101	111	15
-3	4	11	198	195	11
-2	4	11	17	6	-72
-1	4	11	106	86	15
0	4	11	48	54	-20
1	4	11	18	7	-76
2	4	11	109	112	16
3	4	11	28	27	-53
-9	5	11	19	19	-80
-8	5	11	19	46	-80
-7	5	11	71	70	22

Table 58. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-6	5	11	18	6	-74
-5	5	11	38	30	-33
-4	5	11	90	97	17
-3	5	11	36	20	-35
-2	5	11	18	9	-74
-1	5	11	100	102	16
0	5	11	62	76	16
1	5	11	18	2	-75
2	5	11	46	57	-33
3	5	11	38	30	-39
-9	6	11	44	17	-32
-8	6	11	75	61	21
-7	6	11	18	14	-75
-6	6	11	77	46	19
-5	6	11	133	133	14
-4	6	11	17	19	-73
-3	6	11	18	56	-75
-2	6	11	18	31	-74
-1	6	11	31	33	-43
0	6	11	18	3	-53
1	6	11	18	13	-76
2	6	11	50	57	-30
-9	7	11	19	3	-80
-8	7	11	19	50	-80
-7	7	11	18	2	-74
-6	7	11	18	27	-75
-5	7	11	28	11	-50
-4	7	11	19	59	-78
-3	7	11	73	55	20
-2	7	11	18	12	-74
-1	7	11	158	158	12
0	7	11	56	51	-27
1	7	11	47	34	-29
2	7	11	41	20	-37
-8	8	11	19	27	-80
-7	8	11	52	35	-27
-6	8	11	55	46	-27
-5	8	11	85	80	20
-4	8	11	87	98	18
-3	8	11	18	6	-74
-2	8	11	33	0	-41
-1	8	11	34	9	-40
0	8	11	37	10	-31
1	8	11	40	17	-34
-8	9	11	82	74	22
-7	9	11	19	33	-79
-6	9	11	44	18	-33
-5	9	11	44	18	-32
-4	9	11	18	7	-75
-3	9	11	18	5	-76
-2	9	11	18	51	-76
-1	9	11	19	24	-78
0	9	11	18	27	-53
1	9	11	29	12	-47
-7	10	11	19	19	-78
-6	10	11	66	49	23
-5	10	11	40	3	-36
-4	10	11	48	44	-31
-3	10	11	44	22	-30
-2	10	11	54	40	-27
-1	10	11	19	11	-78
0	10	11	18	16	-55
-6	11	11	44	32	-36
-5	11	11	31	27	-48
-4	11	11	46	1	-31
-3	11	11	19	37	-78
-2	11	11	32	50	-47
-1	11	11	83	85	20
-8	0	12	52	49	-29
-6	0	12	76	83	20
-4	0	12	19	40	-79
-2	0	12	50	45	-27
0	0	12	74	72	15
2	0	12	76	63	22
-9	1	12	19	24	-80
-8	1	12	31	17	-47
-7	1	12	27	42	-52
-6	1	12	31	43	-46
-5	1	12	42	31	-31
-4	1	12	252	253	11
-3	1	12	17	27	-73
-2	1	12	17	19	-74
-1	1	12	19	3	-78
0	1	12	42	16	-30
1	1	12	44	17	-32
2	1	12	40	47	-38
-9	2	12	58	63	-29
-8	2	12	53	48	-28
-7	2	12	64	51	-24
-6	2	12	86	89	19
-5	2	12	17	1	-74
-4	2	12	18	29	-77

Table 58. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-3	2	12	18	27	-76
-2	2	12	37	8	-37
-1	2	12	159	172	13
0	2	12	42	17	-23
1	2	12	52	41	-28
2	2	12	49	48	-30
-9	3	12	69	54	24
-8	3	12	19	21	-79
-7	3	12	18	45	-77
-6	3	12	78	60	19
-5	3	12	37	28	-37
-4	3	12	45	57	-33
-3	3	12	31	24	-41
-2	3	12	85	89	18
-1	3	12	83	92	20
0	3	12	51	33	-28
1	3	12	27	50	-54
2	3	12	19	0	-81
-9	4	12	29	12	-52
-8	4	12	18	17	-77
-7	4	12	63	37	-23
-6	4	12	82	71	19
-5	4	12	55	44	-25
-4	4	12	70	66	21
-3	4	12	58	36	-22
-2	4	12	81	88	18
-1	4	12	124	117	14
0	4	12	51	44	-27
1	4	12	61	38	-25
2	4	12	19	11	-79
-9	5	12	19	31	-82
-8	5	12	19	3	-79
-7	5	12	18	22	-78
-6	5	12	98	95	17
-5	5	12	18	27	-75
-4	5	12	98	97	18
-3	5	12	62	55	-22
-2	5	12	25	13	-52
-1	5	12	90	84	18
0	5	12	18	11	-54
1	5	12	19	0	-79
-8	6	12	58	59	-28
-7	6	12	19	13	-79
-6	6	12	44	11	-32
-5	6	12	18	28	-76
-4	6	12	18	9	-77
-3	6	12	18	28	-75
-2	6	12	33	40	-44
-1	6	12	18	10	-75
0	6	12	34	24	-33
1	6	12	127	124	15
-8	7	12	35	7	-43
-7	7	12	19	37	-79
-6	7	12	45	24	-32
-5	7	12	28	17	-49
-4	7	12	37	32	-39
-3	7	12	52	65	-28
-2	7	12	61	55	-24
-1	7	12	18	22	-76
0	7	12	36	23	-27
-7	8	12	19	19	-79
-6	8	12	56	47	-28
-5	8	12	57	25	-25
-4	8	12	38	31	-38
-3	8	12	53	35	-27
-2	8	12	47	68	-32
-1	8	12	19	26	-79
0	8	12	18	8	-54
-6	9	12	94	85	20
-5	9	12	18	32	-76
-4	9	12	19	24	-78
-3	9	12	50	53	-30
-2	9	12	97	90	18
-1	9	12	19	1	-79
-5	10	12	19	26	-79
-4	10	12	31	32	-50
-3	10	12	19	3	-79
-8	0	13	30	28	-51
-6	0	13	18	6	-75
-4	0	13	59	50	-24
-2	0	13	135	127	15
0	0	13	28	8	-40
-8	1	13	19	25	-80
-7	1	13	36	29	-40
-6	1	13	18	5	-74
-5	1	13	38	24	-38
-4	1	13	67	61	22
-3	1	13	32	18	-43
-2	1	13	94	88	18
-1	1	13	18	18	-76
0	1	13	19	33	-55
-8	2	13	19	1	-79

Table 58. (cont).
F(obs), F(calc), and σ_F ($-\sigma_F$ indicates ommited data)

H	K	L	$10F_o$	$10F_c$	10σ
-7	2	13	83	75	20
-6	2	13	18	2	-76
-5	2	13	105	114	17
-4	2	13	43	33	-32
-3	2	13	28	33	-52
-2	2	13	98	107	18
-1	2	13	19	15	-78
0	2	13	19	23	-56
-8	3	13	19	10	-79
-7	3	13	59	7	-25
-6	3	13	19	13	-79
-5	3	13	86	62	18
-4	3	13	47	43	-31
-3	3	13	28	26	-50
-2	3	13	19	28	-79
-1	3	13	36	28	-40
0	3	13	42	50	-27
-8	4	13	19	3	-81
-7	4	13	44	55	-35
-6	4	13	18	10	-76
-5	4	13	79	78	20
-4	4	13	73	78	22
-3	4	13	65	69	-24
-2	4	13	32	31	-45
-1	4	13	18	41	-77
0	4	13	19	9	-55
-7	5	13	93	96	21
-6	5	13	44	34	-33
-5	5	13	64	53	-25
-4	5	13	18	3	-77
-3	5	13	45	16	-32
-2	5	13	71	51	21
-1	5	13	19	26	-79
0	5	13	81	69	16
-7	6	13	45	25	-36
-6	6	13	19	20	-80
-5	6	13	19	30	-78
-4	6	13	19	38	-78
-3	6	13	104	87	16
-2	6	13	69	66	-25

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