



The X-ray crystallographic structure study of the 1,2,4 trimethylbenzene thiourea adduct and 1,2,4 trichlorobenzene thiourea adduct
by Thomas Albert Wick

A thesis submitted in partial fulfillment of the requirements for the degree of Master of Science in
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Montana State University
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Abstract:

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The general characteristics of these two structures are consistent with other similar thiourea adduct structures. The possibility of a hydrogen bond between the aromatic ring C-H group and the thiourea sulfur was found in both structures. From the non-bonded distances between the thiourea sulfur atoms and the disordered aromatic, evidence for a dipole-dipole interaction exists.

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by

Thomas Albert Wick

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APPROVAL

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ABSTRACT

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INTRODUCTION

Background

Frequently in industrial chemical processes mixtures of hard-to-separate aromatic compounds turn up. Since the compounds in these mixtures have similar physical and chemical properties, separation is often times difficult and economically poor. Although conventional separation techniques for these systems are diverse, they typically require large amounts of energy to effect a minimal degree of separation.

Distillation has been the standard technique for making such aromatic hydrocarbon separations, but in some cases it is impractical since the mixtures may pyrolyze, may have close boiling isomers and/or form azeotropes. An alternative separation technique useful for aromatic, isomeric hydrocarbon mixtures is extractive crystallization.

Extractive crystallization, by its analogy to the nonideal extractive distillation, is a selective process wherein a given compound preferentially forms an adduct crystal with another component thus effecting a separation (1). Adduct complexes are a class of non-stoichiometric compounds in which "guest" molecules are entrapped in channels or cage-like structures formed by "host" molecules. Adduct crystals will form only with suitable "guest" molecules since the spatial characteristics of the channel places structural constraints on the guest molecules which can be accommodated. When an adduct is

decomposed, the "host" and the "guest" molecules are returned unchanged.

The most prevalent of "host" molecules are urea and thiourea. It is hypothesized that urea and thiourea form complexes easily because of their large dipole moment and zwitterion characteristics (1). Urea forms crystalline adducts with normal hydrocarbons, but usually not with branched or cyclic compounds unless the straight chain portion is sufficiently long enough. Thiourea forms channel adducts similar to the urea adducts, however, due to the larger sulfur atom the channel which entraps the "guest" is larger and thus can accommodate a larger "guest". On the other hand, a straight chain alkane would leave too much of the channel unfilled producing an unstable structure.

The hydrocarbons which can be adducted with thiourea include the branched paraffins, cyclohexyl-paraffins, certain chlorocompounds and some branched cyclic aldehydes, alcohols, naphthalenes, and ketones (2). Recent research has shown that substituted aromatics can be complexed with thiourea. Substituted aromatics known to adduct are o-xylene, 1,2,4 trimethylbenzene, and the isomers of trichlorobenzene. Certain aromatics can be induced to adduct if an additional compound, referred to as an inductor, is present. The inductors' contribution to the complexing is not well understood, yet the inductor appears to be selective with regard to certain aromatics.

Numerous organic compounds have been separated by adduct formation with urea and thiourea by batch or continuous methods. The continuous method uses a fluidized, fixed or moving bed of urea or thiourea with which the organic components are brought into contact.

The adduct crystals are filtered or decanted, then decomposed usually by steam distillation or by heat.

Historical Review

The words complex and adduct came into common use during the formative years of synthetic organic chemistry to designate substances which do not appear to be held together by classical chemical bonds. These substances were designated by early German investigators as "Einschlussverbindungen" or inclusion compounds. The discovery of urea adducts was made accidentally in 1940 by Bengen while studying the action of urea on proteins in pasteurized milk. In these studies frothing and formation of an emulsion were causing difficulties, so Bengen added a small amount of n-octyl alcohol as a defrothing agent. Bengen observed the formation of long crystals at the interface of the liquid layers. On attempting to reproduce these crystals, Bengen discovered that they also form when a saturated aqueous urea solution was mixed with n-octanol. Further investigation extended the urea adduct formation to include higher alcohols, acids, n-paraffins, and other straight chained compounds (2).

Bengen's work came to Lloyd Fetterly's attention in the Technical Oil Mission publications of 1946. Fetterly was attempting to improve the octane ratings of gasoline by using a complexing agent which would readily react with the low octane branched paraffins. Although urea would not complex with these hydrocarbons, he discovered that thiourea would complex with the branched-chained paraffins as well as with naphthenic compounds, some ketones, carbon tetrachloride, and some

other chloro compounds. His studies also showed complex formation with selenourea and tellurorea. Concurrently in 1947 Angla, in France, independently reported similar complexes between thiourea and organic compounds of the terpene, camphene, cyclohexane, and chloroparaffin classes (3).

In 1950 Redlick contributed to the current knowledge of thiourea channel adducts by conducting thermodynamic studies at equilibrium conditions. Using Gibbs free energy relationships and a chemical equilibrium equation, Redlich reported the composition and equilibrium constants for the decomposition of thiourea complexes of various isoparaffins, naphthenes and carbon tetrachloride. He concluded that equilibrium appeared to be that of a normal chemical reaction (4).

The indeterminate structure of the channel adducts prompted Smith (5) and Schlenk (6) to conduct x-ray analysis on urea and thiourea complexes in 1949. Smith examined a number of urea complexes of n-hydrocarbons, alcohols, acids and esters of various chain length C_8 - C_{50} by the powder method. Results indicated essentially identical powder patterns for all complexes. The extinctions and symmetry of the Weissenburg patterns established the space group as $C6_12-D_62$ or its enantiomorph $C6_52-D_63$ (See Appendix A). The unit cell for the complexes is hexagonal with lattice parameters $a = 8.230 \text{ \AA}$ and $c = 11.005 \text{ \AA}$.

The urea molecules were shown to form three interpenetrating helical spirals with the hydrocarbon situated in the center. The urea molecules are held together by spirals of hydrogen bonds between an oxygen atom and a nitrogen atom of adjacent molecules turned 120° with

respect to one another. Each oxygen is hydrogen bonded to four nitrogen atoms and each nitrogen to two oxygen atoms. The hydrogen bonds, which are essentially coplanar with the urea molecules to which the nitrogens are attached, are of two types. The N...O distances are 2.93 Å for the shorter and 3.03 Å in length for the longer. The C-N-H...O bond angles are 136° and 116° respectively for the strong and weak bonds.

The hydrocarbons located inside the channel, are at the special positions (o,o,z) in a zigzag planar configuration with the long axis of the molecule parallel to the c-axis. The hydrocarbon molecules show a disorder parallel to the c-axis. Rotation of the hydrocarbon about the c-axis appears to cause this disorder.

Stability of channel adducts involves several physical and chemical phenomena. Pure urea forms tetragonal crystals, whereas urea adducts are hexagonal. The bond distances between the two forms are in Table 1.

Table 1. Bond distances (Å) in urea.

Urea-Hydrocarbon Complexes		Pure Tetragonal Urea	
C-O	1.28	C-O	1.25
C-N	1.33	C-N	1.37
N-H...O	2.93 Å	N-H...O	2.99 Å
N-H...O	3.03 Å	N-H...O	3.03 Å

The shortening of the N-H...O bond yields a lower energy value which indicates more stability in the hexagonal vs tetragonal form (9). The complexes are further stabilized by the urea-hydrocarbon van der Waals

bonds. Schlenk calculates a value of 2.8 kcal per CH_2 group in urea complexes. Smith, however, refuted any unusually strong interaction between the hydrocarbons and the urea such as that indicated by Schlenk. Smith suggests that the closest possible approach between a carbon atom of the hydrocarbon and an oxygen atom of the urea is approximately 4.1 Å which is as large as or larger than normal van der Waals distances for these atoms.

Fetterly (2) points out a new concept that a stronger hydrogen bond can exist only when it is supported by an otherwise inert surface (i.e., the channel hydrocarbon) capable of exerting only weak dispersion forces. Without the presence of a hydrocarbon, urea or thiourea complexes cannot exist. Fetterly referred to these additionally stabilized bonds as "supported hydrogen bonds." It was this phenomenon that Fetterly claimed stabilized urea and thiourea adducts.

Another factor that may contribute to the stability of the complexes is that the van der Waals forces in the tetragonal urea may be less than normal because of the relatively open structure (Figure 1), while those in the complex would appear to be normal (5). This is also indicated by the smaller volume occupied by the complex compared to the same number of urea molecules and guest hydrocarbon molecules in their standard, pure crystalline states.

The complexes of non-aromatic thiourea discovered by Fetterly and Angla are similar to urea complexes in almost every respect. The arrangement of thiourea molecules in the adducts is rhombohedral, forming a pseudohexagonal but similar cell to that of urea complexes.

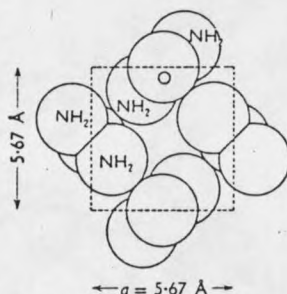


Figure 1. Tetragonal urea showing the relatively open structure.

There are 18 thiourea molecules per unit cell with space group $R\bar{3}2/C$ and $a = b = 15.8 \text{ \AA}$, $c = 12.5 \text{ \AA}$ along the channel length (3). As with urea, the crystal structure of thiourea in an adduct is different from that of the pure reagent. Pure reagent thiourea crystalizes in space group $Pbnm$ and is orthorhombic. The unit cell constants of the thiourea adducts apparently vary slightly with the nature of the adducted hydrocarbon, hence, so will the channel dimensions vary slightly.

The larger size of the sulfur atom in thiourea, compared with the oxygen in urea, results in a channel of larger dimensions capable of adducting larger cross-sectional guest hydrocarbons. In Figure 2 the cross-sections show the thiourea adduct schematically containing the larger guest molecule. The distance between two molecules lying one above another is 4.2 \AA , and the edge length of the cell is 5.4 \AA ,

these values compare with 3.7 Å, and 4.8 Å respectively for the urea adduct.

Figure 2 shows only the oxygen or sulfur atoms with arrows pointing toward the carbons. The dotted lines in the urea hexagonal prism connect oxygen atoms of the same elementary cell and indicate the helical structure. The three shaded regions in the thiourea adduct represent planes formed by three coplaner sulfur atoms pointing directly into the channel. Schlenk suggested that because of the optimal positions of the three coplaner thiourea molecules and their strong dipole moments that these planes were regions of maximum attraction (6). Coplaner sulfur atoms occur every third sulfur along an edge and since each atom is approximate 4.2 Å apart, the distance between planes is 12.5 Å which is the c-axis unit cell dimensions.

A number of researchers conducted composition studies on urea and thiourea complexes. In urea and thiourea complexes the ratio of urea or thiourea molecules to guest hydrocarbon molecules increases linearly with the length of the guest hydrocarbon (Table 2). Exception to this relationship is with guest hydrocarbons which exhibit what Schlenk referred to as compressibility. Table 2 uses w-w'-methylene bridged dicyclohexyls as an example of compressible guest hydrocarbons.

Schlenk (6) recognized that dicyclohexylmethane, 1, 2 dicyclohexylethane and 1, 3 dicyclohexylpropane showed an almost constant mole ratio of 6:1. Their x-ray patterns shows a compression of the slender paraffinic portion of the guest molecule in the channel. In this way several w,w - dicyclohexyl derivatives can fit into the

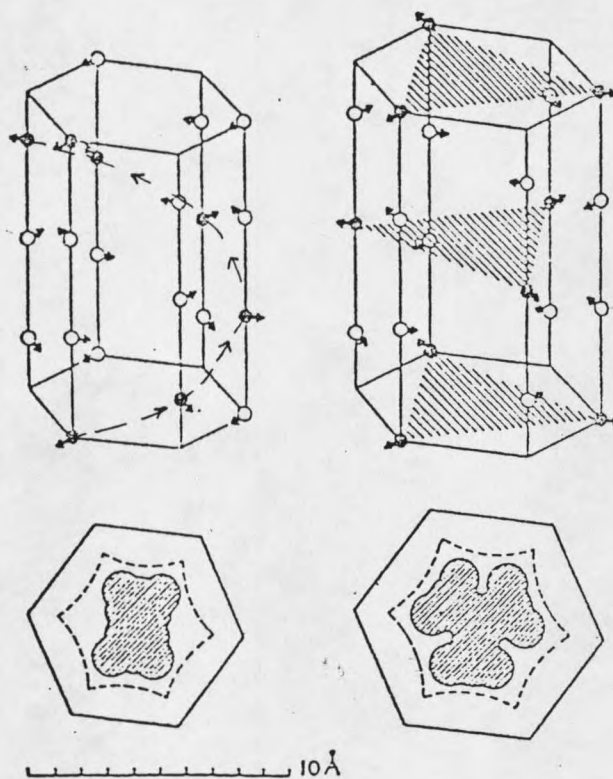
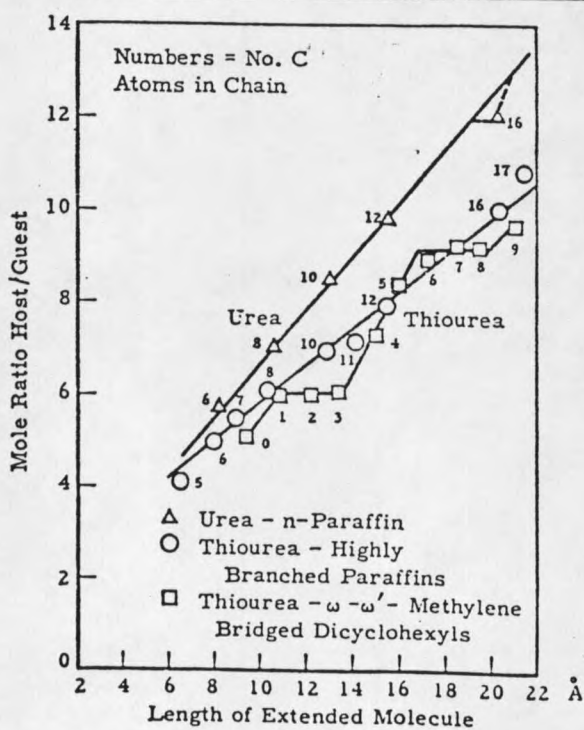


Figure 2. Lattice of urea (left) and thiourea (right) adducts. Top: each circle represents a urea or thiourea molecule, the arrow points from the oxygen or carbon atom toward the sulfur atom. Bottom: cross-section with included hydrocarbons [reproduced from Schlenk (6)].

same channel space. Thus, if the fully extended length of the guest hydrocarbon exceeds an integral multiple of $c/2$ only slightly, there is a tendency for the enclosed molecule to take up a somewhat less extended form whenever possible to fit the repeating half unit of the thiourea complex. In this way the terminal cyclohexyl rings coincide with the zones of maximum attraction (12). Since only one site of maximum attraction occurs per unit cell, molecule ratios of multiples of three (i.e. 3:1, 6:1, 9:1 etc) will preferentially occur when the guest hydrocarbon can compress. In Table 2 the plateaus at molecule ratio 6:1 and 9:1 exhibit this behavior. Guest molecules which cannot compress will form complexes of multiples other than three.

Table 2. Lengths of the guest hydrocarbon plotted against the molar ratio thiourea: guest for compressible and noncompressible guest.





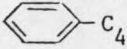

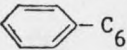
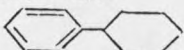
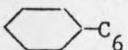
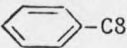
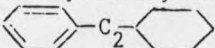
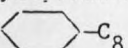
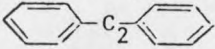
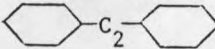
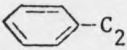
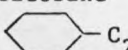
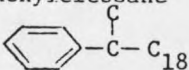
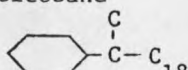
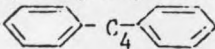
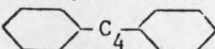




McLaughlin compiled a comparison list (Table 3) of organics, of similar size and shape, that will or will not adduct with thiourea. Although the dimension of the benzoid ring is very close to those of the cyclohexyl ring, no adduction occurs. This suggests that adduction with thiourea requires the guest hydrocarbon to have other properties besides the appropriate cross-sectional dimensions.

Some compounds which are non adducting by themselves can be induced to form a thiourea complex when mixed with certain adduct formers called "inductors". Examples of induced compounds are toluene, benzene, the xylenes, neptane, decane, dipentene, and 1, 3 - dimethylcyclohexane. Some examples of inductors are, cyclohexane, dicyclohexyl, 2, 2, 4 trimethylpentane and decahydronaphtholene (2).

McCandless (10) reported the inductors which would adduct C_8 and C_9 alkylbenzenes. His work exemplified the ability of extractive crystallization with thiourea to be an effective separation technique for aromatic isomers and aromatics of close boiling points. For example CCl_4 as an inductor exhibited a selectivity of ethylbenzene > o-xylene > p-xylene > m-xylene while the use of 1,2,4 trichlorobenzene (inductor) resulted in a selectivity of o-xylene > p-xylene > m-xylene > ethylbenzene. With the C_9 alkylbenzenes, CCl_4 as an inductor was selective for n-propylbenzene while 1,2,4 trichlorobenzene was selective for 1,2,4 trimethylbenzene. Similarly o-xylene and 1,2,4 trimethylbenzene exhibited the same selectivity as 1,2,4 trichlorobenzene when used with mixtures of the C_9 and C_8 aromatics, respectively. All of the inductors mentioned above also form complexes alone.

Table 3. Compound which form adducts with thiourea compared to similar compounds which do not form adducts.

<u>Nonadducting</u>	<u>Adducting</u>	<u>Adducting</u>
Benzene 		Cyclohexane 
Toluene 		Methylcyclohexane 
n-Butylbenzene 		n-Butylcyclohexane 
n-Hexylbenzene 	Phenylcyclohexane 	n-Hexylcyclohexane 
n-Octylbenzene 	1-Phenyl-2-cyclohexylethane 	n-octylcyclohexane 
1,2-Diphenylethane 		1,2-Dicyclohexylethane 
1-Phenyleicosane 		2-Cyclohexyleicosane 
2-Phenyleicosane 		2-Cyclohexyleicosane 
1,4-Diphenylbutane 		1,4-Dicyclohexylbutane 
Tetraline 		Decalin 

Welling measured the unit cell dimensions of the binary 1,2,4 TCB/1,2,4 TMB thiourea adduct and found $a=12.64\text{\AA}$, $b=15.3\text{\AA}$, $c=9.8\text{\AA}$, $\alpha = \gamma = 90.0^\circ$ and $\beta = 113.85^\circ$. Welling also enlisted the Molecular Structure Corporation to obtain a structure for the 1,2,4 TMB thiourea adduct. Unit cell dimensions obtained were $a=12.3\text{\AA}$, $b=15.1\text{\AA}$, $c=10.0\text{\AA}$, $\alpha = \gamma = 90.0$, and $\beta = 112.7^\circ$ (12). Due to the disordered arrangement from a translational view as well as through the inversion center, a conclusive structure was not obtained from the Molecular Structure Corporation. However, Welling did postulate some ideas about the thiourea lattice and 1,2,4 TMB interactions from intermolecular distances.

Initially Welling reasoned that benzene did not adduct because the pi clouds, which lie both above and below the plane of the carbon atoms, form a repulsive force with the lone pairs of electrons on the nitrogen and sulfur of thiourea. With this idea Welling speculated that 1,2,4 TMB adducted because of an interaction between the methyl groups and the thiourea lattice. The isomers of 1,2,4 TMB (ie 1,3,5 TMB and 1,2,3 TMB) did not adduct indicating a steric hinderance toward adduction. The methyl groups on 1,3,5 trimethylbenzene are symmetrically dispersed about the benzene ring and the methyl groups on 1,2,3 trimethylbenzene are concentrated to one side of the ring. Both isomers are larger in diameter than that permitted by the thiourea lattice and hence no adduction occurs.

In 1,2,4 TMB the benzene ring increases the electron density of the carbon atom on the methyl group (13). The methyl groups become slightly acidic, or partially positive, through this resonance effect

and will induce weak hydrogen bonding with the sulfur atom in the thiourea molecules. Welling reasoned that if a hydrogen bond were to be possible, the distance between the C-H group and sulfurs must be closer than the non-bonded van der waal distance. Since the covalent radii for a C-H group is 1.08 A, the van der Waals radii for hydrogen is 1.15 A, and the van der Waals radii for sulfur is 1.85 A, the non-bonded distance is the sum of these radii, or 4.08 A. The Molecular Structure Corporation reported the observed contacts between sulfur and carbon. These distances are tabulated in Table 4. All of the distances are less than the non-bonded distance (4.08 A) and thus hydrogen bonding is a possibility (12).

Table 4. Interatomic distances between sulfur and carbon in the 1,2,4 TMB-thiourea adduct.

Atom 1	Atom 2	Distance A
S1	C11	3.90
S1	C12	3.65
S1	C13	3.81
S2	C13	3.91

At Montana State University researchers Fait and Spinti, et al, have conducted structural analysis on non-aromatic isostructural thiourea adducts. Fait reproduced Lennes' crystal structure for the cyclohexane-thiourea adduct and independently determined the crystal structure of the carbon tetrachloride-thiourea adduct and the bicyclo (2.2.2) octane-thiourea adduct. Spinti obtained a crystal structure for the cis-paramenthane thiourea adduct. All three complexes crystallize in the rhombohedral space group, $R\bar{3}c$, as is

characteristic for non-aromatic complexes. In addition, the honeycomb shaped thiourea lattice formed with all three complexes. The lattice parameters are tabulated in Table 5. The guest hydrocarbon was disordered translationally as well as around the axis of symmetry in all three adducts. Figure 3 shows the thiourea lattice with the guest hydrocarbon, cis-paramenthane, (Fig. 4) disordered in the channel. Fait reported sulfur atoms pointing into the channel and hydrogen bonded to other thiourea molecules. He concluded that dipole-dipole interactions between the three coplaner thiourea sulfurs and the CCl_4 carbon and between the three coplaner thiourea sulfurs and cyclohexane hydrogens are responsible for binding of the substrate hydrocarbon in these complexes. Fait recognized that the sulfur-carbon double bond distance for thiourea in these non-aromatic complexes was lengthed in comparison with that of pure thiourea. Table 6 shows the magnitude of these bond distances. If a linear relationship between bond strength and the $\text{c} = \text{s}$ bond distance is assumed then the conclusion which can be drawn is that the dipole interaction between the coplaner sulfurs and the guest hydrocarbon is stronger than the hydrogen bonding interaction in pure thiourea.

Table 5. Unit cell parameters for cis-paramenthane, cyclohexane and carbon tetrachloride adducts. All distances and angstroms.

Hydrocarbon Adducted with	A	B	C	α	γ	β	Space Group
Cyclohexane	15.708(1)	15.708(1)	12.431(2)	90.0	90.0	120.0	R3bar
CCl ₄	15.539(1)	15.539(1)	12.529(2)	90.0	90.0	120.0	R3bar
Cis-paramenthane	15.935(1)	15.935(1)	12.489(2)	90.0	90.0	120.0	R3bar

Table 6. Sulfur-carbon double bond distances in the thiourea for various non-aromatic adducts.

Crystal	Thiourea Sulfur = Carbon Bond Distance
Cyclohexane-Thiourea Adduct	1.725 (9)
CCl ₄ -Thiourea Adduct	1.744 (8)
Bicyclo [2.2.2] Octane Thiourea Urea Adduct	1.731 (5)
Pure Thiourea	1.708 (5)

Research Objectives

The purpose of this research was to continue the investigation of the selectivity mechanism of aromatic thiourea adducts begun at Montana State University. This objective would be facilitated by:

1. Obtaining a crystal structure of a 1,2,4 TMB-thiourea complex using a more correct model than that employed by Welling and the Molecular Structure Corporation.
2. Obtaining a crystal structure of a 1,2,4, Trichlorobenzene-thiourea adduct in order that the heavier chlorine atoms might resolve the disorder problem associated with the guest hydrocarbons in thiourea complexes.
3. From the intermolecular distances and positions yielded from these structures, ascertain the interactive forces between the thiourea honeycomb lattice and an aromatic guest hydrocarbon.

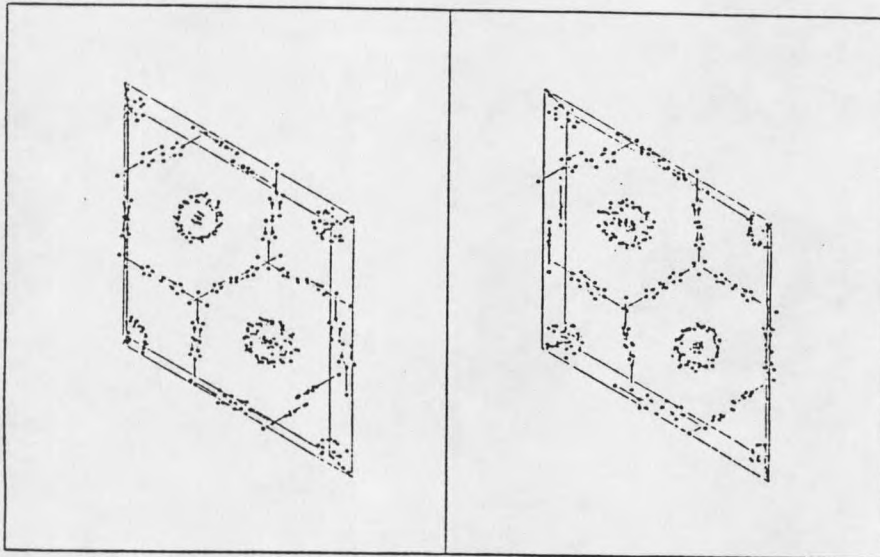


Figure 3. Cis para-menthane adduct viewed down the a-c diagonal.

EXPERIMENTAL

Crystal Preparation

The preparation of 1,2,4 trimethylbenzene-thiourea adducts and 1,2,4 trichlorobenzene-thiourea adducts has already been reported (10,11,12). However, an alternative technique was employed to avoid twinning and enhance slow crystal growth. A 20 ml saturated solution of pure reagent thiourea and methanol was heated in a constant temperature bath of 40°C. Approximately three to four milliliters of 1,2,4 TMB or 1,2,4 TCB was added to this solution and the mixture was sealed to avoid evaporation. After one-half hour the mixture was taken from the 40°C bath and placed in a 17°C constant temperature bath. Crystals from each aromatic system formed within 24 hours. The adduct crystals formed were long, clear, hexagonal, and needle-like. Any white, flat or plate-like crystals were known to be pure thiourea crystals and were avoided when crystals were selected for x-ray analysis.

Crystal Analysis

To ensure the reagent 1,2,4 TCB was not contaminated with its isomers, a distillation was performed. At the time of distillation the barometric pressure was 638 mm Hg and the reflux ratio was 20:1. In addition, both adduct systems were analyzed by an elemental analysis and by using a Varion Aerograph Series 1400 Gas Chromatograph.

Elemental analysis was conducted on the 1,2,4 TCB adduct 1,2,4 TMB adduct and pure reagent thiourea. The instrument employed was a Carlo Erba Strumentazione Elemental Analyzer.

Crystals were prepared for both analyses by vacuum filtering crystals, then placing them on filter paper to air dry for one hour. If crystals are exposed to air for any extended length of time the guest hydrocarbon will evaporate and the adduct will decompose. Crystals to be analyzed with the gas chromatograph were then placed in a minimum amount of boiling, distilled water. The thiourea dissolved in the water layer and the 1,2,4 TMB or 1,2,4 TCB formed a separate, immiscible layer. The organic layer and the aqueous layer were separated with a separatory funnel. The organic cut was analyzed with the Varion Gas Chromatograph using a 5% diisodecylphthalate and 5% bentone 34 on Chromosorb W column at 150° C. The carrier gas used was helium. Pure reagent 1,2,4 TMB and 1,2,4 TCB were analyzed with the gas chromatograph to compare as standards.

The dried crystals to be analyzed with the elemental analyzer were placed in small silver capsules and sealed with pliers. Each capsule was placed in a electrobalance which measured to the nearest 10^{-4} mg. To ensure that the capsule was sealed and not losing weight, due to evaporation of the 1,2,4 TMB or 1,2,4 TCB, the weight was monitored for 5 minutes. If in that time no change in weight was recorded, the capsule was removed from the balance and placed in the analyzer. Cicloesanone and Sulfanamide were used as the standards. Weight percentages of carbon, nitrogen and hydrogen were measured for each sample.

Adduct Density

The density of an adduct was determined by suspending the adduct in a mixture of miscible liquids, one more dense than the adduct and one less dense. The density of the solution which is in gravity equilibrium with the adduct is also the density of the adduct (21). In the case of 1,2,4 TCB a medium of carbon tetrachloride and methanol was used to suspend the adducts and for the 1,2,4 TMB system the medium used composed of heptane and 1,2,4 trichlorobenzene. Once the crystals would neither sink nor float in the medium, a known volume was weighed and the density calculated. The densities were 1.49 g/ml and 1.19 g/ml for the 1,2,4, TCB adduct and 1,2,4 TMB adduct respectively.

Crystal Mounting

Selecting an appropriate crystal for x-ray analysis required placing crystals on a microscope slide and positioning the slide under a dissecting microscope. Ample room was allowed for the crystals to be cut or fragmented along their length. Crystals were cut or fragmented to the appropriate size using a sharp razor blade or dissecting scalpel. Once a crystal fragment of suitable size and shape was selected, a glass fiber dipped in adhesive Paratone-N was used to transport the crystal from the microscope slide to a low lead glass capillary tube of approximately 0.8 mm in diameter. Care was taken not to choose pure thiourea crystals which might have crystallized out of the mother liquor.

The capillaries were sealed by heat or glue to prevent air exposure from decomposing the crystal. To check for twinning (multiple crystal growth), the crystals were examined under polarized light. Crystals which extinguished upon rotation between crossed nickle prisms were used for x-ray analysis. The 1,2,4 TMB adduct crystal used for data collection was cylindrical in shape measuring 0.6 mm in diameter and 0.8 mm in length. The 1,2,4 TCB adduct crystal was also cylindrical in shape and had dimensions 0.7 mm in diameter and length of 0.9 mm.

Photographic Film Studies

A Weissenburg camera was employed to check crystal quality and estimate unit cell dimensions. The radiation source used was copper with a nickel filter. Weissenburg photographs taken for a deteriorated adduct would show few, if any, layer lines and those lines which were present would contain indefinite spots. Once a suitable crystal was obtained, oscillation, zero level, first level, and second level photographs were collected to determine approximate unit cell dimensions.

Numerous Buerger Precession photographs were taken for the 1,2,4 TCB complex. These photographs were expected to provide support for, as well as clarification of, the unit cell dimensions. Problems were encountered which involved the alignment of the crystal for precession photographs and this method was abandoned since the photographs were not necessary to proceed with the diffractometer data collection.

Diffraction Data Collection

Intensity data for both adduct systems were collected on a Nicolet R3mE automatic four circle diffractometer using the omega scan technique with the 1,2,4 TCB complex and the theta-two-theta scanning technique with the 1,2,4 TMB complex. The x-ray source used was MoK_2 radiation of $\lambda = 0.71069 \text{ \AA}$, and monochromated with a graphite crystal monochromator. Both data sets were collected at room temperature. Throughout the course of the data collection three standard reflections were measured every one hundred reflections. There was no decrease in the intensity of these standards over the course of the data collection. For instance, the decrease in the average value of these standards was about 7% by the end of the data collection for the 1,2,4 TMB complex. All intensities were corrected for the changes in the standards. Lattice parameters for the 1,2,4 TCB complex were obtained from the least squares fit of 20 centered reflections for which $25^\circ < 2\theta < 35^\circ$. For the 1,2,4 trimethylbenzene thiourea complex the same procedure was followed using 25 centered reflections with $28^\circ < 2\theta < 31^\circ$. The data collected on each complex ranged from 3° to 50° on 2θ . Asmuithal adsorption correction data was taken for both complexes.

For the 1,2,4 TMB complex the linear absorption coefficient, $\mu (\text{MoK}_2)$ was 4.01 cm^{-1} and no correction was made for absorption. For the 1,2,4 TCB complex, $\mu (\text{MoK}_2) = 8.89 \text{ cm}^{-1}$ and an empirical absorption correction was made to the intensity data. The two data sets were reduced in the usual manner with appropriate Lorentz and polarization corrections. Scattering factors for Cl, S, O, N, C and H and anomalous

scattering terms for all types except H were taken from the International Tables for X-ray Crystallography (18); all atoms were assumed to be in the zero ionization state.

For the 1,2,4 TCB-Thiourea complex, 3397 intensities collected yielded 1610 observed reflections. The data set for the 1,2,4 TMB-Thiourea complex had 3161 intensities collected of which 1536 were observed reflections. Criterion for observed reflections was $I > 3\sigma$. The data sets for both complexes reveal the monoclinic primitive lattice. In addition, both sets showed the following extinctions in Table 7.

Table 7. Extinctions and associated symmetries of the 1,2,4 TMB-thiourea complex and the 1,2,4 TCB-thiourea complex.

Reflections Absent	Symmetry Indicated
U00	
U0G	n glide perpendicular
U0U	to b
OUO	2 fold screw axis on b

From these extinctions the space group P21/c was determined for both structures.

A least squares fit of 25 centered reflections produced the unit cell dimension of $a = 10.037 \text{ \AA}$, $b = 15.155 \text{ \AA}$, $c = 12.255 \text{ \AA}$, $\beta = 112.77^\circ$, and $a = 9.779 \text{ \AA}$, $b = 15.355 \text{ \AA}$, $c = 12.293 \text{ \AA}$, $\beta = 111.85^\circ$ for the 1,2,4 TMB-thiourea complex and the 1,2,4 TCB-thiourea complex respectively.

Solution of Structure and Refinement

The 1,2,4 TCB complex was solved initially by direct methods. Since the two complexes are isostructural with respect to the thiourea honeycomb lattice, sulfur positions from the 1,2,4 TCB complex were used for the initial phasing of the 1,2,4 TMB-thiourea complex. Once the sulfur positions were found, the thiourea nitrogens and carbon appeared on the difference maps. These atoms, along with any other strong peaks, were added to a model and the model's structure factors were compared to the observed structure factors. A resultant R value was obtained and if the R value decreased, the peaks were left in the model. At this point the thiourea positions were well-defined, yet the channel atoms were disordered.

Refinement for both complexes was done using a block cascade least-squares refinement program where the minimization function;

$$M = \sum \text{weight} (|F_{\text{obs}}| - |F_{\text{calc}}|)^2$$

used to refine 101 parameters in each full matrix block. F_{obs} was the observed structure factor and F_{calc} was the calculated structure factor (22).

The thiourea molecules were well-behaved and thus a model was easily fit to the thiourea lattice. Once the carbon, sulfur and nitrogen atoms of the thiourea were well defined, hydrogen atoms of the thiourea began to appear on the difference maps and the thiourea molecules were refined anisotropically.

The 1,2,4 TMB or 1,2,4 TCB remained disordered in the channel and were refined isotropically. In the final refinement the weighting factor used was

$$\text{Weight } 1/[\sigma^{**2}(F) + (.0004F*F)].$$

The 1,2,4 TMB-thiourea structure refined to $R = .1053$, $R_w = .0911$, $R_g = .0990$, $R_m = .0990$, and goodness of fit = 2.399. The 1,2,4 TCB-thiourea structure with the two ring disordered model refined to $R = .0951$, $R_w = .0927$, $R_g = .1061$, $R_m = .1061$, and goodness of fit = 2.650. Without the models, both structures refined to about $R = 0.15$.

RESULTS AND DISCUSSION

Discussion of X-ray Crystallography

An ideal crystalline substance is a homogeneous solid in which the atomic or molecular arrangement repeats by translation in three dimensions; the repeat distance and direction can be described by a three dimensional coordinate system. A crystal is composed of atoms oscillating about regular positioning of a lattice, repeating in accordance with the crystal system and symmetry (26). If x-rays are passed through a crystal the incident beam is diffracted by the electrons of the atoms according to Bragg's law of diffraction;

$$n\lambda = 2d\sin\theta$$

n = (1,2,3,4, . . .)

λ = wavelength of incident radiation

d = distance between reflecting planes

θ = angle between the incident or reflecting surface

The intensity and coordinates of the reflecting or diffracted radiation are collected by the diffractometer using a radiation counter. The intensity of a diffracted wave is dependent upon the atomic position and the atomic scattering factor, which is a function of the number of electrons in the atom. Furthermore, since changes in temperature of crystals affects the thermal vibrations of the atoms, the intensities must be corrected for this temperature effect. In

general the greater the vibrations the more the intensities will be lowered.

The intensities of the reflections from the diffracted x-rays are directly obtainable from a radiation counter; however, the phases of the reflections are not directly obtainable, yet they are essential for crystal structure determination. Crystallographers have shown that the wave scattered by a crystal can be characterized by a quantity, F_{hkl} , referred to as the structure factor (23). More generally, the structure factor for any given configuration of matter is the ratio of the amplitude of the wave scattered by all the matter in that configuration in any direction to that scattered by a single electron under corresponding conditions. Thus, following this definition, the structure factor of an electron is always unity (24). The amplitude of a scattered wave is proportional to the intensity, only after scaling, Lorentz-Polarization corrections, absorption and other comperical corrections are applied to the intensity.

Mathematically:

$$I_{hkl \text{ cal}} = (F_{hkl \text{ cal}})^2$$

$$F_{hkl} = \sum_j f_j e^{2\pi i(hx_j + ky_j + lz_j)}$$

or,

$$F_{hkl} = \sum_j f_j e^{i\phi_j}$$

where I_{hkl} = intensity of hkl reflection

$$\begin{matrix} x_j \\ y_j \\ z_j \end{matrix} = \text{fractional coordinators}$$

$$f_j = \text{scattering power of an atom at angle } \theta$$

The scattering power of an atom is tabulated in the literature for all elements. The term θ , is referred to as the phase of the reflected wave. Each F_{hkl} is complex; that is, it is characterized by both a magnitude, $|F_{hkl}|$, and a phase θ_{hkl} . The magnitude can be experimentally observed but, as mentioned previously, the phase cannot (25).

If, in studying the arrangement of atoms in a given crystal a particular model is proposed, the set of F_{hkl} 's of the model can be computed. The test for correctness of a crystal-structure model to be correct is that the set of structure factors computed, $F_{hkl} \text{ calc.}$ match the observed structure factors, $F_{hkl} \text{ obs.}$ It is, however, possible to obtain a good agreement with an incorrect structure. This calculation is greatly simplified by fast computers.

The ultimate goal in the determination of a crystal's structure is finding the positions of all the atoms in the unit cell. These atomic positions are not found directly but are deduced from the electron density. Atomic positions are found where the electron density is at a maximum. The electron density, $\rho(x,y,z)$, is computed using the equation:

$$\rho(x,y,z) = 1/V^* \sum \sum \sum F_{hkl} e^{-2\pi i(hx + ky + lz)}$$

where V = volume
 F_{hkl} = structure factor of hkl reflection
 x
 y = fractional coordinates
 z

Thus, once structure factors are determined, the electron density can be computed using Fourier synthesis. The F_{hkl} calc and F_{hkl} obs determined are refined using least squares calculations. The measure used to quantify the agreement between the model and the actual data is the R value. The R value equation used for the 1,2,4 TMB complex and the 1,2,4 TCB complex was:

$$R = \frac{\sum ||F_o| - |F_c||}{\sum |F_o|}$$

$$R_w = \frac{\sum [||F_o| - |F_c|| * (\text{weight})^{1/2}]}{\sum [F_o * (\text{weight})^{1/2}]}$$

$$R_g = \frac{[\sum (\text{weight} * [||F_o| - |F_c||]^2)]^{1/2}}{\sum [\text{weight} * F_o^2]}$$

$$R_m = R_g \text{ (calculated for the scale factor which minimizes } R_g \text{) (22).}$$

Conventionally, R values less than about 0.07 reveal that the model has "solved" the crystal structure, although technically it only means that the model fits the data within reasonable agreement. To claim the model represents the true crystal structure, the agreement (R value) between F_{obs} and F_{calc} must be acceptable and the model must adhere to chemical and physical laws.

Aromatic-Thiourea Complexes

The Molecular Structure Corporation's x-ray analysis of 1,2,4 TMB-thiourea complex was unable to resolve the disorder of the 1,2,4 TMB in the channel. This motivated a new structure determination using a different model solution. Furthermore, it was hypothesized that if the methyl groups in 1,2,4 trimethylbenzene were replaced with chlorines, forming 1,2,4 trichlorobenzene, that these heavier chlorine atoms would appear more defined in an x-ray analysis. If the chlorine atoms were more defined in an x-ray data set, a correct model would be assembled easier.

From floatability the densities of 1,2,4 TMB-thiourea and 1,2,4 TCB-thiourea were 1.19 g/ml and 1.49 g/ml respectively. The elemental analysis listed in Appendix B proved the thiourea to be of pure reagent grade and a balance on nitrogen showed the mole ratio of thiourea to aromatic to be 4.38 and 3.55 for 1,2,4 TMB-Thiourea and 1,2,4 TCB-Thiourea respectively. These mole ratios were confirmed by the density measurements which yielded mole ratios of 4.40 and 3.55 for the 1,2,4 TMB-Thiourea and 1,2,4 TCB-Thiourea respectively. The distillation of 1,2,4 TCB and the gas chromatography analysis proved

the adducts to contain only the pure reagents (i.e. no isomeric impurities).

Additional structures studied for comparison in this work are listed in Table 8. As can be seen, the non-aromatics crystallize in the same space group $R\bar{3}m$ and have similar cell dimensions. The adduct containing a 50 mole percent of both 1,2,4 TCB and 1,2,4 TMB crystallizes in the same space group as the 1,2,4 TMB-thiourea and 1,2,4 TCB-thiourea complexes and has approximately the same cell dimensions. This change in space group between aromatic and non-aromatic adducts suggests that there is a fundamental change in the thiourea channel shape. This change indicates a possible different kind of interaction between the aromatic and the thiourea lattice than that between non-aromatics and thiourea.

The two adduct systems were proved to be isostructural when the thiourea positions from the 1,2,4 TCB-thiourea were successfully used for the initial phasing for the thiourea positions in the 1,2,4 trimethylbenzene-thiourea adduct. Figures 4 and 5 exhibit the similarities between both complexes' thiourea lattice. The structures show a pseudo hexagonal lattice with distorted channel walls. The view is down the a - c diagonal. Both structures have very similar atomic positions for the thiourea molecules. The graphics software in the SHELXTL package allowed for interatomic distances between bonded and non-bonded atoms to be found (22).

The graphics program showed each sulfur atom to be hydrogen bonded to NH_2 groups on four adjacent thiourea molecules. This is illustrated in Figures 6, 7, and 8 where the hydrogen bonding scheme in

Table 8. Structural data for related thiourea complexes. All distances and angstroms.

Hydrocarbon Adducted with	A	B	C	α	β	γ	Space Group	DENSITY (g/cm ³)
Cyclohexane	15.708(1)	15.708(1)	12.431(2)	90.0	90.0	120.0	R3bar	1.138
CCl ₄	15.539(1)	15.539(1)	12.529(2)	90.0	90.0	120.0	R3bar	1.415
cis para-menthane	15.935(2)	15.935(2)	12.489(2)	90.0	90.0	120.0	R3bar	1.16
1,2,3 TCB and 1,2,4 TMB	12.64	15.3	9.8	90.0	113.8	90.0	P2 ₁ /c	1.27
1,2,4 TCB and 1,2,3 TMB							P2 ₁ /c	1.3
1,2,4 TCB	9.779(1)	15.355(1)	12.293(2)	90.0	111.85	90.0	P2 ₁ /c	1.49
1,2,4 TMB	12.3 (1)	15.1 (1)	10.0 (2)	90.0	112.7	90.0	P2 ₁ /c	1.19
1,2,4 TCB and 1,2,4 TMB	9.886(7)	15.245(8)	12.313(6)	90.0	112.48(4)	90.0	P2 ₁ /c	1.28

the thiourea network of the 1,2,4 TMB-thiourea adduct is shown. The four hydrogen bonds, denoted as dotted or dashed lines, are of lengths 3.314 Å, 3.402 Å, 3.454 Å, and 3.452 Å. The corresponding lengths for the 1,2,4 TCB-thiourea adduct are 3.433 Å, 3.348 Å, 3.446 Å, and 3.408 Å. At room temperature pure crystalline thiourea has three sulfur-nitrogen hydrogen bonds of 3.526 Å, 3.394 Å, and 3.696 Å in length (15). The shortening of these hydrogen bonds in the complexes indicates a lower energy state and correspondingly a greater stability. Although Smith contends that compacting of the adduct structures is solely responsible for holding the adduct together, a review of Table 2 suggests other factors seem at work. For example, evidence of this is the fact that cyclohexane adducts, but benzene does not.

Schlenk suggests a zone of maximum attraction in each unit cell, corresponding to three coplaner sulfur atoms (see Figure 2). These zones are evident in both the 1,2,4 TCB-thiourea adduct and the 1,2,4 TMB-thiourea adduct. Figure 9 shows three coplaner sulfur in the 1,2,4 TMB-thiourea adduct, pointing directly into the channel exhibiting a zone of maximum attraction. The three thioureas do not form an equilateral triangle, but instead are slightly distorted about the a-c diagonal.

The thiourea lattice in each complex is by and large responsible for the space group symmetry and therefore the positions and intermolecular distances and angles are nearly identical for both structures. Figure 10 shows the three coplaner sulfur atoms for the 1,2,4 TCB-thiourea adduct with open lines forming a triangle. The

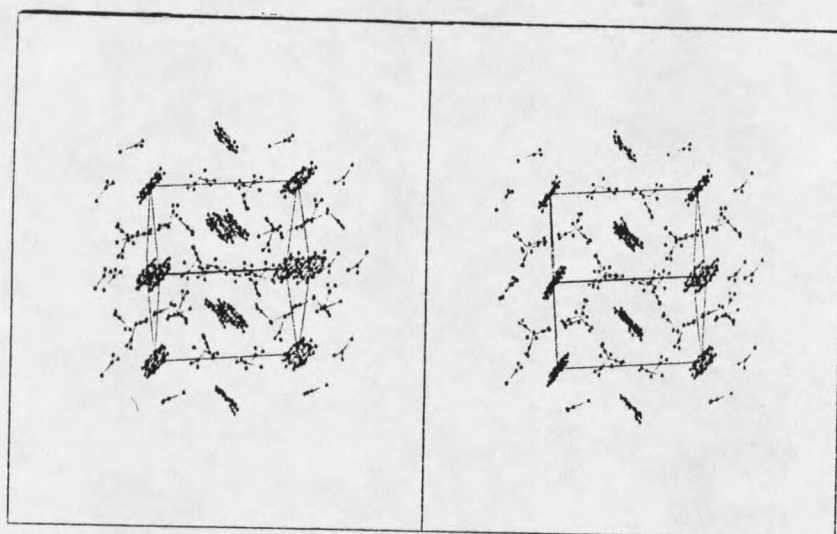


Figure 4. 1,2,4 TMB-thiourea complex viewed down the a-c diagonal.

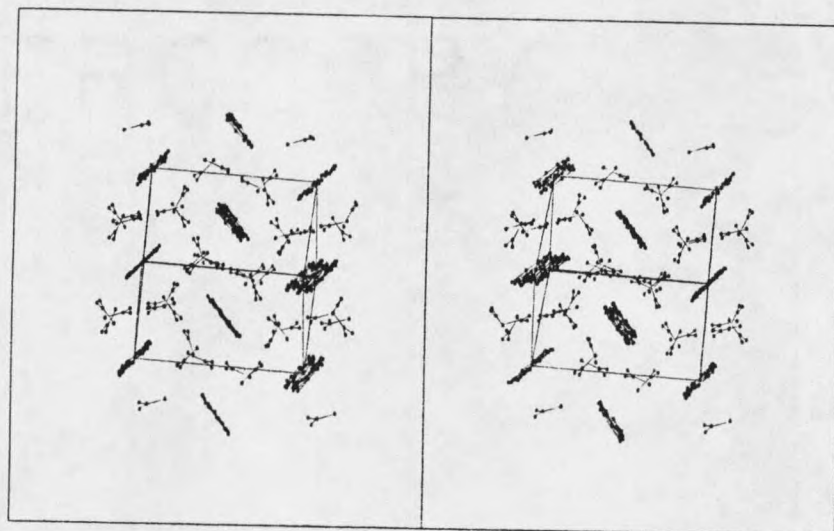


Figure 5. 1,2,4 TCB-thiourea complex viewed down the a-c diagonal.

center-to-center intermolecular distances and angles represented by this triangle are given in Table 9 for both complexes.

In order to obtain an idea of how the aromatic in the channel was situated a series of electron density difference maps were generated for the 1,2,4 TCB-thiourea adduct. The electron density difference map shown in Figure 11 was generated using only the refined thiourea. The view is looking down on the plane of the 1,2,4 trichlorobenzene. The contours range from -0.1 to 2.3 electrons per cubic angstrom.

Table 9. Center-to-center intermolecular bond distances and angles for the three coplaner sulfur atoms in the 1,2,4 TMB and 1,2,4 TCB adducts.

1,2,4 TMB-Thiourea		1,2,4 TCB-Thiourea
Distances Å		
S1-S2	9.043	9.067
S2-S3	7.053	7.073
S3-S1	8.165	7.944
Angles in Degrees		
<S1	48.1	48.6
<S2	59.4	57.4
<S3	72.5	74.0

The dotted lines are levels 0 and -0.1, the dashed lines are levels 0.1 to 1.1 and the solid lines are levels 1.1 to 2.3 electrons per cubic angstroms. The plot clearly shows the repeat down the channel of four peaks.

Upon superimposing an idealized 1,2,4 trichlorobenzene molecule in the channel it was evident that there are at least four different arrangements for which the molecule can satisfy the electron density

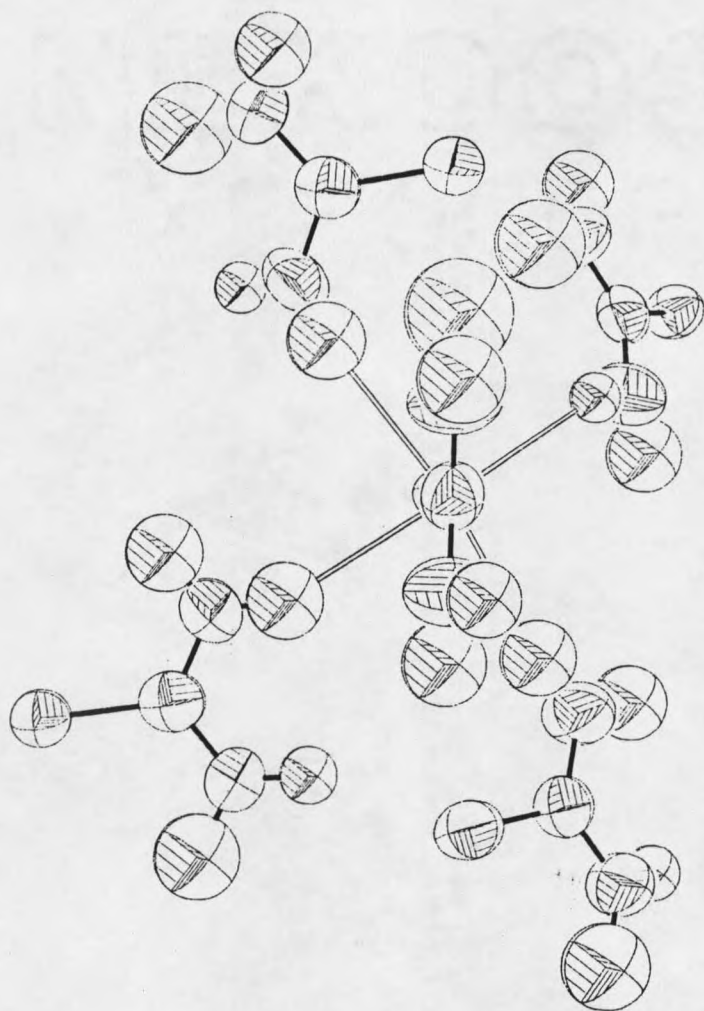


Figure 6. Hydrogen bonding scheme in the thiourea Lattice of the 1,2,4, TMB-thiourea adduct. The open lines are hydrogen bonds. The view is down the carbon=sulfur double bond.

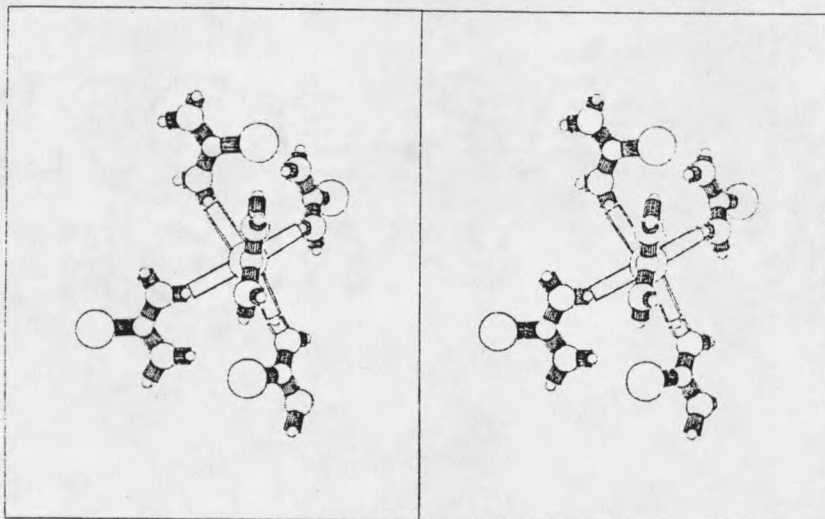


Figure 7. Steroview, down the carbon=sulfur double bond, of the hydrogen bonding network in within the thiourea lattice. Open lines are hydrogen bonds.

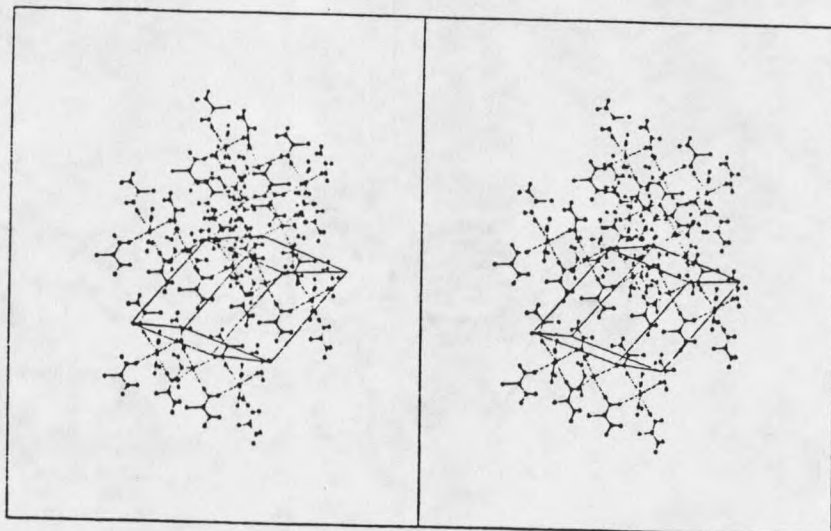


Figure 8. Steroview of the thiourea hydrogen bonding network, viewed down the a-c diagonal. Hydrogen bonds are drawn as dotted lines.

scheme. The combination of these arrangements yielded aromatic ring carbons overlapping chlorines and adjacent ring carbons. This gave an indication of the disorder which arose when constructing a model to describe the aromatic positioning in the channel. Figure 12 exhibits the electron density difference map with an idealized 1,2,4 trichlorobenzene molecule superimposed in one of at least four possible arrangements.

Models for the aromatics in both complexes were constructed by constraining atoms in the channel which resembled a benzene ring and refining them using least squares. For the 1,2,4 TMB-thiourea complex this resulted in four benzene rings seen in Figure 13. The benzene rings are in pairs which are planar. The two planar pairs of rings are nearly in the same plane. The 1,2,4 TCB-thiourea complex yielded two benzene rings in the same plane. This model is shown in Figure 14. The open lines indicate that it is not known to which aromatic carbon the substituent is bonded. In both models, atoms were added where peaks on the difference maps indicated a possible chlorine or methyl group.

Explanation of the disorder of the aromatics requires examination of the size and orientation of the guest and thiourea lattice. Within the thiourea lattice, coplanar sulfurs occur every third sulfur on the c-axis and this interplanar distance for both complexes is 12.54 Å (Figure 2). The maximum lengths of a 1,2,4 trichlorobenzene molecule and of a 1,2,4 trimethylbenzene molecule are 9.77 Å and 9.25 Å, respectively, including their van der Waal radii. Since the aromatics are found only within the region of the three coplanar sulfurs and

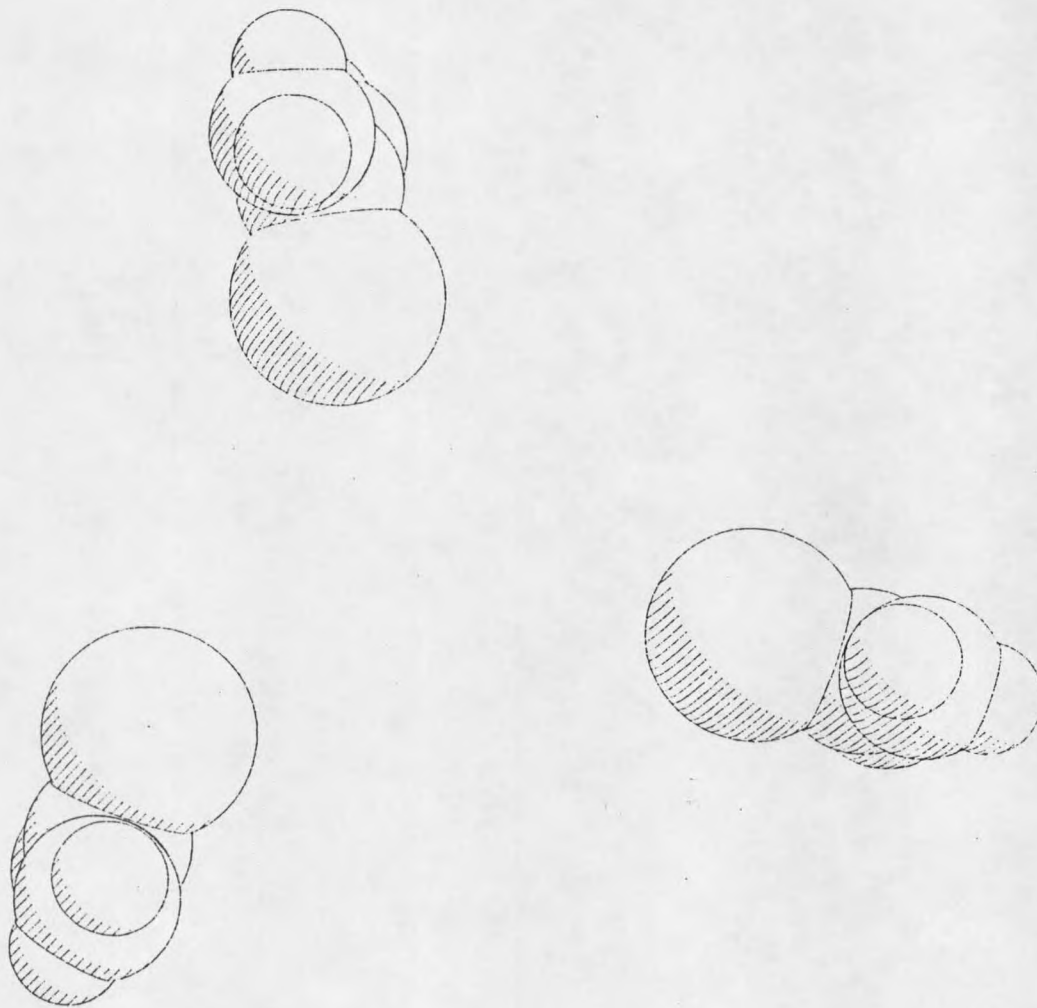


Figure 9. Space filling plot of the three coplaner suffer atoms of the 1,2,4, TCB-thiourea adduct pointing directly into the channel.

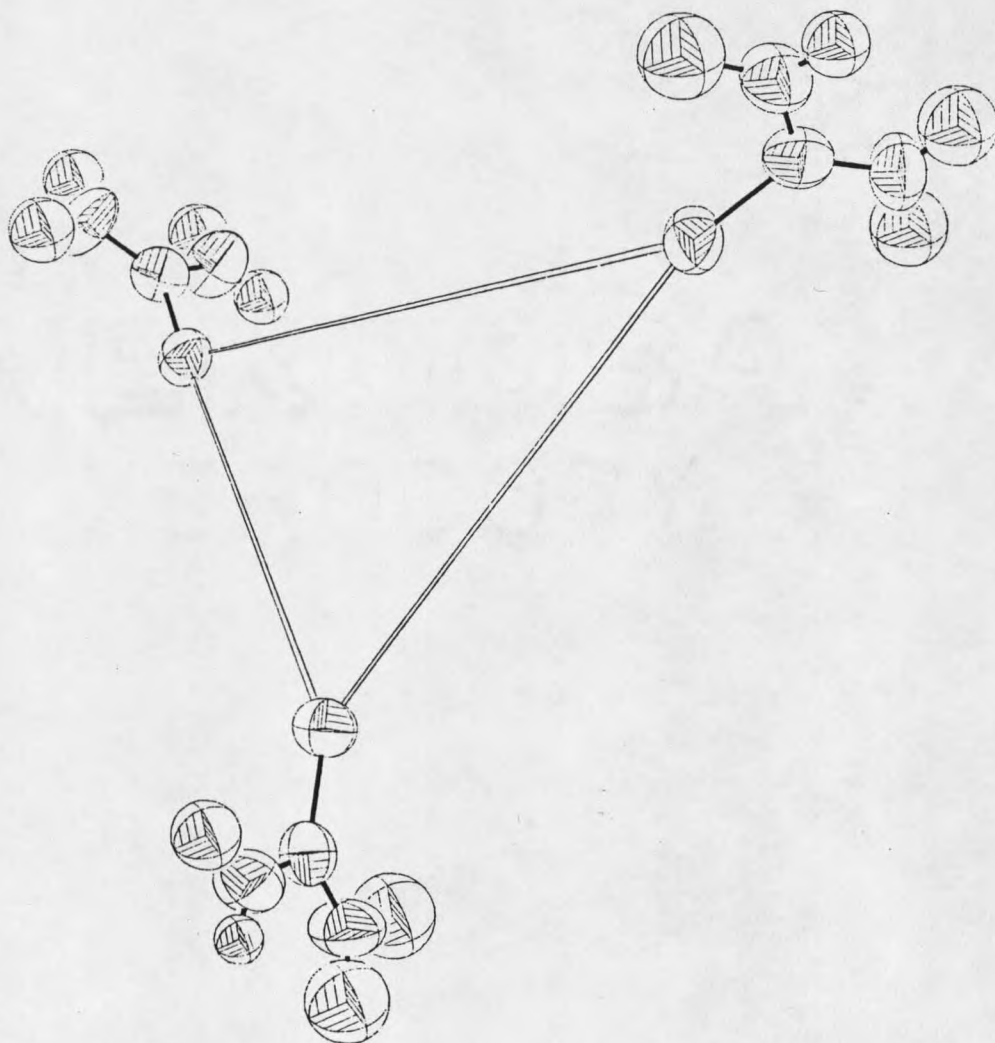


Figure 10. Three coplaner sulfur atoms of the 1,2,4 TCB-thiourea adduct with open lines defining the triangle formed by the sulfur atoms.

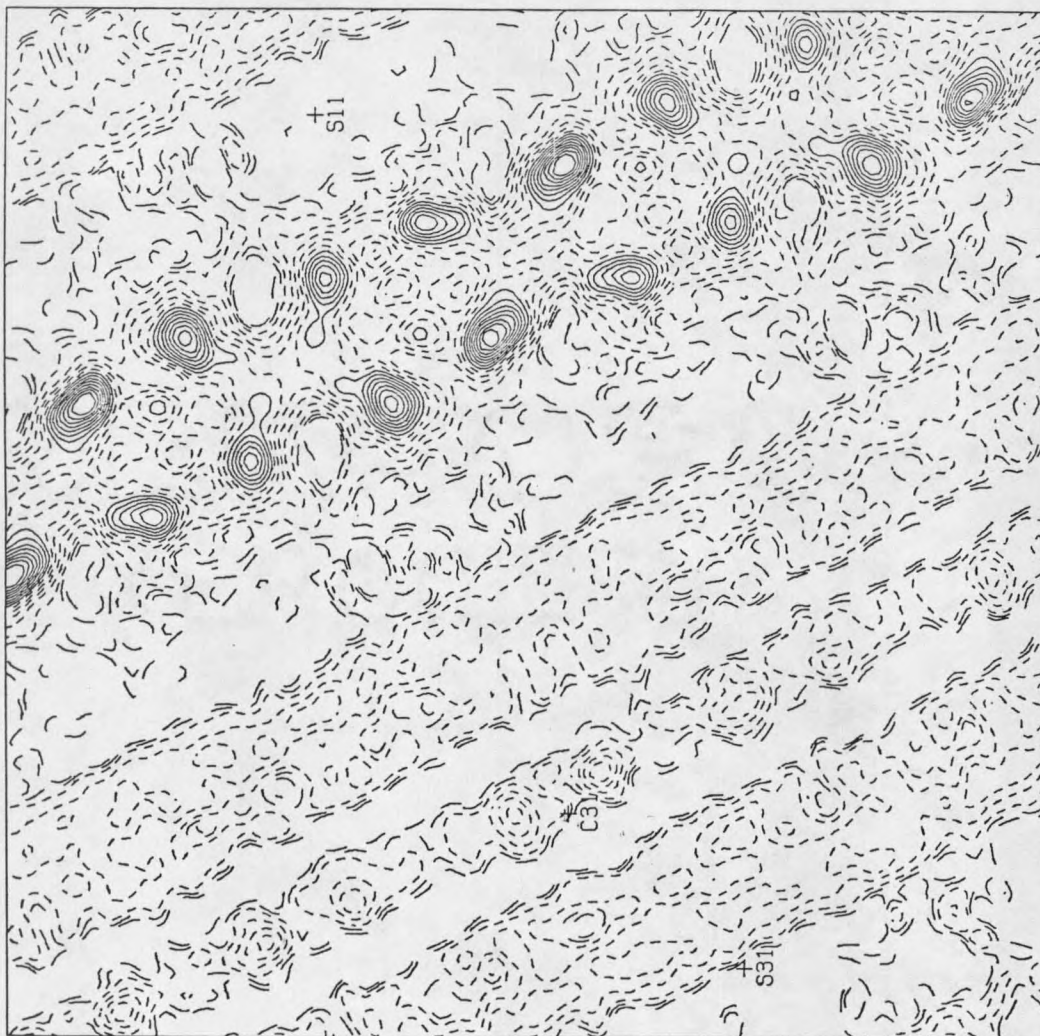


Figure 11. Electron density difference map of the 1,2,4 TCB-thiourea adduct. $X = 24.107 \text{ \AA}$, $Y = 24.107 \text{ \AA}$

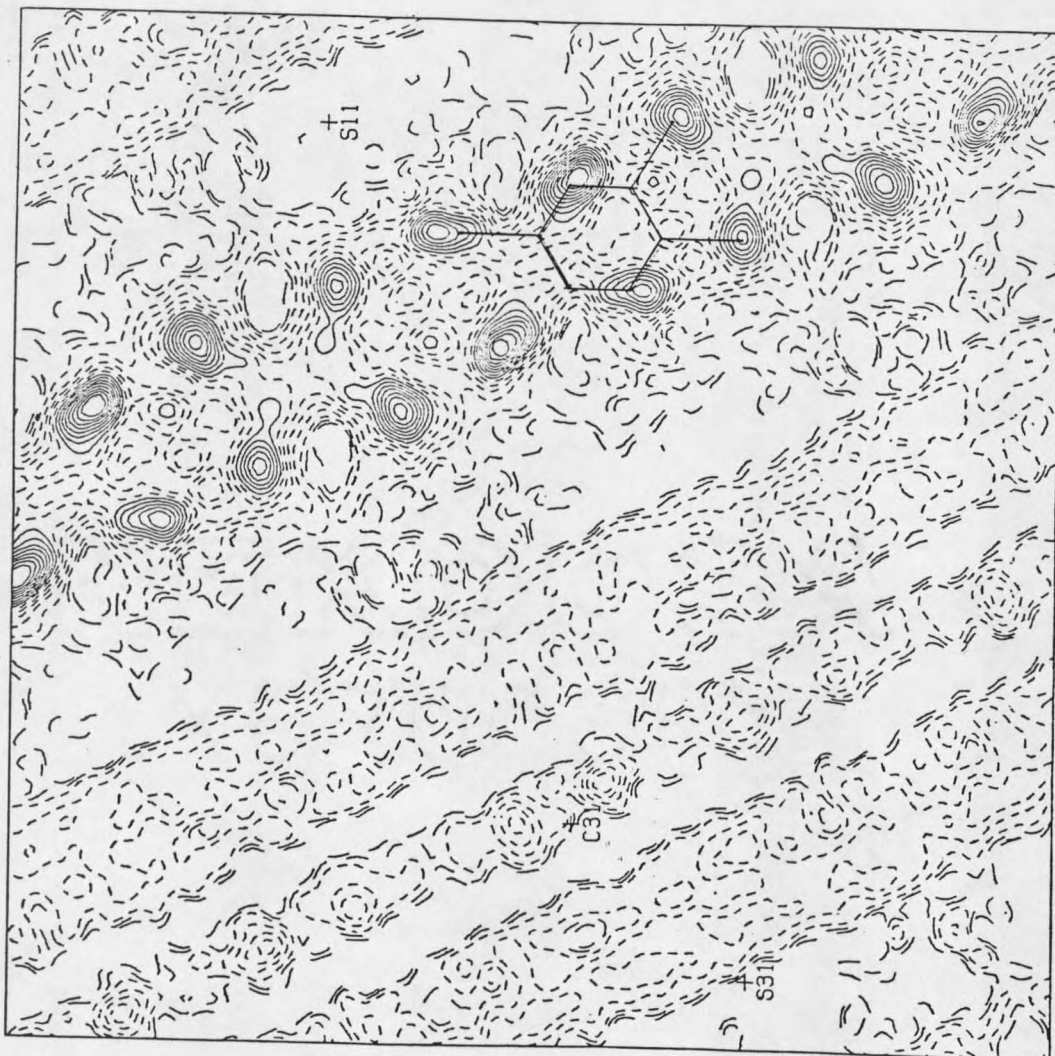


Figure 12. Electron density difference map of the 1,2,4 TCB-thiourea adduct with an idealized 1,2,4 TCB molecule superimposed. X = 24.107 Å, Y = 24.107 Å

their lengths are shorter than 12.54 Å, disorder translationally seems to arise from site disorder and or orientation disorder and not adjacent aromatics overlapping into the next unit cell.

When the adducts are formed, the aromatics are equivalently positioned in the same channel unless there is a zone of maximum attraction unoccupied, then the preceding aromatics may initiate another positioning along the channel which is different than that before the empty zone. Site disorder arises when the aromatics in a channel are positioned differently than aromatics in another channel. The disorder arises because the crystallographic data is an average of all the positions. If diffraction data could be obtained for each unit cell, the disorder could be resolved. The empty or unoccupied zones of maximum attraction are responsible for the non-stoichiometry of these complexes.

In the 1,2,4 TCB-thiourea complex and the 1,2,4 TMB-thiourea complex the aromatic ring might be positioned equally in any of two or more unit cells, however, the chlorines or methyl groups on the rings might be oriented differently. This is referred to as orientation disorder. This occurs since the aromatic ring can remain constant while the chlorines or methyl groups are moved by rotating the aromatic 180°. It is site and or orientation disorder which are responsible for the 1,2,4 TCB and 1,2,4 TMB models having overlap of atoms.

The disordered aromatics prevent the precise location of the thiourea and aromatic interactions. Generally it can be said that the aromatic interacts with one or all of the three coplaner sulfurs. The

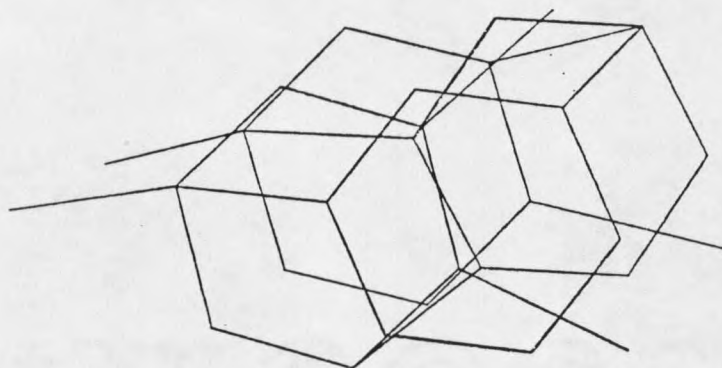


Figure 13. Model of the 1,2,4 TMB molecule in the 1,2,4, TMB-thiourea adduct.

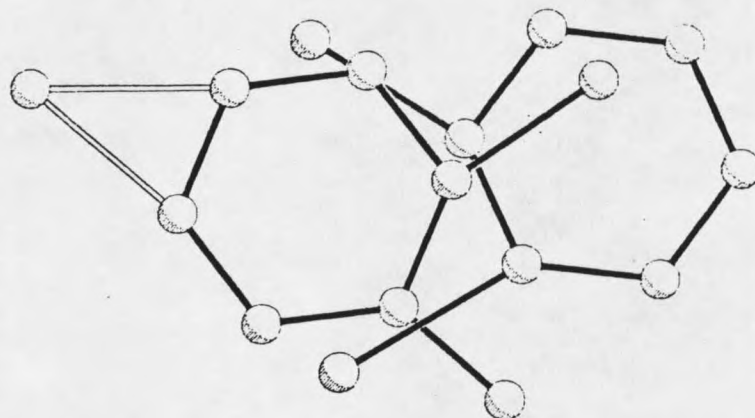


Figure 14. Model of the 1,2,4 TCB adduct in the 1,2,4 TCB-thiourea adduct. The open lines indicate that it is not known to which ring carbon the substituent is bonded.

nature of the strength of this interaction can be understood by studying the sulfur-carbon double bond length in the three coplaner sulfurs.

The sulfur-carbon double bond lengths in the three coplaner thiourea are 1.698(9) Å, 1.706(10) Å, 1.707(8) Å, and 1.707(8) Å, 1.698(9) Å, 1.706(10) Å for the 1,2,4, TCB adduct and the 1,2,4 TMB adduct respectively. These bond distances are about the same as the sulfur-carbon double bond distance found in pure thiourea. It can be concluded that the interaction between thiourea and the aromatic in an adduct is of the same magnitude as that of the hydrogen bonding in pure thiourea. Table 9 shows non-aromatic adducts having a stronger interaction due to the increased sulfur-carbon double bond distances. This could account for the greater stability of non-aromatic adducts versus aromatic adducts.

A view of the 1,2,4, TCB model in the plane of the three coplaner sulfurs can be seen in Figure 15. The two non-solid bonds in the aromatic model indicate that it is not known which of the two aromatic carbons are bonded to the chlorine. Figure 15 and 16 show the relationship between the sulfur atoms and the aromatic. The three planer sulfur atoms can be seen pointing in at the 1,2,4 TCB model. Figure 16 is a view looking down the third thiourea's carbon-sulfur double bond. The angle of this figure shows that one sulfur is pointing directly into the middle of the planer rings while the other two are pointing into the sides of the rings. The non-bonded distances from each of these sulfur atoms to the rings are in Table 10.

The relationship between the coplaner sulfurs and the 1,2,4 TMB can be seen in Figures 17 through 20. Each of these figures exhibits only one of the four rings used in the model. If Figures 17 through 20 were superimposed, the result would be the four ring model positioned in the zone of the coplaner sulfurs. As in the 1,2,4, TCB-thiourea adduct, there is one sulfur pointing in at the plane of the 1,2,4 TMB model and the remaining two are pointing in at the sides. The non-bonded distances from each sulfur atom to the rings are listed in Table 11.

In both adducts, the distances from the sulfur pointing directly into the plane of the rings, and the aromatic carbons are all too long for a strong interaction to occur. The remaining two sulfurs oriented to the sides of the aromatic, are closer to some of the ring carbons. For a hydrogen bond to be possible, the atoms must be closer than the sum of their van der Waal radii and the carbon, hydrogen and sulfur must be linear. The van der Waal radius of sulfur is 1.76 and that for hydrogen is 1.20 A. The radius for a carbon-hydrogen covalent bond is 1.08 A. Thus, the shortest non-bonded distance between a linear carbon, hydrogen and sulfur is the sum of these radii, or 4.04 A. From Tables 10 and 11 only one sulfur-carbon nonbonded distance, S1A to B14 for the 1,2,4 TCB adduct and S1A to F4 for the 1,2,4 TMB adduct, are of the appropriate distance and angles necessary to be considered a hydrogen bond. Both these bonds are linear with a hydrogen in the middle and their distances are 4.001 A and 3.761 A for the 1,2,4 TCB adduct and 1,2,4 TMB adduct respectively. This indicates that a hydrogen bond is a possibility.

Table 10. Interatomic distances between sulfur and carbon in the 1,2,4 TCB-thiourea adduct structure. Only distances less than about 4.5 Å are tabulated.

Atom 1	Atom 2	Distance in Å
S1A	B1	3.991
S1A	B2	4.485
S1A	B14	4.001
S2A	B11	4.111
S2A	B12	3.709
S2A	B13	4.026
S2A	B1	4.439
S2A	B4	4.108
S2A	B5	3.713
S2A	B6	3.899
S3A	B11	4.355
S3A	B12	4.243
S3A	B4	4.550
S3A	B5	4.078

The other most likely form of interaction is a dipole-dipole attraction between the sulfurs and the aromatic carbons. This would require the two unshared pairs of electrons on the sulfurs inducing an added dipole in the aromatic C-H group. Whether the interaction between the thiourea and the aromatic is of a hydrogen bonding type and, or a dipole-dipole type the interaction does contribute to lowering the energy state of the complex.

The possibility of hydrogen bonding and the evidence of dipole-dipole interactions might contribute to the predicting of which hydrocarbon will or will not adduct.

Table 11. Interatomic distances between sulfur and carbon in the 1,2,4 TMB-thiourea adduct structure. Only distances less than about 4.5A are tabulated.

Atom 1	Atom 2	Distance in A
S1A	B4	4.234
S1A	F3	4.539
S1A	F4	3.761
S1A	B25	4.424
S1A	B26	4.483
S2A	B1	3.925
S2A	B6	3.784
S2A	T3	3.724
S2A	T1	3.965
S2A	T2	3.744
S2A	F1	3.569
S2A	F2	4.066
S2A	F6	3.825
S2A	B21	3.763
S2A	B22	3.735
S3A	B1	3.875
S3A	B6	4.116
S3A	T3	4.127
S3A	T1	3.894
S3A	T2	3.410
S3A	F1	3.950
S3A	F2	4.440
S3A	F6	4.584
S3A	B21	4.396
S3A	B22	3.823

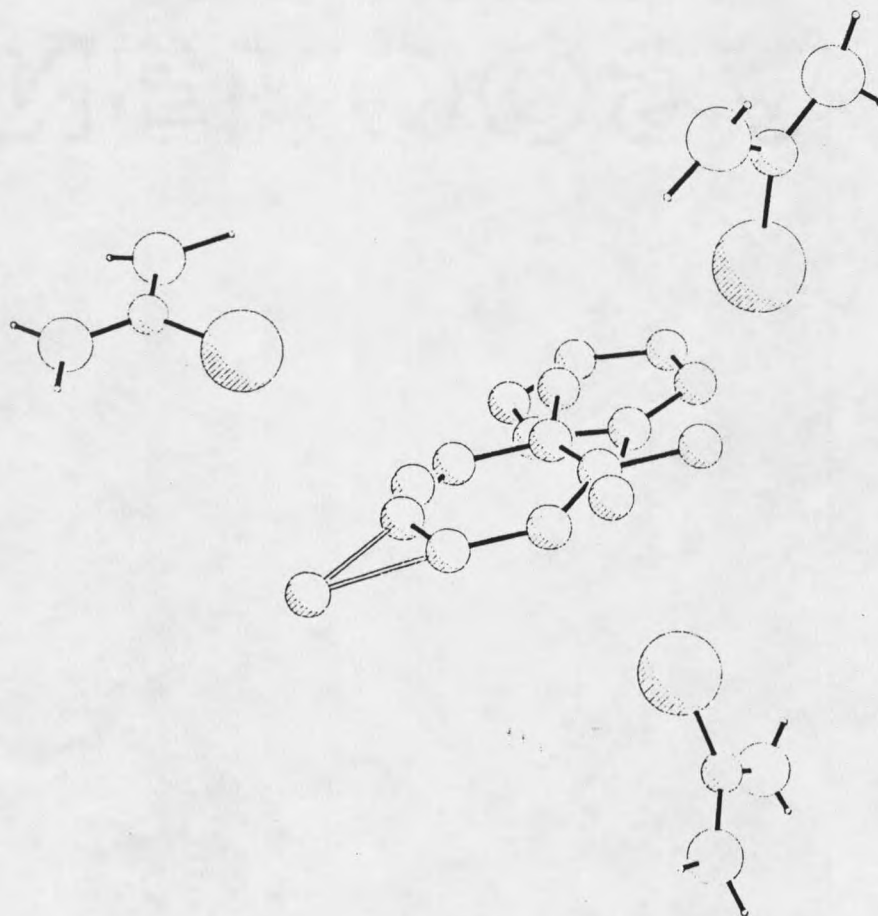


Figure 15. View of the 1,2,4 TCB model in the region of the three coplaner sulfurs.

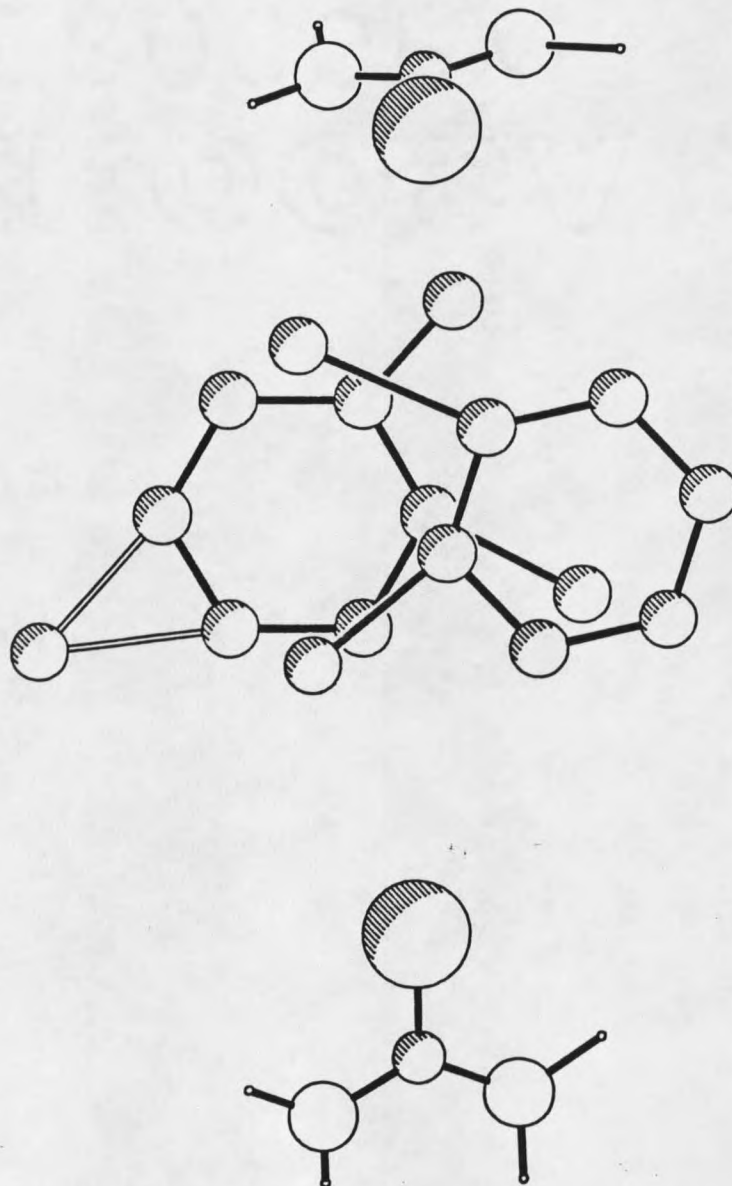


Figure 16. Two thiourea molecules with planer sulfur atoms pointing into the sides of the 1,2,4 TCB model view in looking down the sulfur=carbon double bond of the third coplaner sulfur.

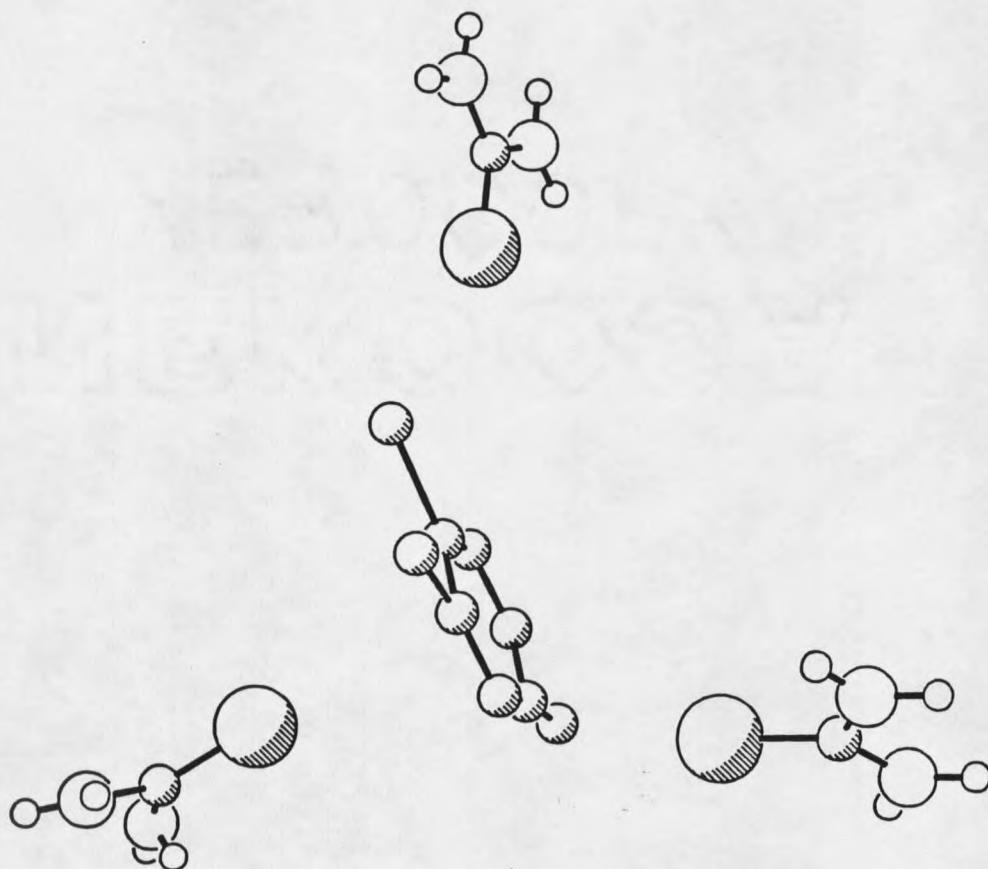


Figure 17. One of the four model rings of the 1,2,4, TMB shown in the region of the three coplaner sulfurs.

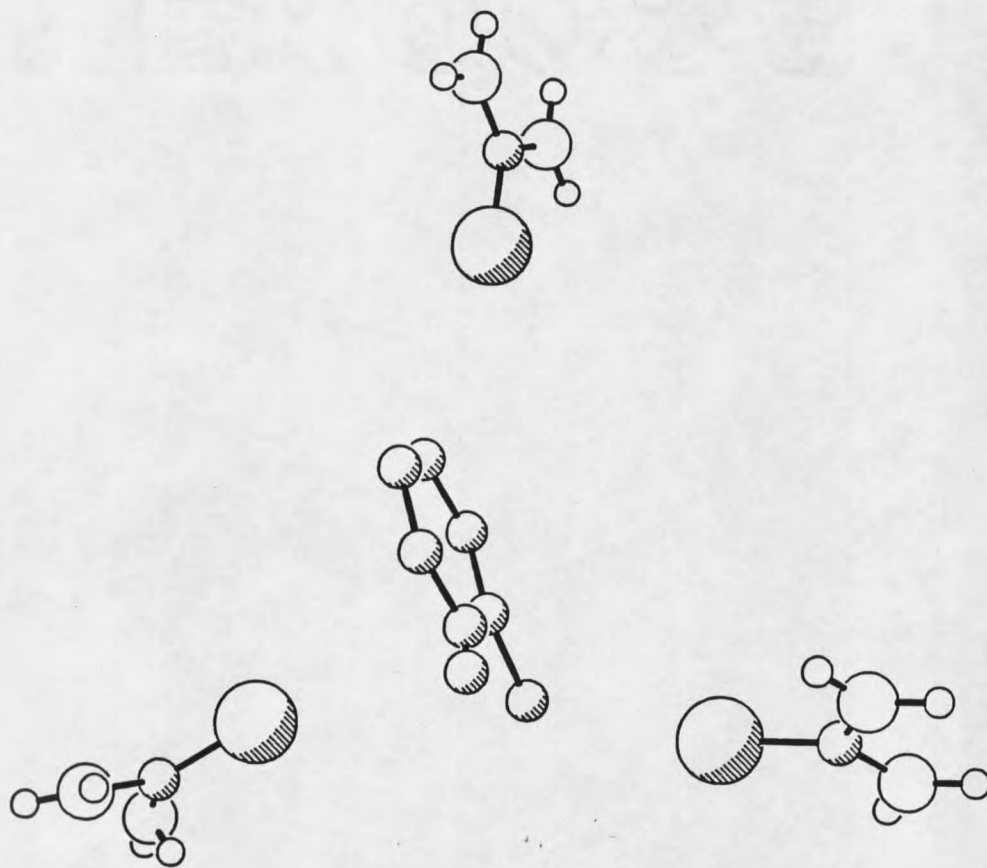


Figure 18. One of the four model rings of the 1,2,4 TMB shown in the region of the three coplaner sulfurs.

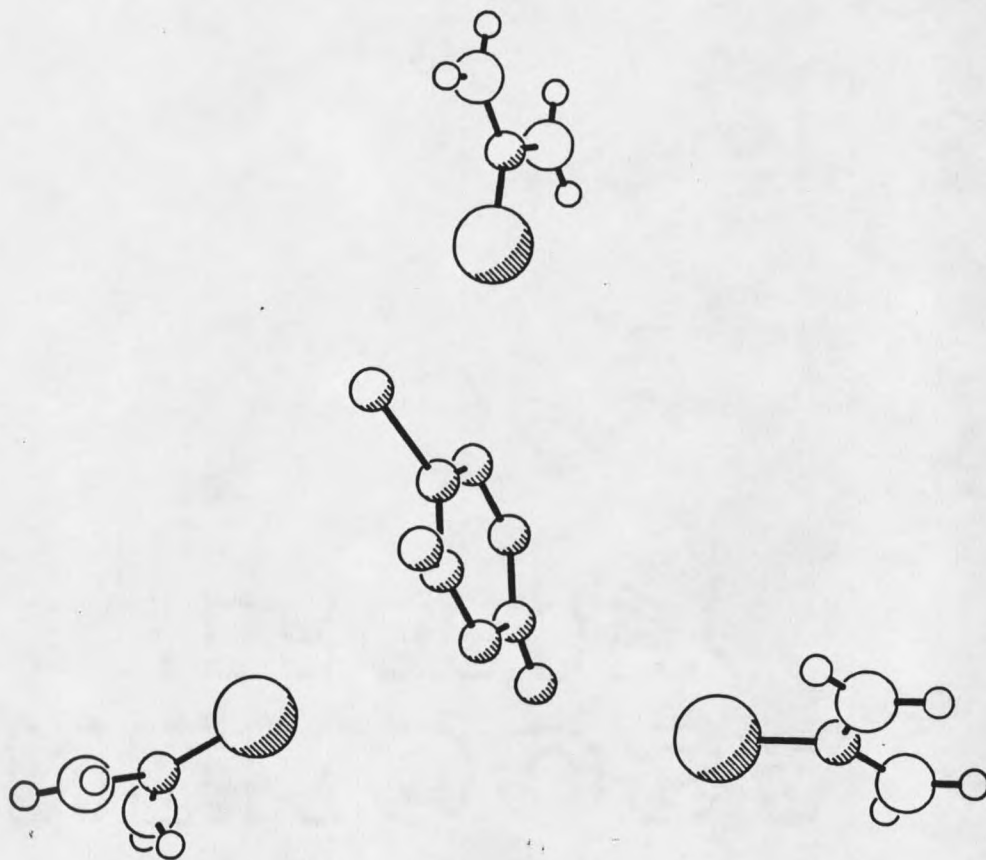


Figure 19. One of the four model rings of the 1,2,4 TMB shown in the region of the three coplaner sulfurs.

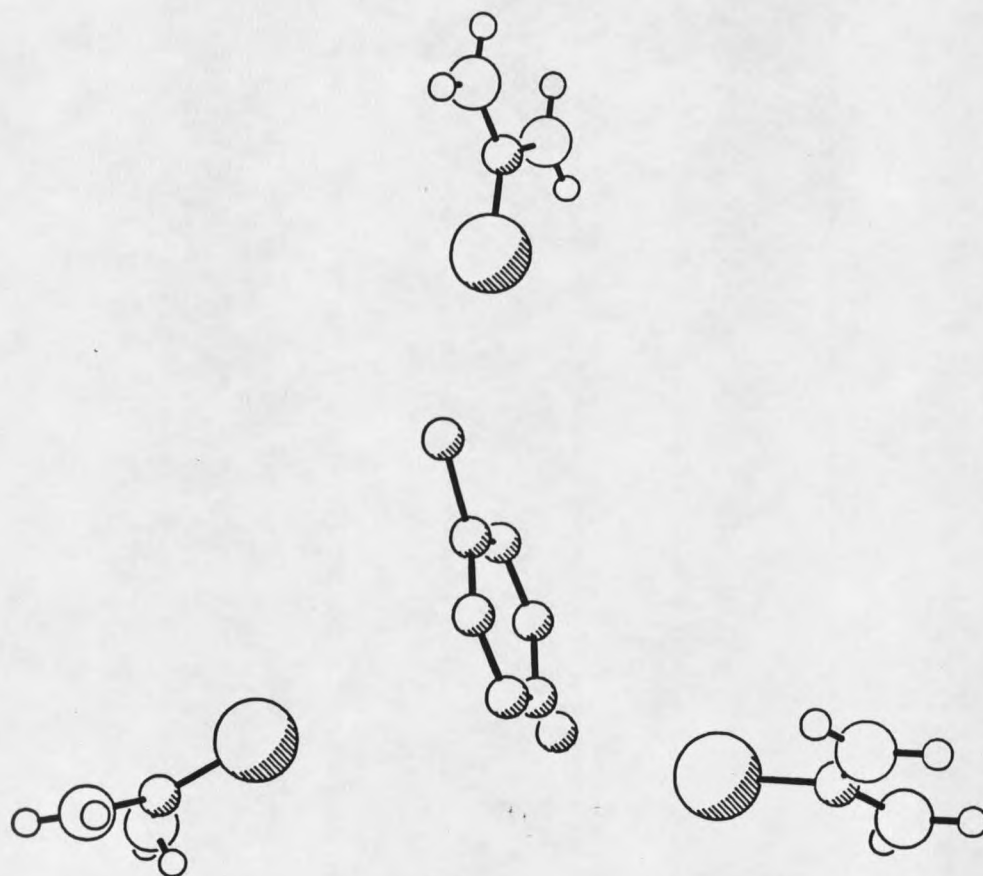


Figure 20. One of the four model rings of the 1,2,4 TMB shown in the region of the three coplaner sulfurs.

CONCLUSIONS

Extractive crystallization with thiourea is a novel separations technique which separates hydrocarbons and notably aromatic systems. In the extractive crystallization process, a unique crystalline complex is formed when thiourea spirals around a selected hydrocarbon and forms a cage-like entrapment. Thiourea is selective for classes of hydrocarbons and is even selective between isomers of the same empirical formula. The entrapped hydrocarbon can be recovered from the complex by steam stripping, followed by phase separation of the products.

Knowledge of the atomic positions, intermolecular distances and the intermolecular forces of interaction in these thiourea complexes might allow an understanding of their selectivity and stability. From x-ray crystallographic data the thiourea lattice is well defined in these complexes. Schlenk discovered the zones of maximum attraction occurring in each unit cell where three coplaner sulfur atoms are pointing directly into the channel. The thiourea molecules are bonded to one another via hydrogen bonds. This accounts for a part of the stability, but not the selectivity of these thiourea adducts. The key to the selectivity of these complexes is thought to lie in the thiourea/hydrocarbon interaction.

Supporting evidence for an interaction lies in the fact that thiourea will form adducts with some compounds yet not with other

compounds of similar size and shape. In addition, the carbon-sulfur double bond distance in thiourea varies between aromatic and non-aromatic complexes. This is an indication that there is an interaction and that it is flexible in nature. Finally, the nonbonded distances between the coplaner sulfurs and the aromatic are almost at the distance equal to the sum of the van der Waal radii and, in each adduct one nonbonded distance is within the appropriate length and geometry to indicate a possible hydrogen bond. The nonbonded distances close to the van der Waal radii of the aromatic indicate a dipole-dipole interaction.

If in fact a hydrogen bond does exist some credibility might be added to Fetterly's notion of a "supported hydrogen bond". However, the probability of dipole-dipole attractions occurring should not be ruled out. Fetterly's idea does not explain explain adducts which have no possibilities of hydrogen bonding, i.e. carbon tetrachloride adduct. No evidence was found to support Welling's suggestion of a chlorine/ NH_2 group hydrogen bond in the 1,2,4 TCB thiourea adduct. Furthermore, no hydrogen bonding was seen between a methyl group and a sulfur in the 1,2,4 TMB-thiourea adduct.

Diffraction data sets collected on both the 1,2,4 TMB-thiourea and 1,2,4 TCB-thiourea adducts showed both adducts crystallizing in the space group $P21/c$, which is characteristic of aromatic complexes. The most difficult problem associated with both complexes was the disorder of the aromatic in the channel. The disorder arose from site and or orientation disorder and not adjacent aromatics overlapping each other. A model which take into account the disorder was found

for each complex. Refinement of these models resulted in an R value of .1053 for the 1,2,4 TBM adduct and .0951 for the 1,2,4 TCB adduct. Both aromatic models were found to lie in the zone of maximum attraction created by the three coplaner sulfur atoms in the thiourea lattice. It is hoped that the information concerning the structures of these adduct can be used in future research to determine the overall selectivity mechanism of these thiourea adducts.

Recommendations

Many aromatic and non-aromatic hydrocarbons form adducts with thiourea. The wide range of stability and selectivity of these adducts pose many questions regarding their structures and chemical interactions. The knowledge of the exact nature of the thiourea and hydrocarbon interaction appears to be vital if the selectivity mechanism and chemical structures are to be known. The primary obstacle is resolving the disorder associated with the channel hydrocarbon.

Steps taken to reduce the disorder might entail utilizing a guest hydrocarbon, such as carbon tetrabromide, which possesses heavy atoms that could appear less disordered in the difference maps. Alternatively, a better 1,2,4 TCB model refined using a full matrix least squares in the XTAL system might enhance locating the chlorine atoms in the 1,2,4 TCB adduct. Another approach might be to find a guest hydrocarbon which is geometrically large enough so that the number of orientations possible in the channel are minimized, thus reducing the orientation disorder. Furthermore, if a larger guest

hydrocarbon could be found that occupied two or more zones of maximum attraction the site disorder might be reduced. The quality of the x-ray diffraction data could be enhanced if data set were obtained using low temperatures.

Although 1,2,4 trichlorobenzene is considered to be an inductor, the role of inductors in thiourea complexes was not fully investigated in the two aromatic adducts studied. It appears that the role of an inductor must be studied in adducts which contain the inductor and selected hydrocarbon. For instance, CCl_4 is selective for ethylbenzene in the aromatic mixture of ethylbenzene and oxylene. In the same mixture, 1,2,4 trichlorobenzene is selective for the o-xylene. Since CCl_4 adducts in space group $R\bar{3}c$ and 1,2,4, TCB adducts in $P2_1/c$ it would be interesting to see which space group forms when CCl_4 inducts ethylbenzene and when 1,2,4 TCB inducts o-xylene.

The same intermolecular forces which appear in the crystalline adduct are also present in solution. Therefore, nuclear magnetic resonance (nmr) spectroscopy and infrared spectroscopy may shed light on the intermolecular interaction between the thiourea and the hydrocarbon.

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APPENDICES

21

APPENDIX A
CLASSIFICATION OF CRYSTALS

APPENDIX A

There are seven three-dimensional coordinate systems which are used to classify crystals (18). In general, the unit cell is characterized by a certain symmetry and six parameters, three axial lengths and three interaxial angles. The lengths of the unit cell edges are designated a , b , c and the interaxial angles α, β, γ where α is the angle between b and c , β is the angle between a and c , and γ is between a and b .

The following table specifies the seven crystal systems along with the corresponding unit cell parameters:

Table 12. The seven possible crystal systems.

Crystal System	No. Independent Parameters	Parameters	Lattice Symmetry
Triclinic	6	$a \neq b \neq c; \alpha \neq \beta \neq \gamma$	1
Monoclinic	4	$a \neq b \neq c; \alpha = \gamma = 90^\circ; \beta \neq 90^\circ$	2/m
Orthorhombic	3	$a \neq b \neq c; \alpha = \beta = \gamma = 90^\circ$	mmm
Tetragonal	2	$a = b \neq c; \alpha = \beta = \gamma = 90^\circ$	4/mmm
Rhombohedral	2	$a = b = c; \alpha = \beta = \gamma \neq 90^\circ$	3/m
Hexagonal	2	$a = b \neq c; \alpha = \beta = \gamma = 90^\circ$	6/mmm
Cubic	1		m3m

The essential symmetries of a structure can be categorized into systems referred to as the Laue Space Groups. There are 230 space groups, each unique in describing a particular crystal's internal

(i.e. molecular) symmetry. A crystal's space group can be determined by systematic x-ray reflection absences, and the space group is listed in the "International Tables for X-Ray Crystallography." All symmetry elements are represented by symbols, figures and letters which are arranged together to indicate a space group.

Table 13. Symbols for symmetry elements and for the corresponding symmetry operations in one-, two-, and three-dimensions [reproduced from (8)].

Printed symbol	Symmetry element and its orientation	Generating symmetry operation with glide or screw vector
m	Reflection plane, mirror plane	Reflection through a plane
	Reflection line, mirror line (two dimensions)	Reflection through a line
	Reflection point, mirror point (one dimension)	Reflection through a point
$a, b, \text{ or } c$	'Axial' glide plane	Glide reflection through a plane, with glide vector
a	$\perp[010]$ or $\perp[001]$	$\frac{1}{2}a$
b	$\perp[001]$ or $\perp[100]$	$\frac{1}{2}b$
c	$\perp[100]$ or $\perp[010]$	$\frac{1}{2}c$
	$\perp[1\bar{1}0]$ or $\perp[110]$	$\frac{1}{2}c$
	$\perp[100]$ or $\perp[010]$ or $\perp[1\bar{1}0]$	$\frac{1}{2}c$
	$\perp[1\bar{1}0]$ or $\perp[120]$ or $\perp[2\bar{1}0]$	$\frac{1}{2}c$ } hexagonal coordinate system
n	'Diagonal' glide plane	Glide reflection through a plane, with glide vector
	$\perp[001]: \perp[100]: \perp[010]$	$\frac{1}{2}(a+b): \frac{1}{2}(b+c): \frac{1}{2}(a+c)$
	$\perp[1\bar{1}0]$ or $\perp[01\bar{1}]$ or $\perp[10\bar{1}]$	$\frac{1}{2}(a+b+c)$
d	$\perp[110]: \perp[011]: \perp[101]$	$\frac{1}{2}(-a+b+c): \frac{1}{2}(a-b+c): \frac{1}{2}(a+b-c)$
	'Diamond' glide plane	Glide reflection through a plane, with glide vector
	$\perp[001]: \perp[100]: \perp[010]$	$\frac{1}{4}(a \pm b): \frac{1}{4}(b \pm c): \frac{1}{4}(a \pm c)$
g	$\perp[1\bar{1}0]: \perp[01\bar{1}]: \perp[10\bar{1}]$	$\frac{1}{4}(a+b \pm c): \frac{1}{4}(\pm a+b+c): \frac{1}{4}(a \pm b+c)$
	$\perp[110]: \perp[011]: \perp[101]$	$\frac{1}{4}(-a+b \pm c): \frac{1}{4}(\pm a-b+c): \frac{1}{4}(a \pm b-c)$
	Glide line (two dimensions)	Glide reflection through a line, with glide vector
$\bar{2} = m, \bar{3}, \bar{4}, \bar{6}$	$\perp[01]: \perp[10]$	$\frac{1}{2}a: \frac{1}{2}b$
	None	Identity
2, 3, 4, 6	n -fold rotation axis, n	Counter-clockwise rotation of $360/n$ degrees around an axis
	n -fold rotation point, n (two dimensions)	Counter-clockwise rotation of $360/n$ degrees around a point
$\bar{1}$	Centre of symmetry, inversion centre	Inversion through a point
2_1 $3_1, 3_2$ $4_1, 4_2, 4_3$ $6_1, 6_2, 6_3, 6_4, 6_5$	Rotoinversion axis, \bar{n}	Counter-clockwise rotation of $360/n$ degrees around an axis, followed by inversion through a point on the axis
		Right-handed screw rotation of $360/n$ degrees around an axis, with screw vector (pitch) $(p/n) t$; here t is the shortest lattice translation vector parallel to the axis in the direction of the screw
	n -fold screw axis, n_p	

Table 14. Symbols for one-, two-, and three-dimensional cells [reproduced from (8)].

Printed symbol	Centring type of cell	Number of lattice points per cell	Coordinates of lattice points within cell
<i>One dimension</i>			
<i>a</i>	Primitive	1	0
<i>Two dimensions</i>			
<i>p</i>	Primitive	1	0,0
<i>c</i>	Centred	2	0,0; $\frac{1}{2},\frac{1}{2}$
<i>h</i>	Hexagonally centred	3	0,0; $\frac{2}{3},\frac{1}{3};\frac{1}{3},\frac{2}{3}$
<i>Three dimensions</i>			
<i>P</i>	Primitive	1	0,0,0
<i>C</i>	C-face centred	2	0,0,0; $\frac{1}{2},\frac{1}{2},0$
<i>A</i>	A-face centred	2	0,0,0; $0,\frac{1}{2},\frac{1}{2}$
<i>B</i>	B-face centred	2	0,0,0; $\frac{1}{2},0,\frac{1}{2}$
<i>I</i>	Body centred	2	0,0,0; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$
<i>F</i>	All-face centred	4	0,0,0; $\frac{1}{2},\frac{1}{2},0;0,\frac{1}{2},\frac{1}{2};\frac{1}{2},0,\frac{1}{2}$
<i>R</i>	Rhombohedrally centred (description with 'hexagonal axes')	3	{ 0,0,0; $\frac{2}{3},\frac{1}{3},\frac{1}{3};\frac{1}{3},\frac{2}{3},\frac{2}{3}$ ('obverse setting')
	Primitive (description with 'rhombohedral axes')	1	{ 0,0,0; $\frac{1}{3},\frac{2}{3},\frac{1}{3};\frac{2}{3},\frac{1}{3},\frac{2}{3}$ ('reverse setting')
<i>H</i>	Hexagonally centred	3	0,0,0; $\frac{2}{3},\frac{1}{3},0;\frac{1}{3},\frac{2}{3},0$

APPENDIX B
ELEMENTAL ANALYSIS

APPENDIX B

Table 15. Elemental analysis for the 1,2,4 TCB-thiourea adduct, the 1,2,4 TMB-thiourea adduct, and pure thiourea.

(I) 1,2,4 TCB-Thiourea Adduct

Sample Weight (mg)	Nitrogen %	Carbon %	Hydrogen %
1.2829	22.00	24.68	3.83
1.1389	22.46	24.35	3.85
1.8014	21.61	24.66	3.84

(II) 1,2,4 TMB-Thiourea Adduct

Sample Weight (mg)	Nitrogen %	Carbon %	Hydrogen %
1.4673	26.93	35.58	6.68
1.5272	27.07	35.40	6.68
1.4972	25.77	37.04	6.81

(III) Pure Thiourea

% C	% H	% N	% S	% O
15.83	5.29	37.18	41.65	0.06

APPENDIX C

TABLES FOR PUBLICATION FOR THE
1,2,4 TCB-THIOUREA ADDUCT STRUCTURE

APPENDIX C

Table 16. Atomic coordinates and isotropic thermal parameters for the 1,2,4 TCB-thiourea adduct structure.

	Atomic coordinates ($\times 10^4$) and isotropic thermal parameters ($\text{\AA}^2 \times 10^3$)			
	x	y	z	U
B(5)	3317(28)	10410(13)	2589(15)	211(10)
B(6)	2143	9865	2511	362
B(1)	2198	9366	3475	374(17)
B(2)	3427	9413	4518	184(7)
B(3)	4601	9958	4596	264(19)
B(4)	4546	10457	3632	131(8)
B(11)	1635(21)	10462(11)	667(15)	186(8)
B(12)	2507	10258	1824	513(46)
B(13)	1982	9687	2461	687(49)
B(14)	584	9318	1940	139(4)
B(15)	-288	9522	783	356(43)
B(16)	237	10094	146	746
S(1)	3975(2)	6472(1)	4397(2)	73(1)*
S(2)	-88(2)	6370(1)	1410(2)	67(1)*
S(3)	3182(2)	3030(1)	2024(2)	70(1)*
C(1)	2765(9)	6881(5)	4970(7)	69(4)*
C(2)	899(8)	7081(5)	936(7)	66(3)*
C(3)	2719(7)	4073(5)	2226(6)	66(3)*
N(11)	1337(6)	6951(5)	4296(5)	82(3)*
N(12)	3228(7)	7157(4)	6067(5)	89(3)*
N(21)	2294(9)	7263(6)	1570(8)	91(4)*
N(22)	268(11)	7465(6)	-88(8)	88(4)*
N(31)	1774(7)	4529(4)	1362(5)	91(3)*
N(32)	3271(10)	4437(6)	3285(7)	95(4)*
Cl(1)	4042(65)	11046(40)	2154(54)	423(34)
Cl(2)	4819(27)	9341(16)	6008(20)	122(8)
Cl(3)	482(59)	9615(29)	1213(39)	235(20)
Cl(5)	4425(14)	10714(8)	3105(11)	55(3)
Cl(6)	2411(20)	10740(12)	867(15)	85(5)
Cl(7)	2848(29)	10757(20)	1335(25)	116(11)
Cl(4)	2515(23)	9275(14)	3948(19)	94(6)

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

Table 17. Anisotropic thermal parameters for the 1,2,4 TCB-thiourea adduct structure.

Anisotropic thermal parameters ($\text{\AA}^2 \times 10^3$)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S(1)	61(1)	90(1)	64(1)	-13(1)	17(1)	3(1)
S(2)	60(1)	73(1)	62(1)	9(1)	18(1)	-2(1)
S(3)	81(1)	69(1)	54(1)	-2(1)	18(1)	12(1)
C(1)	71(6)	69(6)	65(5)	3(5)	24(5)	-8(5)
C(2)	67(5)	70(6)	63(5)	-4(4)	26(4)	7(4)
C(3)	65(4)	65(5)	68(4)	-6(4)	24(4)	-4(4)
N(11)	56(3)	107(5)	83(4)	3(4)	24(3)	2(4)
N(12)	78(4)	120(6)	70(4)	-24(4)	30(3)	1(4)
N(21)	63(5)	116(7)	89(6)	7(5)	23(5)	-21(5)
N(22)	116(7)	87(7)	70(5)	17(4)	43(5)	-11(5)
N(31)	98(5)	72(4)	77(4)	3(4)	4(4)	13(4)
N(32)	120(7)	65(5)	82(5)	-9(5)	15(5)	7(5)

The anisotropic temperature factor exponent takes the form:

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

Table 18. H-atom coordinates and isotropic thermal parameters for the 1,2,4 TCB-thiourea adduct structure.

	H-Atom coordinates ($\times 10^4$) and isotropic thermal parameters ($\text{\AA}^2 \times 10^3$)			
	x	y	z	U
H(12a)	2541	7399	6375	105
H(12b)	4252	7111	6557	105
H(1)	635(66)	7443(39)	4594(52)	83(19)
H(2)	600(133)	6539(80)	2967(109)	255(50)
H(21)	2889(81)	7142(52)	2386(67)	144(29)
H(22)	2875(104)	7473(65)	1416(85)	115(40)
H(23)	615(69)	7640(43)	-258(58)	6(19)
H(24)	-530(132)	7252(79)	-1218(114)	269(53)
H(31)	3753(78)	4065(48)	3801(60)	84(26)
H(32)	3319(65)	4929(37)	3279(51)	36(19)
H(33)	1653(92)	5087(65)	1248(81)	181(38)
H(34)	1354(75)	4214(47)	629(62)	106(24)

Table 19. Bond lengths for the 1,2,4 TCB-thiourea adduct structure.

Bond lengths (Å)			
S(1)-C(1)	1.706(10)	S(2)-C(2)	1.698(9)
S(2)-H(2)	1.796(124)	S(3)-C(3)	1.707(8)
C(1)-N(11)	1.337(9)	C(1)-N(12)	1.322(10)
C(2)-N(21)	1.325(10)	C(2)-N(22)	1.318(11)
C(3)-N(31)	1.320(8)	C(3)-N(32)	1.332(10)
N(11)-H(1)	1.168(69)	N(21)-H(21)	0.973(69)
N(21)-H(22)	0.736(113)	N(22)-H(23)	0.532(77)
N(22)-H(24)	1.356(125)	N(31)-H(33)	0.869(101)
N(31)-H(34)	0.969(72)	N(32)-H(31)	0.853(66)
N(32)-H(32)	0.757(58)	Cl(1)-B(5)	1.423(73)
Cl(1)-B(4)	1.922(66)	Cl(1)-B(12)	1.851(64)
Cl(1)-Cl(5)	1.200(64)	Cl(1)-Cl(6)	1.841(53)
Cl(1)-Cl(7)	1.303(57)	Cl(2)-B(2)	1.834(26)
Cl(2)-B(3)	1.918(32)	Cl(2)-B(3a)	1.530(36)
Cl(2)-B(4a)	0.687(31)	Cl(2)-Cl(5a)	1.069(24)
Cl(3)-B(6)	1.844(47)	Cl(3)-B(11)	1.993(60)
Cl(3)-B(13)	1.685(45)	Cl(3)-B(14)	0.975(52)
Cl(3)-B(15)	0.756(47)	Cl(3)-B(16)	1.443(52)
Cl(3)-B(16a)	1.617(47)	Cl(5)-B(5)	1.133(26)
Cl(5)-B(4)	0.730(24)	Cl(5)-Cl(2a)	1.069(24)
Cl(6)-B(11)	0.825(27)	Cl(6)-B(12)	1.363(26)
Cl(6)-Cl(7)	0.576(29)	Cl(7)-B(5)	1.531(35)
Cl(7)-B(11)	1.250(30)	Cl(7)-B(12)	1.099(38)
Cl(4)-B(6)	1.896(30)	Cl(4)-B(1)	0.566(26)
Cl(4)-B(2)	0.931(28)	Cl(4)-B(13)	1.818(29)

Table 20. Bond angles for the 1,2,4 TMB-thiourea adduct structure.

Bond angles (°)	
B(6)-B(5)-Cl(1)	154.0(23)
B(12)-B(5)-Cl(1)	97.9(29)
B(6)-B(5)-Cl(5)	151.3(12)
B(12)-B(5)-Cl(5)	151.1(30)
Cl(1)-B(5)-Cl(5)	54.6(25)
B(4)-B(5)-Cl(7)	137.7(14)
B(13)-B(5)-Cl(7)	101.8(16)
Cl(5)-B(5)-Cl(7)	106.6(22)
B(1)-B(6)-Cl(3)	111.4(18)
B(13)-B(6)-Cl(3)	55.0(44)
B(5)-B(6)-Cl(4)	110.8(9)
B(12)-B(6)-Cl(4)	153.5(21)
B(14)-B(6)-Cl(4)	88.9(14)
B(6)-B(1)-Cl(4)	147.5(35)
B(13)-B(1)-Cl(4)	157.5(47)
B(1)-B(2)-Cl(2)	168.5(12)
B(1)-B(2)-Cl(4)	16.3(21)
Cl(2)-B(2)-Cl(4)	152.2(28)
B(4)-B(3)-Cl(2)	174.8(9)
Cl(2)-B(3)-Cl(2a)	148.1(14)
B(3)-B(4)-Cl(1)	167.5(20)
B(3)-B(4)-Cl(5)	173.4(23)
Cl(1)-B(4)-Cl(2a)	104.5(35)
B(12)-B(11)-Cl(3)	73.6(13)
B(12)-B(11)-Cl(6)	70.5(17)
Cl(3)-B(11)-Cl(6)	144.1(23)
B(16)-B(11)-Cl(7)	167.6(19)
Cl(6)-B(11)-Cl(7)	22.0(20)
Cl(6)-B(11)-B(15a)	123.2(27)
Cl(3)-B(11)-B(15a)	48.7(15)
Cl(7)-B(11)-B(16a)	170.8(25)
B(6)-B(12)-Cl(1)	127.3(25)
B(13)-B(12)-Cl(1)	136.5(20)
B(6)-B(12)-Cl(6)	160.2(21)
B(13)-B(12)-Cl(6)	154.7(11)
B(5)-B(12)-Cl(7)	93.2(24)
B(11)-B(12)-Cl(7)	58.8(15)
Cl(1)-B(12)-Cl(7)	43.8(24)
B(5)-B(13)-Cl(3)	120.8(22)
B(1)-B(13)-Cl(3)	129.2(27)
B(14)-B(13)-Cl(3)	35.3(20)
B(6)-B(13)-Cl(4)	100.0(45)
B(12)-B(13)-Cl(4)	139.1(9)
Cl(3)-B(13)-Cl(4)	136.0(24)
B(1)-B(14)-Cl(3)	129.5(34)
B(15)-B(14)-Cl(3)	31.3(32)
B(16)-B(14)-Cl(3)	78.1(44)
Cl(3)-B(14)-B(16a)	100.0(50)
B(15)-B(16)-Cl(3)	30.8(21)
Cl(3)-B(16)-B(15a)	168.4(34)
Cl(3)-B(16)-Cl(3a)	160.3(14)
S(1)-C(1)-N(11)	119.9(7)
N(11)-C(1)-N(12)	119.2(9)
S(2)-C(2)-N(22)	119.5(7)
S(3)-C(3)-N(32)	121.6(5)
N(31)-C(3)-N(32)	118.2(7)
C(2)-N(21)-H(21)	131.0(54)
H(21)-N(21)-H(22)	97.3(83)
C(2)-N(22)-H(24)	139.3(51)
C(3)-N(31)-H(33)	131.6(48)
H(33)-N(31)-H(34)	110.9(71)
C(3)-N(32)-H(32)	114.4(45)
B(5)-Cl(1)-Cl(5)	50.3(28)
B(12)-Cl(1)-Cl(5)	82.5(37)
B(4)-Cl(1)-Cl(6)	121.9(36)
Cl(5)-Cl(1)-Cl(6)	125.9(46)
B(4)-Cl(1)-Cl(7)	114.3(45)
Cl(5)-Cl(1)-Cl(7)	118.3(55)
B(5)-Cl(5)-Cl(1)	75.1(31)
Cl(1)-Cl(5)-Cl(2a)	151.0(34)
B(12)-Cl(6)-Cl(1)	68.7(24)
B(12)-Cl(6)-Cl(7)	51.3(37)
B(5)-Cl(7)-Cl(1)	59.6(34)
B(12)-Cl(7)-Cl(1)	100.5(38)
B(11)-Cl(7)-Cl(6)	32.5(30)
Cl(1)-Cl(7)-Cl(6)	154.9(61)
B(4)-B(5)-Cl(1)	86.0(22)
B(13)-B(5)-Cl(1)	154.0(25)
B(4)-B(5)-Cl(5)	31.4(12)
B(13)-B(5)-Cl(5)	151.1(17)
B(6)-B(5)-Cl(7)	102.1(14)
B(12)-B(5)-Cl(7)	45.8(17)
Cl(1)-B(5)-Cl(7)	52.2(25)
B(5)-B(6)-Cl(3)	128.4(19)
B(12)-B(6)-Cl(3)	83.8(21)
B(14)-B(6)-Cl(3)	31.8(18)
B(1)-B(6)-Cl(4)	9.2(9)
B(13)-B(6)-Cl(4)	70.8(45)
Cl(3)-B(6)-Cl(4)	120.6(22)
B(2)-B(1)-Cl(4)	27.5(35)
B(14)-B(1)-Cl(4)	156.6(39)
B(3)-B(2)-Cl(2)	71.4(12)
B(3)-B(2)-Cl(4)	136.3(20)
B(2)-B(3)-Cl(2)	65.0(10)
Cl(2)-B(3)-B(3a)	52.5(23)
B(5)-B(4)-Cl(1)	47.6(19)
B(5)-B(4)-Cl(5)	54.1(21)
Cl(1)-B(4)-Cl(5)	6.6(24)
Cl(5)-B(4)-Cl(2a)	97.9(37)
B(16)-B(11)-Cl(3)	46.4(13)
B(16)-B(11)-Cl(6)	169.2(16)
B(12)-B(11)-Cl(7)	48.7(17)
Cl(3)-B(11)-Cl(7)	122.2(22)
Cl(3)-B(11)-B(15a)	92.6(18)
Cl(7)-B(11)-B(15a)	145.2(26)
Cl(6)-B(11)-B(16a)	167.1(27)
B(5)-B(12)-Cl(1)	49.6(25)
B(11)-B(12)-Cl(1)	102.4(19)
B(5)-B(12)-Cl(6)	117.3(22)
B(11)-B(12)-Cl(6)	34.8(10)
Cl(1)-B(12)-Cl(6)	67.9(22)
B(6)-B(12)-Cl(7)	165.7(26)
B(13)-B(12)-Cl(7)	174.3(20)
Cl(6)-B(12)-Cl(7)	24.1(15)
B(6)-B(13)-Cl(3)	116.3(48)
B(12)-B(13)-Cl(3)	84.7(20)
B(5)-B(13)-Cl(4)	102.4(12)
B(1)-B(13)-Cl(4)	6.8(14)
B(14)-B(13)-Cl(4)	100.7(9)
B(6)-B(14)-Cl(3)	85.1(32)
B(13)-B(14)-Cl(3)	88.8(32)
B(14)-B(15)-Cl(3)	42.0(44)
Cl(3)-B(15)-B(11a)	150.7(53)
B(11)-B(16)-Cl(3)	89.2(21)
Cl(3)-B(16)-B(11a)	92.9(24)
Cl(3)-B(16)-B(16a)	98.3(46)
C(2)-S(2)-H(2)	103.7(43)
S(1)-C(1)-N(12)	120.8(6)
S(2)-C(2)-N(21)	121.8(7)
N(21)-C(2)-N(22)	118.7(9)
S(3)-C(3)-N(32)	120.1(6)
C(1)-N(11)-H(1)	117.3(26)
C(2)-N(21)-H(22)	131.7(65)
C(2)-N(22)-H(23)	117.4(62)
H(23)-N(22)-H(24)	85.8(86)
C(3)-N(31)-H(34)	114.4(39)
C(3)-N(32)-H(31)	111.0(49)
H(31)-N(32)-H(32)	130.9(57)
B(4)-Cl(1)-Cl(5)	4.0(15)
B(5)-Cl(1)-Cl(6)	75.8(27)
B(12)-Cl(1)-Cl(6)	43.3(15)
B(5)-Cl(1)-Cl(7)	68.2(34)
B(12)-Cl(1)-Cl(7)	35.7(23)
Cl(6)-Cl(1)-Cl(7)	7.6(18)
B(4)-Cl(5)-Cl(1)	169.4(38)
B(11)-Cl(6)-Cl(1)	142.7(32)
B(11)-Cl(6)-Cl(7)	125.4(47)
Cl(1)-Cl(6)-Cl(7)	17.4(43)
B(11)-Cl(7)-Cl(1)	171.7(48)
B(5)-Cl(7)-Cl(6)	145.4(47)
B(12)-Cl(7)-Cl(6)	104.6(43)

Table 21. F(obs) and sigma (F) for the 1,2,4 TCB-thiourea adduct structure.

F(obs) and sigma(F) (-sigma = unobserved): Trichlorobenzene Thiourea Adduct

h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s
2	0	0	88	1	5	3	0	18	1	1	6	0	28	1	10	8	0	8	2	0	12	0	42	1
4	0	0	41	1	6	3	0	6	2	2	6	0	46	1	11	8	0	3	-6	1	12	0	25	1
6	0	0	35	1	7	3	0	38	1	3	6	0	13	1	1	9	0	18	1	2	12	0	6	2
8	0	0	14	1	8	3	0	4	-3	4	6	0	44	1	2	9	0	86	1	3	12	0	9	1
10	0	0	24	1	9	3	0	9	2	5	6	0	45	1	3	9	0	7	1	4	12	0	4	-3
12	0	0	3	-6	10	3	0	3	-4	6	6	0	3	-4	4	9	0	3	-4	5	12	0	6	2
1	1	0	16	1	11	3	0	7	3	7	6	0	9	1	5	9	0	17	1	6	12	0	16	1
2	1	0	64	1	12	3	0	10	2	8	6	0	9	1	6	9	0	7	2	7	12	0	10	2
3	1	0	115	1	0	4	0	59	1	9	6	0	17	1	7	9	0	3	-4	8	12	0	3	-4
4	1	0	38	1	1	4	0	164	1	10	6	0	15	1	8	9	0	3	-4	10	12	0	8	2
5	1	0	36	1	2	4	0	102	1	11	6	0	6	-3	9	9	0	7	2	1	13	0	3	-4
6	1	0	25	1	3	4	0	28	1	12	6	0	3	-6	10	9	0	3	-6	2	13	0	6	2
7	1	0	30	1	4	4	0	6	1	1	7	0	8	1	11	9	0	3	-6	3	13	0	11	2
8	1	0	12	1	5	4	0	5	2	2	7	0	19	1	0	10	0	33	1	4	13	0	7	2
9	1	0	3	-4	6	4	0	3	-3	3	7	0	20	1	1	10	0	21	1	5	13	0	23	1
10	1	0	10	1	7	4	0	39	1	4	7	0	15	1	2	10	0	69	1	6	13	0	4	-3
11	1	0	6	-3	8	4	0	32	1	5	7	0	100	1	3	10	0	5	-2	7	13	0	6	-3
0	2	0	30	1	9	4	0	4	-3	6	7	0	11	2	4	10	0	3	-4	10	13	0	3	-7
1	2	0	4	1	10	4	0	16	1	7	7	0	18	2	5	10	0	12	1	0	14	0	31	1
2	2	0	13	1	11	4	0	3	-6	8	7	0	16	2	6	10	0	3	-4	1	14	0	19	1
3	2	0	92	1	12	4	0	3	-6	9	7	0	3	-4	7	10	0	7	2	2	14	0	13	1
4	2	0	10	1	1	5	0	37	1	10	7	0	5	-3	8	10	0	15	1	3	14	0	4	-3
5	2	0	6	1	2	5	0	92	1	11	7	0	6	-3	9	10	0	3	-4	4	14	0	3	-4
6	2	0	3	-3	3	5	0	25	1	12	7	0	3	-5	10	10	0	3	-6	5	14	0	10	2
7	2	0	62	1	4	5	0	69	1	0	8	0	103	1	11	10	0	3	-6	6	14	0	4	-3
8	2	0	3	-4	5	5	0	69	1	1	8	0	4	-2	1	11	0	25	1	1	15	0	9	2
9	2	0	8	1	6	5	0	7	1	2	8	0	110	1	2	11	0	32	1	2	15	0	12	2
10	2	0	7	2	7	5	0	6	2	3	8	0	16	1	3	11	0	17	1	3	15	0	24	1
11	2	0	3	-6	8	5	0	15	1	4	8	0	34	1	4	11	0	13	1	4	15	0	7	2
12	2	0	3	-6	9	5	0	9	1	5	8	0	7	2	5	11	0	45	1	5	15	0	6	2
1	3	0	12	1	10	5	0	11	1	6	8	0	6	2	6	11	0	4	-3	6	15	0	9	2
2	3	0	68	1	11	5	0	7	3	7	8	0	16	1	7	11	0	3	-4	0	16	0	7	2
3	3	0	150	1	12	5	0	3	-6	8	8	0	24	1	8	11	0	3	-4	1	16	0	7	2
4	3	0	8	1	0	6	0	45	1	9	8	0	9	2	10	11	0	3	-6	2	16	0	6	2

Table 21. (Continued)

F(obs) and sigma(F) (-sigma = unobserved): Trichlorobenzene Thiourea Adduct

h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s
3	16	0	10	1	3	1	1	8	1	-10	3	1	10	2	1	4	1	23	1	12	5	1	10	2
4	16	0	5	-3	4	1	1	32	1	-9	3	1	17	1	2	4	1	54	1	-10	6	1	8	2
5	16	0	4	-3	5	1	1	39	1	-8	3	1	3	-5	3	4	1	29	1	-9	6	1	12	1
1	17	0	5	-3	6	1	1	17	1	-7	3	1	20	1	4	4	1	58	1	-8	6	1	9	2
2	17	0	3	-4	7	1	1	7	2	-6	3	1	75	1	5	4	1	60	1	-7	6	1	3	-5
3	17	0	10	1	8	1	1	9	2	-5	3	1	17	1	6	4	1	47	1	-6	6	1	31	1
0	18	0	20	1	9	1	1	21	1	-4	3	1	27	1	7	4	1	10	1	-5	6	1	35	1
1	18	0	3	-6	10	1	1	7	2	-3	3	1	69	1	8	4	1	3	-5	-4	6	1	24	1
-10	0	1	3	-6	11	1	1	9	2	-2	3	1	137	1	9	4	1	10	2	-3	6	1	157	1
-8	0	1	10	2	12	1	1	3	-6	-1	3	1	333	1	10	4	1	3	-6	-2	6	1	21	1
-6	0	1	18	1	-11	2	1	14	1	0	3	1	29	1	11	4	1	3	-6	-1	6	1	29	1
-4	0	1	160	1	-10	2	1	3	-6	1	3	1	32	1	12	4	1	7	-3	0	6	1	72	1
-2	0	1	27	1	-9	2	1	3	-5	2	3	1	26	1	-10	5	1	15	1	1	6	1	16	1
0	0	1	2	-1	-8	2	1	10	2	3	3	1	41	1	-9	5	1	6	-3	2	6	1	29	1
2	0	1	134	1	-7	2	1	6	2	4	3	1	26	1	-8	5	1	33	1	3	6	1	66	1
4	0	1	84	1	-6	2	1	2	-5	5	3	1	11	1	-7	5	1	10	1	4	6	1	11	1
6	0	1	60	1	-5	2	1	73	1	6	3	1	5	-2	-6	5	1	60	1	5	6	1	2	-5
8	0	1	3	-5	-4	2	1	74	1	7	3	1	3	-5	-5	5	1	11	1	6	6	1	28	1
10	0	1	3	-6	-3	2	1	72	1	8	3	1	6	2	-4	5	1	20	1	7	6	1	35	1
12	0	1	10	2	-2	2	1	72	1	9	3	1	35	1	-3	5	1	2	-4	8	6	1	3	-6
-11	1	1	3	-6	-1	2	1	79	1	10	3	1	6	-3	-2	5	1	19	1	9	6	1	9	2
-10	1	1	8	2	0	2	1	3	1	11	3	1	10	2	-1	5	1	48	1	10	6	1	9	2
-9	1	1	10	1	1	2	1	20	1	12	3	1	3	-6	0	5	1	147	1	11	6	1	6	-4
-8	1	1	72	1	2	2	1	73	1	-10	4	1	14	1	1	5	1	112	1	-10	7	1	3	-6
-7	1	1	2	-5	3	2	1	96	1	-9	4	1	8	2	2	5	1	102	1	-9	7	1	11	2
-6	1	1	49	1	4	2	1	25	1	-8	4	1	9	2	3	5	1	14	1	-8	7	1	17	1
-5	1	1	46	1	5	2	1	82	1	-7	4	1	3	-5	4	5	1	2	-4	-7	7	1	5	-3
-4	1	1	27	1	6	2	1	13	1	-6	4	1	39	1	5	5	1	12	1	-6	7	1	34	1
-3	1	1	57	1	7	2	1	30	1	-5	4	1	23	1	6	5	1	3	-5	-5	7	1	4	-3
-2	1	1	13	1	8	2	1	3	-5	-4	4	1	45	1	7	5	1	36	1	-4	7	1	7	2
-1	1	1	22	1	9	2	1	3	-6	-3	4	1	49	1	8	5	1	7	2	-3	7	1	58	1
0	1	1	3	1	10	2	1	3	-6	-2	4	1	63	1	9	5	1	6	-3	-2	7	1	39	1
1	1	1	21	1	11	2	1	7	-3	-1	4	1	341	1	10	5	1	8	2	-1	7	1	33	1
2	1	1	229	1	12	2	1	9	2	0	4	1	78	1	11	5	1	3	-6	0	7	1	58	1

Table 21. (Continued)

F(obs) and sigma(F) (-sigma = unobserved): Trichlorobenzene Thiourea Adduct

h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s
1	7	1	109	1	-7	9	1	3	-5	6	10	1	3	-5	3	12	1	5	-3	6	14	1	7	3
2	7	1	12	1	-6	9	1	49	1	7	10	1	3	-6	4	12	1	3	-6	-6	15	1	10	2
3	7	1	8	1	-5	9	1	28	1	8	10	1	3	-6	5	12	1	10	2	-5	15	1	11	2
4	7	1	5	-3	-4	9	1	4	-3	10	10	1	3	-6	6	12	1	7	2	-4	15	1	9	2
5	7	1	12	1	-3	9	1	3	-5	11	10	1	3	-6	7	12	1	12	2	-3	15	1	3	-6
6	7	1	27	1	-2	9	1	17	1	-8	11	1	3	-6	10	12	1	3	-6	-2	15	1	10	2
7	7	1	32	1	-1	9	1	16	1	-7	11	1	3	-6	-7	13	1	11	2	-1	15	1	22	1
8	7	1	5	-3	0	9	1	91	1	-6	11	1	17	1	-6	13	1	3	-6	0	15	1	14	1
9	7	1	15	1	1	9	1	6	2	-5	11	1	3	-5	-5	13	1	3	-6	1	15	1	4	-4
10	7	1	8	2	2	9	1	12	1	-4	11	1	19	1	-4	13	1	12	1	2	15	1	14	1
11	7	1	7	-3	3	9	1	22	1	-3	11	1	3	-5	-3	13	1	3	-6	3	15	1	10	2
-9	8	1	3	-6	4	9	1	45	1	-2	11	1	15	1	-2	13	1	15	1	4	15	1	3	-6
-8	8	1	14	1	5	9	1	12	1	-1	11	1	31	1	-1	13	1	3	-5	5	15	1	8	2
-7	8	1	5	-3	6	9	1	7	2	0	11	1	17	1	0	13	1	8	2	-5	16	1	9	2
-6	8	1	28	1	7	9	1	6	-3	1	11	1	45	1	1	13	1	35	1	-4	16	1	3	-6
-5	8	1	9	2	8	9	1	6	-3	2	11	1	12	1	2	13	1	27	1	-3	16	1	3	-6
-4	8	1	2	-5	9	9	1	8	2	3	11	1	3	-6	3	13	1	6	-3	-2	16	1	3	-6
-3	8	1	89	1	10	9	1	9	2	4	11	1	14	1	4	13	1	17	1	-1	16	1	17	1
-2	8	1	54	1	11	9	1	10	2	5	11	1	3	-5	5	13	1	15	1	0	16	1	4	-4
-1	8	1	7	1	-9	10	1	3	-6	6	11	1	8	2	6	13	1	10	2	1	16	1	3	-6
0	8	1	38	1	-8	10	1	3	-6	7	11	1	16	1	7	13	1	14	1	2	16	1	13	1
1	8	1	36	1	-7	10	1	9	2	8	11	1	11	2	-7	14	1	9	2	3	16	1	3	-6
2	8	1	7	1	-6	10	1	37	1	10	11	1	5	-4	-6	14	1	7	3	4	16	1	3	-6
3	8	1	26	1	-5	10	1	3	-5	-8	12	1	8	2	-5	14	1	9	2	-4	17	1	11	2
4	8	1	76	1	-4	10	1	4	-4	-7	12	1	3	-6	-4	14	1	12	1	-3	17	1	8	2
5	8	1	13	1	-3	10	1	25	1	-6	12	1	3	-6	-3	14	1	17	1	-2	17	1	8	2
6	8	1	6	2	-2	10	1	11	1	-5	12	1	10	1	-2	14	1	3	-6	-1	17	1	13	2
7	8	1	35	1	-1	10	1	32	1	-4	12	1	10	2	-1	14	1	24	1	0	17	1	6	-3
8	8	1	4	-4	0	10	1	4	-3	-3	12	1	54	1	0	14	1	3	-5	1	17	1	3	-6
9	8	1	3	-6	1	10	1	20	1	-2	12	1	8	2	1	14	1	10	2	2	17	1	9	2
10	8	1	3	-6	2	10	1	3	-5	-1	12	1	8	2	2	14	1	10	2	3	17	1	5	-4
11	8	1	8	3	3	10	1	25	1	0	12	1	11	1	3	14	1	3	-6	-1	18	1	3	-6
-9	9	1	3	-6	4	10	1	69	1	1	12	1	4	-4	4	14	1	16	1	0	18	1	6	-3
-8	9	1	6	-3	5	10	1	10	2	2	12	1	6	2	5	14	1	7	3	1	18	1	8	2

Table 21. (Continued)

F(obs) and sigma(F) (-sigma = unobserved): Trichlorobenzene Thiourea Adduct

h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s
-10	0	2	3	-5	11	1	2	9	2	-3	3	2	115	1	9	4	2	5	-3	2	6	2	8	1
-8	0	2	14	1	12	1	2	5	-4	-2	3	2	341	1	11	4	2	9	2	3	6	2	38	1
-6	0	2	73	1	-11	2	2	3	-6	-1	3	2	4	2	-10	5	2	6	-3	4	6	2	32	1
-4	0	2	6	1	-10	2	2	6	-3	0	3	2	46	1	-9	5	2	19	1	5	6	2	34	1
-2	0	2	235	1	-9	2	2	37	1	1	3	2	45	1	-8	5	2	3	-5	6	6	2	14	1
0	0	2	19	1	-8	2	2	17	1	2	3	2	78	1	-7	5	2	28	1	7	6	2	6	-3
2	0	2	30	1	-7	2	2	22	1	3	3	2	27	1	-6	5	2	28	1	8	6	2	16	1
4	0	2	94	1	-6	2	2	41	1	4	3	2	24	1	-5	5	2	5	-2	9	6	2	15	1
6	0	2	16	1	-5	2	2	33	1	5	3	2	31	1	-4	5	2	118	1	10	6	2	3	-6
8	0	2	44	1	-4	2	2	66	1	6	3	2	43	1	-3	5	2	49	1	11	6	2	3	-6
10	0	2	7	2	-3	2	2	79	1	7	3	2	13	1	-2	5	2	36	1	-10	7	2	11	2
12	0	2	3	-6	-2	2	2	114	1	8	3	2	5	-3	-1	5	2	121	1	-9	7	2	3	-6
-11	1	2	7	2	-1	2	2	38	1	9	3	2	7	-3	0	5	2	14	1	-8	7	2	3	-5
-10	1	2	3	-6	0	2	2	93	1	11	3	2	7	-3	1	5	2	32	1	-7	7	2	3	-5
-9	1	2	18	1	1	2	2	270	1	-11	4	2	8	2	2	5	2	2	-4	-6	7	2	7	2
-8	1	2	7	2	2	2	2	151	1	-10	4	2	3	-6	3	5	2	18	1	-5	7	2	8	2
-7	1	2	11	1	3	2	2	89	1	-9	4	2	13	1	4	5	2	38	1	-4	7	2	8	1
-6	1	2	39	1	4	2	2	62	1	-8	4	2	13	1	5	5	2	6	2	-3	7	2	9	1
-5	1	2	30	1	5	2	2	2	-5	-7	4	2	13	1	6	5	2	51	1	-2	7	2	90	1
-4	1	2	24	1	6	2	2	2	-5	-6	4	2	49	1	7	5	2	4	-3	-1	7	2	150	1
-3	1	2	112	1	7	2	2	3	-5	-5	4	2	42	1	8	5	2	18	1	0	7	2	56	1
-2	1	2	241	1	8	2	2	25	1	-4	4	2	51	1	9	5	2	3	-6	1	7	2	7	1
-1	1	2	8	1	9	2	2	15	1	-3	4	2	82	1	-10	6	2	3	-6	2	7	2	14	1
0	1	2	30	1	10	2	2	6	-3	-2	4	2	83	1	-9	6	2	9	2	3	7	2	55	1
1	1	2	25	1	11	2	2	13	2	-1	4	2	5	2	-8	6	2	5	-3	4	7	2	17	1
2	1	2	20	1	12	2	2	10	2	0	4	2	9	1	-7	6	2	59	1	5	7	2	14	1
3	1	2	17	1	-11	3	2	10	2	1	4	2	154	1	-6	6	2	53	1	6	7	2	22	1
4	1	2	143	1	-10	3	2	5	-3	2	4	2	74	1	-5	6	2	5	-2	7	7	2	3	-6
5	1	2	30	1	-9	3	2	32	1	3	4	2	10	1	-4	6	2	2	-5	8	7	2	6	-3
6	1	2	2	-5	-8	3	2	3	-5	4	4	2	40	1	-3	6	2	11	1	9	7	2	12	2
7	1	2	12	1	-7	3	2	24	1	5	4	2	2	-5	-2	6	2	3	-3	10	7	2	3	-6
8	1	2	26	1	-6	3	2	42	1	6	4	2	9	2	-1	6	2	147	1	11	7	2	3	-6
9	1	2	6	2	-5	3	2	24	1	7	4	2	3	-5	0	6	2	28	1	-10	8	2	3	-6
10	1	2	3	-6	-4	3	2	68	1	8	4	2	10	2	1	6	2	28	1	-9	8	2	9	2

Table 21. (Continued)

F(obs) and sigma(F) (-sigma = unobserved): Trichlorobenzene Thiourea Adduct

h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s
-8	8	2	21	1	6	9	2	60	1	2	11	2	6	2	3	13	2	20	1	-1	16	2	8	2
-7	8	2	31	1	7	9	2	3	-6	3	11	2	26	1	4	13	2	18	1	0	16	2	3	-6
-6	8	2	3	-5	8	9	2	16	1	4	11	2	12	1	5	13	2	8	2	1	16	2	27	1
-5	8	2	6	2	10	9	2	3	-6	5	11	2	3	-6	6	13	2	5	-4	2	16	2	3	-6
-4	8	2	37	1	-9	10	2	10	2	6	11	2	28	1	-7	14	2	5	-4	3	16	2	3	-6
-3	8	2	11	1	-8	10	2	11	2	7	11	2	3	-6	-6	14	2	15	1	4	16	2	4	-4
-2	8	2	24	1	-7	10	2	10	2	10	11	2	3	-6	-5	14	2	18	1	-4	17	2	3	-6
-1	8	2	54	1	-6	10	2	7	2	-8	12	2	3	-6	-4	14	2	5	-3	-3	17	2	7	-3
0	8	2	52	1	-5	10	2	11	1	-7	12	2	11	2	-3	14	2	14	1	-2	17	2	16	1
1	8	2	29	1	-4	10	2	40	1	-6	12	2	13	1	-2	14	2	3	-6	-1	17	2	3	-6
2	8	2	6	2	-3	10	2	7	2	-5	12	2	3	-5	-1	14	2	8	2	0	17	2	7	3
3	8	2	54	1	-2	10	2	46	1	-4	12	2	3	-6	0	14	2	3	-5	1	17	2	3	-6
4	8	2	7	2	-1	10	2	42	1	-3	12	2	7	2	1	14	2	23	1	2	17	2	3	-6
5	8	2	4	-3	0	10	2	40	1	-2	12	2	3	-5	2	14	2	12	1	3	17	2	3	-6
6	8	2	18	1	1	10	2	15	1	-1	12	2	37	1	3	14	2	8	2	-1	18	2	6	-3
7	8	2	7	2	2	10	2	56	1	0	12	2	14	1	4	14	2	18	1	0	18	2	3	-6
8	8	2	3	-6	3	10	2	36	1	1	12	2	7	2	5	14	2	3	-6	-10	0	3	30	1
10	8	2	3	-6	4	10	2	19	1	2	12	2	5	-3	6	14	2	3	-6	-8	0	3	7	2
11	8	2	3	-6	5	10	2	3	-5	3	12	2	45	1	-6	15	2	6	-3	-6	0	3	13	1
-9	9	2	4	-4	6	10	2	3	-6	4	12	2	6	-3	-5	15	2	3	-6	-4	0	3	170	1
-8	9	2	3	-6	7	10	2	5	-4	5	12	2	6	-3	-4	15	2	12	2	-2	0	3	151	1
-7	9	2	16	1	8	10	2	3	-6	6	12	2	6	-3	-3	15	2	12	1	0	0	3	211	4
-6	9	2	8	2	10	10	2	3	-6	7	12	2	10	2	-2	15	2	5	-3	2	0	3	17	1
-5	9	2	7	2	-9	11	2	8	2	-8	13	2	5	-4	-1	15	2	7	2	4	0	3	42	1
-4	9	2	80	1	-8	11	2	10	2	-7	13	2	3	-6	0	15	2	5	-3	6	0	3	37	1
-3	9	2	2	-5	-7	11	2	5	-3	-6	13	2	9	2	1	15	2	4	-4	8	0	3	22	1
-2	9	2	6	2	-6	11	2	3	-5	-5	13	2	3	-6	2	15	2	5	-3	-11	1	3	3	-6
-1	9	2	48	1	-5	11	2	4	-4	-4	13	2	18	1	3	15	2	10	2	-10	1	3	3	-6
0	9	2	46	1	-4	11	2	29	1	-3	13	2	11	1	4	15	2	8	2	-9	1	3	8	2
1	9	2	20	1	-3	11	2	6	2	-2	13	2	32	1	5	15	2	9	2	-8	1	3	13	1
2	9	2	7	2	-2	11	2	3	-5	-1	13	2	35	1	-5	16	2	8	2	-7	1	3	56	1
3	9	2	4	-4	-1	11	2	23	1	0	13	2	22	1	-4	16	2	7	2	-6	1	3	12	1
4	9	2	11	1	0	11	2	3	-5	1	13	2	3	-5	-3	16	2	5	-4	-5	1	3	69	1
5	9	2	3	-5	1	11	2	21	1	2	13	2	11	1	-2	16	2	8	2	-4	1	3	131	1

Table 21. (Continued)

F(obs) and sigma(F) (-sigma = unobserved): Trichlorobenzene Thiourea Adduct

h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s
-3	1	3	142	1	9	2	3	3	-6	-1	4	3	2	-4	-10	6	3	11	2	2	7	3	6	2
-2	1	3	28	1	11	2	3	9	2	0	4	3	95	1	-9	6	3	26	1	3	7	3	31	1
-1	1	3	63	1	-11	3	3	3	-6	1	4	3	17	1	-8	6	3	13	1	4	7	3	33	1
0	1	3	183	1	-10	3	3	7	2	2	4	3	13	1	-7	6	3	29	1	5	7	3	33	1
1	1	3	24	1	-9	3	3	13	1	3	4	3	2	-5	-6	6	3	17	1	6	7	3	3	-5
2	1	3	7	1	-8	3	3	11	1	4	4	3	15	1	-5	6	3	36	1	7	7	3	10	2
3	1	3	59	1	-7	3	3	85	1	5	4	3	20	1	-4	6	3	29	1	8	7	3	9	2
4	1	3	25	1	-6	3	3	9	1	6	4	3	25	1	-3	6	3	111	1	10	7	3	3	-6
5	1	3	21	1	-5	3	3	10	1	7	4	3	30	1	-2	6	3	67	1	-10	8	3	10	2
6	1	3	12	1	-4	3	3	82	1	8	4	3	22	1	-1	6	3	5	2	-9	8	3	11	2
7	1	3	5	-3	-3	3	3	29	1	9	4	3	4	-4	0	6	3	89	1	-8	8	3	19	1
8	1	3	9	2	-2	3	3	81	1	11	4	3	5	-4	1	6	3	33	1	-7	8	3	3	-5
9	1	3	5	-3	-1	3	3	2	-4	-11	5	3	9	2	2	6	3	11	1	-6	8	3	3	-5
11	1	3	3	-6	0	3	3	10	1	-10	5	3	3	-6	3	6	3	4	-3	-5	8	3	29	1
-11	2	3	10	2	1	3	3	18	1	-9	5	3	6	-3	4	6	3	9	1	-4	8	3	9	1
-10	2	3	14	1	2	3	3	89	1	-8	5	3	29	1	5	6	3	68	1	-3	8	3	8	1
-9	2	3	8	2	3	3	3	185	1	-7	5	3	20	1	6	6	3	19	1	-2	8	3	112	1
-8	2	3	6	2	4	3	3	21	1	-6	5	3	9	1	7	6	3	3	-6	-1	8	3	26	1
-7	2	3	22	1	5	3	3	12	1	-5	5	3	68	1	8	6	3	14	1	0	8	3	11	1
-6	2	3	2	-5	6	3	3	3	-5	-4	5	3	48	1	9	6	3	7	2	1	8	3	43	1
-5	2	3	25	1	7	3	3	17	1	-3	5	3	52	1	10	6	3	3	-6	2	8	3	10	1
-4	2	3	43	1	8	3	3	12	1	-2	5	3	54	1	11	6	3	3	-7	3	8	3	11	1
-3	2	3	15	1	9	3	3	6	-3	-1	5	3	24	1	-10	7	3	3	-6	4	8	3	18	1
-2	2	3	163	1	11	3	3	3	-6	0	5	3	122	1	-9	7	3	15	1	5	8	3	41	1
-1	2	3	7	1	-11	4	3	8	2	1	5	3	6	2	-8	7	3	7	2	6	8	3	3	-6
0	2	3	95	1	-10	4	3	12	1	2	5	3	24	1	-7	7	3	18	1	7	8	3	3	-6
1	2	3	4	2	-9	4	3	9	2	3	5	3	18	1	-6	7	3	3	-5	8	8	3	11	2
2	2	3	25	1	-8	4	3	13	1	4	5	3	4	-3	-5	7	3	61	1	10	8	3	3	-6
3	2	3	50	1	-7	4	3	23	1	5	5	3	14	1	-4	7	3	19	1	-10	9	3	7	3
4	2	3	22	1	-6	4	3	15	1	6	5	3	3	-5	-3	7	3	113	1	-9	9	3	3	-6
5	2	3	25	1	-5	4	3	59	1	7	5	3	22	1	-2	7	3	4	-3	-8	9	3	7	2
6	2	3	9	2	-4	4	3	39	1	8	5	3	3	-6	-1	7	3	28	1	-7	9	3	3	-5
7	2	3	47	1	-3	4	3	84	1	9	5	3	7	2	0	7	3	30	1	-6	9	3	18	1
8	2	3	5	-3	-2	4	3	234	1	11	5	3	5	-4	1	7	3	93	1	-5	9	3	10	1

Table 21. (Continued)

F(obs) and sigma(F) (-sigma = unobserved): Trichlorobenzene Thiourea Adduct

h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s
-4	9	3	12	1	-7	11	3	13	1	-4	13	3	6	-3	-5	16	3	3	-6	-3	1	4	42	1
-3	9	3	35	1	-6	11	3	16	1	-3	13	3	24	1	-4	16	3	3	-6	-2	1	4	109	1
-2	9	3	2	-5	-5	11	3	39	1	-2	13	3	6	2	-3	16	3	11	2	-1	1	4	137	1
-1	9	3	26	1	-4	11	3	3	-5	-1	13	3	6	2	-2	16	3	3	-6	0	1	4	81	1
0	9	3	4	-3	-3	11	3	3	-5	0	13	3	16	1	-1	16	3	6	-3	1	1	4	16	1
1	9	3	7	2	-2	11	3	17	1	1	13	3	11	1	0	16	3	7	3	2	1	4	33	1
2	9	3	80	1	-1	11	3	3	-5	2	13	3	19	1	1	16	3	9	2	3	1	4	6	2
3	9	3	11	1	0	11	3	15	1	3	13	3	4	-4	2	16	3	3	-6	4	1	4	3	-3
4	9	3	3	-5	1	11	3	46	1	4	13	3	3	-6	3	16	3	9	2	5	1	4	32	1
5	9	3	8	2	2	11	3	37	1	5	13	3	10	2	-4	17	3	10	2	6	1	4	39	1
6	9	3	5	-3	3	11	3	8	2	-7	14	3	8	2	-3	17	3	3	-6	7	1	4	21	1
7	9	3	5	-3	4	11	3	15	1	-6	14	3	3	-6	-2	17	3	3	-6	8	1	4	11	2
8	9	3	16	1	5	11	3	28	1	-5	14	3	3	-6	-1	17	3	3	-6	9	1	4	10	2
10	9	3	3	-7	6	11	3	7	3	-4	14	3	13	1	0	17	3	5	-4	11	1	4	3	-6
-9	10	3	3	-6	7	11	3	3	-6	-3	14	3	11	1	1	17	3	3	-6	-11	2	4	3	-6
-8	10	3	8	2	-8	12	3	3	-6	-2	14	3	24	1	-2	17	3	8	2	-10	2	4	15	1
-7	10	3	3	-5	-7	12	3	3	-6	-1	14	3	3	-6	-10	0	4	16	1	-9	2	4	3	-5
-6	10	3	9	2	-6	12	3	11	1	0	14	3	17	1	-8	0	4	51	1	-8	2	4	10	2
-5	10	3	13	1	-5	12	3	13	1	1	14	3	15	1	-6	0	4	49	1	-7	2	4	25	1
-4	10	3	9	2	-4	12	3	23	1	2	14	3	10	2	-4	0	4	67	1	-6	2	4	29	1
-3	10	3	5	-3	-3	12	3	3	-5	3	14	3	9	2	-2	0	4	54	1	-5	2	4	101	1
-2	10	3	86	1	-2	12	3	14	1	4	14	3	3	-6	0	0	4	124	2	-4	2	4	44	1
-1	10	3	14	1	-1	12	3	16	1	5	14	3	10	2	2	0	4	96	1	-3	2	4	5	1
0	10	3	17	1	0	12	3	31	1	-6	15	3	6	-3	4	0	4	24	1	-2	2	4	57	1
1	10	3	9	2	1	12	3	17	1	-5	15	3	5	-3	6	0	4	16	1	-1	2	4	24	1
2	10	3	12	1	2	12	3	26	1	-4	15	3	9	2	8	0	4	3	-6	0	2	4	42	1
3	10	3	3	-5	3	12	3	3	-6	-3	15	3	11	2	-11	1	4	8	2	1	2	4	4	-2
4	10	3	3	-5	4	12	3	5	-3	-2	15	3	6	-3	-10	1	4	3	-6	2	2	4	42	1
5	10	3	15	1	5	12	3	30	1	-1	15	3	5	-4	-9	1	4	9	2	3	2	4	2	-5
6	10	3	3	-6	6	12	3	9	2	0	15	3	11	2	-8	1	4	70	1	4	2	4	15	1
7	10	3	8	2	-8	13	3	3	-6	1	15	3	3	-6	-7	1	4	10	1	5	2	4	50	1
10	10	3	3	-7	-7	13	3	3	-6	2	15	3	3	-6	-6	1	4	13	1	6	2	4	3	-5
-9	11	3	7	-3	-6	13	3	6	-3	3	15	3	23	1	-5	1	4	51	1	7	2	4	7	2
-8	11	3	3	-6	-5	13	3	20	1	4	15	3	8	2	-4	1	4	23	1	8	2	4	10	2

Table 21. (Continued)

F(obs) and sigma(F) (-sigma = unobserved): Trichlorobenzene Thiourea Adduct

h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s
9	2	4	8	2	-1	4	4	27	1	-7	6	4	16	1	7	7	4	35	1	1	9	4	3	-5
11	2	4	3	-6	0	4	4	35	1	-6	6	4	3	-5	8	7	4	5	-3	2	9	4	3	-5
-11	3	4	9	2	1	4	4	72	1	-5	6	4	12	1	10	7	4	3	-6	3	9	4	26	1
-10	3	4	20	1	2	4	4	129	1	-4	6	4	21	1	-10	8	4	4	-4	4	9	4	16	1
-9	3	4	10	1	3	4	4	37	1	-3	6	4	88	1	-9	8	4	3	-6	5	9	4	5	-3
-8	3	4	27	1	4	4	4	47	1	-2	6	4	12	1	-8	8	4	14	1	6	9	4	5	-3
-7	3	4	3	-5	5	4	4	23	1	-1	6	4	8	1	-7	8	4	19	1	7	9	4	5	-4
-6	3	4	20	1	6	4	4	14	1	0	6	4	5	2	-6	8	4	33	1	10	9	4	7	-3
-5	3	4	2	-5	7	4	4	18	1	1	6	4	34	1	-5	8	4	6	2	-9	10	4	7	2
-4	3	4	42	1	8	4	4	7	2	2	6	4	102	1	-4	8	4	29	1	-8	10	4	12	1
-3	3	4	63	1	11	4	4	9	2	3	6	4	33	1	-3	8	4	44	1	-7	10	4	3	-5
-2	3	4	5	1	-11	5	4	5	-4	4	6	4	18	1	-2	8	4	5	-3	-6	10	4	39	1
-1	3	4	201	1	-10	5	4	24	1	-5	6	4	3	-5	-1	8	4	18	1	-5	10	4	17	1
0	3	4	98	1	-9	5	4	7	2	6	6	4	7	2	0	8	4	5	-2	-4	10	4	7	2
1	3	4	42	1	-8	5	4	27	1	7	6	4	3	-6	1	8	4	69	1	-3	10	4	20	1
2	3	4	15	1	-7	5	4	7	2	8	6	4	3	-6	2	8	4	12	1	-2	10	4	10	1
3	3	4	7	1	-6	5	4	14	1	10	6	4	3	-6	3	8	4	49	1	-1	10	4	7	2
4	3	4	17	1	-5	5	4	44	1	-10	7	4	9	2	4	8	4	48	1	0	10	4	39	1
5	3	4	47	1	-4	5	4	10	1	-9	7	4	3	-6	5	8	4	3	-5	1	10	4	9	2
6	3	4	6	-2	-3	5	4	53	1	-8	7	4	9	2	6	8	4	3	-6	2	10	4	16	1
7	3	4	15	1	-2	5	4	30	1	-7	7	4	3	-5	7	8	4	7	-3	3	10	4	6	-3
8	3	4	3	-6	-1	5	4	45	1	-6	7	4	25	1	8	8	4	3	-6	4	10	4	43	1
9	3	4	13	2	0	5	4	20	1	-5	7	4	8	2	10	8	4	3	-7	5	10	4	7	2
11	3	4	3	-6	1	5	4	57	1	-4	7	4	63	1	-10	9	4	22	1	6	10	4	3	-6
-11	4	4	3	-6	2	5	4	50	1	-3	7	4	107	1	-9	9	4	10	2	7	10	4	3	-6
-10	4	4	3	-6	3	5	4	15	1	-2	7	4	10	1	-8	9	4	8	2	-9	11	4	7	3
-9	4	4	3	-5	4	5	4	28	1	-1	7	4	23	1	-7	9	4	3	-5	-8	11	4	10	2
-8	4	4	27	1	5	5	4	11	1	0	7	4	7	1	-6	9	4	18	1	-7	11	4	4	-4
-7	4	4	5	-2	6	5	4	9	2	1	7	4	39	1	-5	9	4	6	-2	-6	11	4	8	2
-6	4	4	53	1	7	5	4	23	1	2	7	4	6	2	-4	9	4	11	1	-5	11	4	14	1
-5	4	4	110	1	8	5	4	3	-6	3	7	4	3	-5	-3	9	4	23	1	-4	11	4	18	1
-4	4	4	53	1	-10	6	4	5	-4	4	7	4	7	2	-2	9	4	2	-5	-3	11	4	42	1
-3	4	4	84	1	-9	6	4	3	-6	5	7	4	12	1	-1	9	4	11	1	-2	11	4	5	-3
-2	4	4	40	1	-8	6	4	17	1	6	7	4	6	-3	0	9	4	67	1	-1	11	4	9	2

Table 21. (Continued)

F(obs) and sigma(F). (-sigma = unobserved): Trichlorobenzene Thiourea Adduct

h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s
0	11	4	54	1	4	13	4	3	-6	3	16	4	3	-6	7	1	5	12	1	1	3	5	126	1
1	11	4	31	1	5	13	4	9	2	-3	17	4	10	2	8	1	5	3	-6	2	3	5	43	1
2	11	4	5	-3	-7	14	4	5	-4	-2	17	4	7	-3	-11	2	5	21	1	3	3	5	15	1
3	11	4	11	2	-6	14	4	7	3	-1	17	4	10	2	-10	2	5	3	-6	4	3	5	11	1
4	11	4	17	1	-5	14	4	6	-3	0	17	4	3	-6	-9	2	5	38	1	5	3	5	3	-5
5	11	4	3	-6	-4	14	4	8	2	1	17	4	3	-6	-8	2	5	10	1	6	3	5	13	1
6	11	4	6	-3	-3	14	4	13	1	-10	0	5	5	-3	-7	2	5	12	1	7	3	5	4	-4
-8	12	4	3	-6	-2	14	4	7	2	-8	0	5	26	1	-6	2	5	45	1	8	3	5	10	2
-7	12	4	7	2	-1	14	4	12	1	-6	0	5	35	1	-5	2	5	38	1	-11	4	5	7	2
-6	12	4	3	-6	0	14	4	21	1	-4	0	5	2	-4	-4	2	5	24	1	-10	4	5	6	-3
-5	12	4	10	2	1	14	4	5	-3	-2	0	5	94	1	-3	2	5	96	1	-9	4	5	25	1
-4	12	4	21	1	2	14	4	17	1	0	0	5	88	1	-2	2	5	48	1	-8	4	5	26	1
-3	12	4	44	1	3	14	4	8	2	2	0	5	10	1	-1	2	5	41	1	-7	4	5	33	1
-2	12	4	12	1	4	14	4	14	1	4	0	5	16	1	0	2	5	107	1	-6	4	5	6	2
-1	12	4	12	1	5	14	4	6	-3	6	0	5	4	-4	1	2	5	118	1	-5	4	5	48	1
0	12	4	23	1	-6	15	4	3	-6	8	0	5	28	1	2	2	5	21	1	-4	4	5	47	1
1	12	4	19	1	-5	15	4	3	-6	-11	1	5	7	2	3	2	5	5	-2	-3	4	5	25	1
2	12	4	19	1	-4	15	4	6	-3	-10	1	5	9	2	4	2	5	11	1	-2	4	5	54	1
3	12	4	21	1	-3	15	4	9	2	-9	1	5	3	-5	5	2	5	7	2	-1	4	5	18	1
4	12	4	3	-6	-2	15	4	5	-3	-8	1	5	24	1	6	2	5	25	1	0	4	5	29	1
5	12	4	10	2	-1	15	4	23	1	-7	1	5	11	1	7	2	5	18	1	1	4	5	70	1
6	12	4	8	2	0	15	4	9	2	-6	1	5	75	1	8	2	5	15	1	2	4	5	14	1
-8	13	4	10	2	1	15	4	6	-3	-5	1	5	38	1	-11	3	5	3	-6	3	4	5	4	-3
-7	13	4	11	2	2	15	4	4	-4	-4	1	5	71	1	-10	3	5	6	-3	4	4	5	9	2
-6	13	4	5	-3	3	15	4	7	3	-3	1	5	51	1	-9	3	5	3	-6	5	4	5	15	1
-5	13	4	7	2	4	15	4	3	-6	-2	1	5	49	1	-8	3	5	4	-4	6	4	5	37	1
-4	13	4	6	-3	-5	16	4	17	1	-1	1	5	50	1	-7	3	5	13	1	7	4	5	13	1
-3	13	4	24	1	-4	16	4	11	2	0	1	5	5	2	-6	3	5	2	-5	8	4	5	10	2
-2	13	4	8	2	-3	16	4	5	-4	1	1	5	32	1	-5	3	5	52	1	-11	5	5	17	1
-1	13	4	13	1	-2	16	4	5	-3	2	1	5	2	-5	-4	3	5	46	1	-10	5	5	5	-4
0	13	4	14	1	-1	16	4	3	-6	3	1	5	24	1	-3	3	5	107	1	-9	5	5	13	1
1	13	4	3	-6	0	16	4	3	-6	4	1	5	103	1	-2	3	5	15	1	-8	5	5	10	2
2	13	4	10	2	1	16	4	9	2	5	1	5	18	1	-1	3	5	23	1	-7	5	5	9	2
3	13	4	7	2	2	16	4	3	-6	6	1	5	3	-5	0	3	5	23	1	-6	5	5	58	1

Table 21. (Continued)

F(obs) and sigma(F) (-sigma = unobserved): Trichlorobenzene Thiourea Adduct

h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s
-5	5	5	35	1	-10	7	5	8	2	5	8	5	11	2	4	10	5	4	-4	-7	13	5	3	-6
-4	5	5	33	1	-9	7	5	11	2	6	8	5	24	1	5	10	5	9	2	-6	13	5	11	2
-3	5	5	74	1	-8	7	5	3	-5	7	8	5	9	2	6	10	5	26	1	-5	13	5	9	2
-2	5	5	29	1	-7	7	5	25	1	-10	9	5	3	-6	-9	11	5	5	-4	-4	13	5	13	1
-1	5	5	26	1	-6	7	5	3	-5	-9	9	5	3	-6	-8	11	5	3	-6	-3	13	5	3	-6
0	5	5	9	1	-5	7	5	11	1	-8	9	5	13	1	-7	11	5	8	2	-2	13	5	11	2
1	5	5	9	1	-4	7	5	49	1	-7	9	5	7	2	-6	11	5	3	-6	-1	13	5	8	2
2	5	5	22	1	-3	7	5	12	1	-6	9	5	33	1	-5	11	5	16	1	0	13	5	3	-6
3	5	5	28	1	-2	7	5	23	1	-5	9	5	38	1	-4	11	5	27	1	1	13	5	3	-6
4	5	5	53	1	-1	7	5	33	1	-4	9	5	74	1	-3	11	5	14	1	2	13	5	16	1
5	5	5	3	-5	0	7	5	53	1	-3	9	5	3	-5	-2	11	5	11	1	3	13	5	12	2
6	5	5	32	1	1	7	5	13	1	-2	9	5	7	2	-1	11	5	13	1	4	13	5	16	1
7	5	5	5	-4	2	7	5	9	2	-1	9	5	3	-5	0	11	5	10	2	5	13	5	3	-6
8	5	5	3	-6	3	7	5	48	1	0	9	5	11	1	1	11	5	3	-5	-7	14	5	3	-6
-10	6	5	11	2	4	7	5	21	1	1	9	5	7	2	2	11	5	14	1	-6	14	5	4	-4
-9	6	5	3	-6	5	7	5	9	2	2	9	5	48	1	3	11	5	31	1	-5	14	5	7	3
-8	6	5	7	2	6	7	5	5	-4	3	9	5	14	1	4	11	5	7	2	-4	14	5	7	2
-7	6	5	27	1	7	7	5	6	-3	4	9	5	3	-5	5	11	5	3	-6	-3	14	5	6	-3
-6	6	5	25	1	10	7	5	3	-7	5	9	5	10	2	6	11	5	7	3	-2	14	5	13	1
-5	6	5	2	-5	-10	8	5	6	-3	6	9	5	22	1	-8	12	5	3	-6	-1	14	5	12	1
-4	6	5	61	1	-9	8	5	9	2	-7	9	5	9	2	-7	12	5	13	1	0	14	5	6	-3
-3	6	5	25	1	-8	8	5	14	1	-9	10	5	14	1	-6	12	5	3	-6	1	14	5	14	1
-2	6	5	33	1	-7	8	5	3	-5	-8	10	5	21	1	-5	12	5	13	1	2	14	5	3	-6
-1	6	5	109	1	-6	8	5	12	1	-7	10	5	16	1	-4	12	5	3	-6	3	14	5	6	-3
0	6	5	2	-5	-5	8	5	11	1	-6	10	5	10	2	-3	12	5	3	-6	4	14	5	9	2
1	6	5	41	1	-4	8	5	3	-5	-5	10	5	33	1	-2	12	5	18	1	-6	15	5	7	3
2	6	5	10	1	-3	8	5	13	1	-4	10	5	10	1	-1	12	5	52	1	-5	15	5	8	2
3	6	5	14	1	-2	8	5	8	2	-3	10	5	3	-5	0	12	5	11	1	-4	15	5	11	2
4	6	5	16	1	-1	8	5	79	1	-2	10	5	10	1	1	12	5	5	-3	-3	15	5	11	2
5	6	5	7	2	0	8	5	12	1	-1	10	5	50	1	2	12	5	15	1	-2	15	5	14	1
6	6	5	10	2	1	8	5	8	2	0	10	5	23	1	3	12	5	5	-4	-1	15	5	8	2
7	6	5	9	2	2	8	5	20	1	1	10	5	8	2	4	12	5	8	2	0	15	5	8	2
8	6	5	9	2	3	8	5	6	2	2	10	5	44	1	5	12	5	7	3	1	15	5	12	2
10	6	5	3	-6	4	8	5	7	2	3	10	5	18	1	-8	13	5	3	-6	2	15	5	6	-3

Table 21. (Continued)

F(obs) and sigma(F) (-sigma = unobserved): Trichlorobenzene Thiourea Adduct

h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s
3	15	5	4	-4	2	1	6	22	1	-3	3	6	16	1	-7	5	6	13	1	-9	7	6	28	1
-5	16	5	5	-4	3	1	6	38	1	-2	3	6	73	1	-6	5	6	26	1	-8	7	6	9	2
-4	16	5	3	-6	4	1	6	3	-5	-1	3	6	48	1	-5	5	6	16	1	-7	7	6	22	1
-3	16	5	9	-2	5	1	6	8	2	0	3	6	32	1	-4	5	6	8	1	-6	7	6	6	2
-2	16	5	6	-3	6	1	6	15	1	1	3	6	16	1	-3	5	6	2	-4	-5	7	6	4	-3
-1	16	5	8	-2	7	1	6	7	2	2	3	6	27	1	-2	5	6	26	1	-4	7	6	20	1
0	16	5	3	-6	8	1	6	7	-3	3	3	6	47	1	-1	5	6	19	1	-3	7	6	4	-3
1	16	5	18	1	-11	2	6	9	2	4	3	6	3	-5	0	5	6	69	1	-2	7	6	13	1
2	16	5	6	-3	-10	2	6	5	-3	5	3	6	8	2	1	5	6	30	1	-1	7	6	26	1
-2	17	5	14	1	-9	2	6	11	1	6	3	6	4	-4	2	5	6	19	1	0	7	6	2	-5
-1	17	5	3	-6	-8	2	6	3	-5	7	3	6	17	1	3	5	6	7	2	1	7	6	69	1
-10	0	6	3	-6	-7	2	6	37	1	-11	4	6	11	2	4	5	6	8	2	2	7	6	13	1
-8	0	6	10	1	-6	2	6	5	-2	-10	4	6	4	-4	5	5	6	10	2	3	7	6	4	-3
-6	0	6	16	1	-5	2	6	60	1	-9	4	6	14	1	6	5	6	20	1	4	7	6	14	1
-4	0	6	166	1	-4	2	6	89	1	-8	4	6	3	-5	7	5	6	9	2	5	7	6	8	2
-2	0	6	20	1	-3	2	6	47	1	-7	4	6	12	1	-10	6	6	3	-6	6	7	6	3	-6
0	0	6	28	1	-2	2	6	46	1	-6	4	6	39	1	-9	6	6	15	1	7	7	6	7	3
2	0	6	14	1	-1	2	6	36	1	-5	4	6	5	-2	-8	6	6	11	1	-10	8	6	6	-3
4	0	6	4	-3	0	2	6	5	-2	-4	4	6	33	1	-7	6	6	28	1	-9	8	6	9	2
6	0	6	41	1	1	2	6	31	1	-3	4	6	5	2	-6	6	6	7	2	-8	8	6	15	1
8	0	6	3	-6	2	2	6	10	1	-2	4	6	64	1	-5	6	6	40	1	-7	8	6	12	1
-11	1	6	3	-6	3	2	6	101	1	-1	4	6	21	1	-4	6	6	51	1	-6	8	6	6	2
-10	1	6	16	1	4	2	6	24	1	0	4	6	17	1	-3	6	6	2	-5	-5	8	6	29	1
-9	1	6	20	1	5	2	6	8	2	1	4	6	8	1	-2	6	6	14	1	-4	8	6	3	-5
-8	1	6	4	-3	6	2	6	4	-4	2	4	6	15	1	-1	6	6	42	1	-3	8	6	3	-5
-7	1	6	20	1	7	2	6	17	1	3	4	6	65	1	0	6	6	15	1	-2	8	6	68	1
-6	1	6	44	1	-11	3	6	5	-3	4	4	6	3	-6	1	6	6	8	2	-1	8	6	13	1
-5	1	6	8	1	-10	3	6	5	-3	5	4	6	8	2	2	6	6	17	1	-1	8	6	5	-3
-4	1	6	8	1	-9	3	6	14	1	6	4	6	15	1	3	6	6	6	-3	1	8	6	15	1
-3	1	6	2	-4	-8	3	6	23	1	7	4	6	3	-6	4	6	6	3	-6	2	8	6	7	2
-2	1	6	28	1	-8	3	6	60	1	-11	5	6	3	-6	5	6	6	54	1	3	8	6	8	2
-1	1	6	6	2	-6	3	6	29	1	-10	5	6	11	2	6	6	6	12	1	4	8	6	22	1
0	1	6	169	1	-5	3	6	2	-5	-9	5	6	21	1	7	6	6	6	-6	5	8	6	28	1
1	1	6	30	1	-4	3	6	27	1	-8	5	6	3	-5	-10	7	6	7	2	6	8	6	4	-4

Table 21. (Continued)

F(obs) and sigma(F) (-sigma = unobserved): Trichlorobenzene Thiourea Adduct

h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s
-10	9	6	14	1	-8	11	6	6	-3	-1	13	6	5	-3	-2	0	7	26	1	-1	2	7	66	1
-9	9	6	7	2	-7	11	6	8	2	0	13	6	19	1	0	0	7	53	1	0	2	7	2	-5
-8	9	6	8	2	-6	11	6	5	-3	1	13	6	22	1	2	0	7	122	1	1	2	7	23	1
-7	9	6	3	-5	-5	11	6	23	1	2	13	6	7	2	4	0	7	10	1	2	2	7	48	1
-6	9	6	26	1	-4	11	6	10	2	3	13	6	5	-3	6	0	7	3	-5	3	2	7	6	-2
-5	9	6	17	1	-3	11	6	3	-5	4	13	6	11	2	-11	1	7	4	-4	4	2	7	4	-3
-4	9	6	26	1	-2	11	6	41	1	-7	14	6	3	-6	-10	1	7	7	2	5	2	7	5	-4
-3	9	6	10	1	-1	11	6	10	2	-6	14	6	12	2	-9	1	7	3	-5	6	2	7	7	2
-2	9	6	76	1	0	11	6	22	1	-5	14	6	3	-6	-8	1	7	5	-3	7	2	7	6	-3
-1	9	6	5	-3	1	11	6	42	1	-4	14	6	16	1	-7	1	7	11	1	-11	3	7	3	-6
0	9	6	3	-5	2	11	6	3	-6	-3	14	6	20	1	-6	1	7	11	1	-10	3	7	21	1
1	9	6	18	1	3	11	6	5	-3	-2	14	6	13	1	-5	1	7	57	1	-9	3	7	6	-2
2	9	6	32	1	4	11	6	10	2	-1	14	6	9	2	-4	1	7	14	1	-8	3	7	6	2
3	9	6	7	2	5	11	6	3	-6	0	14	6	3	-6	-3	1	7	21	1	-7	3	7	24	1
4	9	6	3	-6	-8	12	6	5	-4	1	14	6	7	2	-2	1	7	37	1	-6	3	7	3	-5
5	9	6	9	2	-7	12	6	9	2	2	14	6	3	-6	-1	1	7	64	1	-5	3	7	71	1
6	9	6	3	-6	-6	12	6	5	-3	-6	15	6	10	2	0	1	7	2	-5	-4	3	7	2	-5
-9	10	6	8	2	-5	12	6	25	1	-5	15	6	3	-6	1	1	7	4	-3	-3	3	7	21	1
-8	10	6	5	-3	-4	12	6	17	1	-4	15	6	3	-6	2	1	7	45	1	-2	3	7	39	1
-7	10	6	3	-6	-3	12	6	7	2	-3	15	6	5	-3	3	1	7	9	2	-1	3	7	52	1
-6	10	6	13	1	-2	12	6	14	1	-2	15	6	3	-6	4	1	7	8	2	0	3	7	12	1
-5	10	6	13	1	-1	12	6	7	2	-1	15	6	10	2	5	1	7	38	1	1	3	7	6	2
-4	10	6	7	2	0	12	6	6	-3	0	15	6	7	3	6	1	7	10	2	2	3	7	6	2
-3	10	6	12	1	1	12	6	14	1	1	15	6	8	2	7	1	7	6	-3	3	3	7	3	-6
-2	10	6	54	1	2	12	6	8	2	2	15	6	3	-6	-11	2	7	8	2	4	3	7	14	1
-1	10	6	15	1	3	12	6	3	-6	-4	16	6	5	-4	-10	2	7	5	-3	5	3	7	46	1
0	10	6	11	1	4	12	6	7	3	-3	16	6	10	2	-9	2	7	7	2	6	3	7	8	2
1	10	6	17	1	5	12	6	20	1	-2	16	6	4	-4	-8	2	7	21	1	7	3	7	10	2
2	10	6	16	1	-7	13	6	5	-4	-1	16	6	3	-6	-7	2	7	26	1	-11	4	7	3	-6
3	10	6	14	1	-6	13	6	12	2	0	16	6	10	2	-6	2	7	16	1	-10	4	7	13	2
4	10	6	14	1	-5	13	6	5	-3	-10	0	7	26	1	-5	2	7	51	1	-9	4	7	3	-6
5	10	6	9	2	-4	13	6	5	-4	-8	0	7	46	1	-4	2	7	15	1	-8	4	7	25	1
6	10	6	8	2	-3	13	6	11	2	-6	0	7	11	1	-3	2	7	39	1	-7	4	7	11	1
-9	11	6	16	1	-2	13	6	16	1	-4	0	7	23	1	-2	2	7	17	1	-6	4	7	24	1

Table 21. (Continued)

F(obs) and sigma(F) (-sigma = unobserved): Trichlorobenzene Thiourea Adduct

h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s
-5	4	7	46	1	-7	6	7	27	1	-7	8	7	25	1	-4	10	7	4	-4	3	12	7	9	2
-4	4	7	22	1	-6	6	7	12	1	-6	8	7	32	1	-3	10	7	11	1	4	12	7	8	2
-3	4	7	2	-5	-5	6	7	21	1	-5	8	7	11	1	-2	10	7	7	2	-7	13	7	3	-6
-2	4	7	53	1	-4	6	7	7	2	-4	8	7	3	-5	-1	10	7	10	2	-6	13	7	6	-3
-1	4	7	55	1	-3	6	7	13	1	-3	8	7	38	1	0	10	7	63	1	-5	13	7	7	2
0	4	7	42	1	-2	6	7	9	2	-2	8	7	23	1	1	10	7	13	1	-4	13	7	6	-3
1	4	7	31	1	-1	6	7	11	1	-1	8	7	21	1	2	10	7	5	-3	-3	13	7	19	1
2	4	7	37	1	0	6	7	17	1	0	8	7	62	1	3	10	7	5	-3	-2	13	7	15	1
3	4	7	12	1	1	6	7	19	1	1	8	7	12	1	4	10	7	6	-3	-1	13	7	13	1
4	4	7	3	-6	2	6	7	28	1	2	8	7	6	-2	5	10	7	7	3	0	13	7	3	-6
5	4	7	9	2	3	6	7	25	1	3	8	7	21	1	-8	11	7	6	3	1	13	7	5	-3
6	4	7	3	-6	4	6	7	8	2	4	8	7	26	1	-7	11	7	3	-6	2	13	7	7	2
7	4	7	3	-6	5	6	7	3	-6	5	8	7	3	-6	-6	11	7	14	1	3	13	7	12	2
-11	5	7	7	3	6	6	7	8	2	6	8	7	6	-3	-5	11	7	15	1	-6	14	7	5	-4
-10	5	7	13	1	-10	7	7	9	2	-9	9	7	4	-4	-4	11	7	7	2	-5	14	7	14	1
-9	5	7	11	2	-9	7	7	3	-6	-8	9	7	13	1	-3	11	7	34	1	-4	14	7	6	-3
-8	5	7	4	-4	-8	7	7	10	2	-7	9	7	3	-5	-2	11	7	3	-5	-3	14	7	10	2
-7	5	7	19	1	-7	7	7	12	1	-6	9	7	19	1	-1	11	7	10	2	-2	14	7	3	-6
-6	5	7	14	1	-6	7	7	3	-5	-5	9	7	3	-5	0	11	7	11	2	-1	14	7	3	-6
-5	5	7	4	-3	-5	7	7	26	1	-4	9	7	9	2	1	11	7	6	2	0	14	7	14	1
-4	5	7	20	1	-4	7	7	9	2	-3	9	7	3	-5	2	11	7	3	-6	1	14	7	6	-3
-3	5	7	79	1	-3	7	7	109	1	-2	9	7	3	-5	3	11	7	17	1	2	14	7	9	2
-2	5	7	43	1	-2	7	7	39	1	-1	9	7	3	-5	4	11	7	10	2	-5	15	7	11	2
-1	5	7	31	1	-1	7	7	18	1	0	9	7	19	1	-8	12	7	14	1	-4	15	7	8	2
0	5	7	14	1	0	7	7	13	1	1	9	7	10	2	-7	12	7	17	1	-3	15	7	3	-6
1	5	7	21	1	1	7	7	8	2	2	9	7	5	-3	-6	12	7	3	-6	-2	15	7	3	-6
2	5	7	13	1	2	7	7	5	-3	3	9	7	3	-6	-5	12	7	6	2	-1	15	7	15	1
3	5	7	24	1	3	7	7	25	1	4	9	7	25	1	-4	12	7	19	1	0	15	7	5	-4
4	5	7	30	1	4	7	7	11	2	5	9	7	3	-6	-3	12	7	3	-6	1	15	7	5	-4
5	5	7	12	1	5	7	7	8	2	-9	10	7	3	-6	-2	12	7	4	-4	-2	16	7	3	-6
6	5	7	3	-6	6	7	7	3	-6	-8	10	7	3	-6	-1	12	7	5	-3	-10	0	8	7	2
-10	6	7	7	3	-10	8	7	3	-6	-7	10	7	3	-6	0	12	7	3	-6	-8	0	8	4	-4
-9	6	7	6	3	-9	8	7	3	-6	-6	10	7	13	1	1	12	7	6	-3	-6	0	8	38	1
-8	6	7	27	1	-8	8	7	5	-3	-5	10	7	6	-3	2	12	7	16	1	-4	0	8	19	1

Table 21. (Continued)

F(obs) and sigma(F) (-sigma = unobserved): Trichlorobenzene Thiourea Adduct

h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s
-2	0	8	62	1	0	2	8	14	1	-1	4	8	22	1	-1	6	8	74	1	1	8	8	3	-6
0	0	8	22	1	1	2	8	12	1	0	4	8	9	1	0	6	8	25	1	2	8	8	18	1
2	0	8	11	1	2	2	8	13	1	1	4	8	18	1	1	6	8	5	-3	3	8	8	9	2
4	0	8	77	1	3	2	8	6	-3	2	4	8	10	2	2	6	8	5	-4	4	8	8	3	-6
6	0	8	3	-6	4	2	8	31	1	3	4	8	14	1	3	6	8	5	-3	5	8	8	5	-4
-11	1	8	4	-4	5	2	8	3	-6	4	4	8	15	1	4	6	8	13	1	-9	9	8	9	2
-10	1	8	6	-3	6	2	8	4	-4	5	4	8	3	-6	5	6	8	7	2	-8	9	8	16	1
-9	1	8	6	2	-11	3	8	11	2	6	4	8	18	1	-10	7	8	3	-6	-7	9	8	6	2
-8	1	8	27	1	-10	3	8	8	2	-10	5	8	9	2	-9	7	8	8	2	-6	9	8	6	2
-7	1	8	7	2	-9	3	8	18	1	-9	5	8	3	-6	-8	7	8	3	-6	-5	9	8	10	1
-6	1	8	49	1	-8	3	8	24	1	-8	5	8	26	1	-7	7	8	16	1	-4	9	8	21	1
-5	1	8	8	1	-7	3	8	10	1	-7	5	8	28	1	-6	7	8	19	1	-3	9	8	4	-4
-4	1	8	21	1	-6	3	8	10	1	-6	5	8	46	1	-5	7	8	28	1	-2	9	8	8	2
-3	1	8	2	-5	-5	3	8	2	-5	-5	5	8	21	1	-4	7	8	31	1	-1	9	8	14	1
-2	1	8	8	1	-4	3	8	46	1	-4	5	8	7	2	-3	7	8	12	1	0	9	8	7	2
-1	1	8	23	1	-3	3	8	3	-5	-3	5	8	25	1	-2	7	8	20	1	1	9	8	3	-6
0	1	8	34	1	-2	3	8	2	-5	-2	5	8	5	-3	-1	7	8	52	1	2	9	8	47	1
1	1	8	54	1	-1	3	8	13	1	-1	5	8	24	1	0	7	8	13	1	3	9	8	10	2
2	1	8	18	1	0	3	8	15	1	0	5	8	16	1	1	7	8	13	1	4	9	8	3	-6
3	1	8	3	-5	1	3	8	62	1	1	5	8	7	2	2	7	8	17	1	-9	10	8	3	-6
4	1	8	46	1	2	3	8	25	1	2	5	8	48	1	3	7	8	16	1	-8	10	8	3	-6
5	1	8	10	2	3	3	8	8	2	3	5	8	13	1	4	7	8	8	2	-7	10	8	6	-3
6	1	8	6	3	4	3	8	3	-6	4	5	8	9	2	5	7	8	6	-3	-6	10	8	16	1
-11	2	8	7	3	5	3	8	5	-3	5	5	8	3	-6	-10	8	8	3	-6	-5	10	8	11	1
-10	2	8	9	2	-11	4	8	3	-6	6	5	8	8	2	-9	8	8	3	-6	-4	10	8	29	1
-9	2	8	18	1	-10	4	8	7	3	-10	6	8	12	2	-8	8	8	13	1	-3	10	8	7	2
-8	2	8	8	2	-9	4	8	17	1	-9	6	8	6	-3	-7	8	8	3	-5	-2	10	8	6	-2
-7	2	8	7	2	-8	4	8	8	2	-8	6	8	3	-5	-6	8	8	17	1	-1	10	8	19	1
-6	2	8	7	2	-7	4	8	18	1	-7	6	8	13	1	-5	8	8	4	-4	0	10	8	5	-3
-5	2	8	15	1	-6	4	8	15	1	-6	6	8	3	-5	-4	8	8	28	1	1	10	8	3	-6
-4	2	8	12	1	-5	4	8	9	1	-5	6	8	14	1	-3	8	8	26	1	2	10	8	8	2
-3	2	8	93	1	-4	4	8	53	1	-4	6	8	25	1	-2	8	8	3	-5	3	10	8	3	-6
-2	2	8	26	1	-3	4	8	49	1	-3	6	8	6	2	-1	8	8	37	1	4	10	8	3	-6
-1	2	8	18	1	-2	4	8	4	-3	-2	6	8	3	-5	0	8	8	23	1	-8	11	8	3	-6

Table 21. (Continued)

F(obs) and sigma(F) (-sigma = unobserved): Trichlorobenzene Thiourea Adduct

h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s
-7	11	8	3	-6	-3	14	8	15	1	-11	2	9	3	-6	-9	4	9	13	1	-7	6	9	11	1
-6	11	8	7	2	-2	14	8	3	-6	-10	2	9	3	-6	-8	4	9	3	-5	-6	6	9	12	1
-5	11	8	3	-6	-1	14	8	8	2	-9	2	9	19	1	-7	4	9	20	1	-5	6	9	44	1
-4	11	8	3	-6	0	14	8	6	-3	-8	2	9	8	2	-6	4	9	31	1	-4	6	9	32	1
-3	11	8	8	2	1	14	8	5	-4	-7	2	9	41	1	-5	4	9	3	-5	-3	6	9	10	1
-2	11	8	11	1	-4	15	8	11	2	-6	2	9	5	-3	-4	4	9	9	2	-2	6	9	16	1
-1	11	8	24	1	-3	15	8	7	-3	-5	2	9	5	-3	-3	4	9	3	-5	-1	6	9	14	1
0	11	8	3	-6	-2	15	8	11	2	-4	2	9	32	1	-2	4	9	12	1	0	6	9	6	-3
1	11	8	10	2	-1	15	8	3	-6	-3	2	9	6	-2	-1	4	9	3	-5	1	6	9	54	1
2	11	8	19	1	-10	0	9	6	-3	-2	2	9	25	1	0	4	9	17	1	2	6	9	8	2
3	11	8	10	2	-8	0	9	10	2	-1	2	9	27	1	1	4	9	8	2	3	6	9	6	-3
-7	12	8	5	-3	-6	0	9	4	-3	0	2	9	5	-3	2	4	9	6	2	4	6	9	12	2
-6	12	8	3	-6	-4	0	9	81	1	1	2	9	16	1	3	4	9	34	1	5	6	9	12	2
-5	12	8	12	1	-2	0	9	30	1	2	2	9	11	1	4	4	9	13	1	-10	7	9	3	-6
-4	12	8	3	-6	0	0	9	51	1	3	2	9	61	1	5	4	9	9	2	-9	7	9	17	1
-3	12	8	7	3	2	0	9	12	1	4	2	9	6	3	-10	5	9	7	2	-8	7	9	11	2
-2	12	8	15	1	4	0	9	4	-4	5	2	9	3	-6	-9	5	9	18	1	-7	7	9	3	-5
-1	12	8	26	1	-11	1	9	8	2	-10	3	9	3	-6	-8	5	9	3	-6	-6	7	9	7	2
0	12	8	8	2	-10	1	9	5	-3	-9	3	9	10	2	-7	5	9	10	2	-5	7	9	11	1
1	12	8	3	-6	-9	1	9	10	2	-8	3	9	16	1	-6	5	9	15	1	-4	7	9	13	1
2	12	8	3	-6	-8	1	9	19	1	-7	3	9	7	2	-5	5	9	12	1	-3	7	9	3	-5
3	12	8	10	2	-7	1	9	5	-3	-6	3	9	5	-3	-4	5	9	42	1	-2	7	9	21	1
-7	13	8	3	-6	-6	1	9	13	1	-5	3	9	20	1	-3	5	9	13	1	-1	7	9	12	1
-6	13	8	21	1	-5	1	9	7	2	-4	3	9	19	1	-2	5	9	56	1	0	7	9	8	2
-5	13	8	16	1	-4	1	9	60	1	-3	3	9	13	1	-1	5	9	21	1	1	7	9	23	1
-4	13	8	3	-6	-3	1	9	2	-5	-2	3	9	62	1	0	5	9	24	1	2	7	9	3	-6
-3	13	8	3	-6	-2	1	9	24	1	-1	3	9	50	1	1	5	9	28	1	3	7	9	3	-6
-2	13	8	11	2	-1	1	9	26	1	0	3	9	3	-5	2	5	9	3	-6	4	7	9	8	2
-1	13	8	3	-6	0	1	9	33	1	1	3	9	10	2	3	5	9	3	-6	-9	8	9	12	1
0	13	8	3	-6	1	1	9	9	2	2	3	9	9	9	4	5	9	7	3	-8	8	9	3	-6
1	13	8	3	-6	2	1	9	3	-5	3	3	9	12	2	5	5	9	11	2	-7	8	9	9	2
2	13	8	3	-6	3	1	9	12	2	4	3	9	6	-3	-10	6	9	3	-6	-6	8	9	23	1
-5	14	8	3	-6	4	1	9	3	-6	5	3	9	3	-6	-9	6	9	11	2	-5	8	9	3	-5
-4	14	8	3	-6	5	1	9	3	-6	-10	4	9	3	-6	-8	6	9	5	-3	-4	8	9	20	1

Table 21. (Continued)

F(obs) and sigma(F) (-sigma = unobserved): Trichlorobenzene Thiourea Adduct

h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s
-3	8	9	6	-3	-6	11	9	5	-4	0	0	10	3	-5	-9	3	10	5	-3	-5	5	10	32	1
-2	8	9	4	-4	-5	11	9	3	-6	2	0	10	11	2	-8	3	10	9	2	-4	5	10	3	-5
-1	8	9	3	-5	-4	11	9	5	-3	4	0	10	5	-4	-7	3	10	23	1	-3	5	10	45	1
0	8	9	3	-6	-3	11	9	7	2	-10	1	10	11	2	-6	3	10	11	1	-2	5	10	6	-3
1	8	9	34	1	-2	11	9	18	1	-9	1	10	3	-6	-5	3	10	63	1	-1	5	10	3	-5
2	8	9	18	1	-1	11	9	3	-6	-8	1	10	7	2	-4	3	10	3	-5	0	5	10	35	1
3	8	9	3	-6	0	11	9	10	2	-7	1	10	16	1	-3	3	10	14	1	1	5	10	5	-3
-9	9	9	5	-4	1	11	9	13	1	-6	1	10	8	2	-2	3	10	18	1	2	5	10	20	1
-8	9	9	8	2	2	11	9	3	-6	-5	1	10	42	1	-1	3	10	3	-5	3	5	10	16	1
-7	9	9	3	-6	-7	12	9	9	2	-4	1	10	19	1	0	3	10	7	2	4	5	10	3	-6
-6	9	9	3	-6	-6	12	9	8	2	-3	1	10	3	-5	1	3	10	17	1	-9	6	10	6	-3
-5	9	9	9	2	-5	12	9	3	-6	-2	1	10	20	1	2	3	10	15	1	-8	6	10	8	2
-4	9	9	3	-6	-4	12	9	18	1	-1	1	10	10	1	3	3	10	7	-3	-7	6	10	19	1
-3	9	9	3	-5	-3	12	9	5	-3	0	1	10	4	-4	4	3	10	7	3	-6	6	10	14	1
-2	9	9	54	1	-2	12	9	3	-6	1	1	10	22	1	-10	4	10	18	1	-5	6	10	16	1
-1	9	9	6	-3	-1	12	9	8	2	2	1	10	38	1	-9	4	10	12	1	-4	6	10	13	1
0	9	9	3	-6	0	12	9	5	-4	3	1	10	3	-6	-8	4	10	3	-6	-3	6	10	33	1
1	9	9	8	2	1	12	9	20	1	4	1	10	3	-6	-7	4	10	14	1	-2	6	10	30	1
2	9	9	3	-6	2	12	9	3	-6	-10	2	10	9	2	-6	4	10	3	-5	-1	6	10	3	-5
3	9	9	5	-4	-5	13	9	3	-6	-9	2	10	7	2	-5	4	10	12	1	0	6	10	10	2
-8	10	9	7	3	-4	13	9	15	1	-8	2	10	16	1	-4	4	10	8	2	1	6	10	8	2
-7	10	9	11	2	-3	13	9	7	3	-7	2	10	4	-3	-3	4	10	3	-5	2	6	10	10	2
-6	10	9	22	1	-2	13	9	7	2	-6	2	10	19	1	-2	4	10	33	1	3	6	10	3	-6
-5	10	9	12	1	-1	13	9	3	-5	-5	2	10	15	1	-1	4	10	17	1	4	6	10	3	-6
-4	10	9	3	-6	0	13	9	9	2	-4	2	10	10	1	0	4	10	38	1	-9	7	10	7	-3
-3	10	9	8	2	-4	14	9	10	2	-3	2	10	19	1	1	4	10	23	1	-8	7	10	6	-3
-2	10	9	7	2	-3	14	9	17	1	-2	2	10	23	1	2	4	10	12	1	-7	7	10	26	1
-1	10	9	7	2	-2	14	9	3	-6	-1	2	10	24	1	3	4	10	3	-6	-6	7	10	9	2
0	10	9	8	2	-1	14	9	3	-6	0	2	10	23	1	4	4	10	3	-6	-5	7	10	3	-5
1	10	9	10	2	-10	0	10	13	1	1	2	10	11	1	-10	5	10	3	-6	-4	7	10	8	2
2	10	9	3	-6	-8	0	10	22	1	2	2	10	11	2	-9	5	10	6	-3	-3	7	10	27	1
3	10	9	8	2	-6	0	10	9	2	3	2	10	3	-6	-8	5	10	10	2	-2	7	10	14	1
-8	11	9	3	-6	-4	0	10	11	1	4	2	10	3	-6	-7	5	10	13	1	-1	7	10	3	-6
-7	11	9	3	-6	-2	0	10	66	1	-10	3	10	3	-6	-6	5	10	8	2	0	7	10	3	-6

Table 21. (Continued)

F(obs) and sigma(F) (-sigma = unobserved): Trichlorobenzene Thiourea Adduct¹

h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s
1	7	10	7	2	-1	10	10	8	2	-6	1	11	28	1	0	3	11	15	1	-5	6	11	28	1
2	7	10	12	1	0	10	10	32	1	-5	1	11	3	-5	1	3	11	20	1	-4	6	11	8	2
3	7	10	28	1	1	10	10	3	-6	-4	1	11	7	2	2	3	11	15	1	-3	6	11	8	2
-9	8	10	8	2	2	10	10	9	2	-3	1	11	24	1	3	3	11	8	2	-2	6	11	6	3
-8	8	10	3	-6	-7	11	10	7	2	-2	1	11	7	2	-9	4	11	5	-4	-1	6	11	11	2
-7	8	10	3	-6	-6	11	10	3	-6	-1	1	11	19	1	-8	4	11	14	1	0	6	11	3	-6
-6	8	10	3	-6	-5	11	10	18	1	0	1	11	46	1	-7	4	11	3	-6	1	6	11	3	-6
-5	8	10	8	2	-4	11	10	17	1	1	1	11	10	2	-6	4	11	14	1	2	6	11	7	3
-4	8	10	10	2	-3	11	10	12	2	2	1	11	9	2	-5	4	11	3	-5	-9	7	11	3	-6
-3	8	10	26	1	-2	11	10	4	-4	3	1	11	3	-6	-4	4	11	22	1	-8	7	11	7	3
-2	8	10	8	2	-1	11	10	3	-6	-10	2	11	3	-6	-3	4	11	44	1	-7	7	11	3	-6
-1	8	10	8	2	0	11	10	3	-6	-9	2	11	3	-6	-2	4	11	6	-3	-6	7	11	4	-4
0	8	10	33	1	1	11	10	3	-6	-8	2	11	10	2	-1	4	11	24	1	-5	7	11	3	-6
1	8	10	3	-6	-6	12	10	3	-6	-7	2	11	3	-5	0	4	11	10	2	-4	7	11	16	1
2	8	10	7	3	-5	12	10	13	1	-6	2	11	14	1	1	4	11	3	-6	-3	7	11	13	1
3	8	10	5	-4	-4	12	10	3	-6	-5	2	11	13	1	2	4	11	23	1	-2	7	11	3	-6
-8	9	10	3	-6	-3	12	10	12	2	-4	2	11	11	1	3	4	11	3	-6	-1	7	11	31	1
-7	9	10	3	-6	-2	12	10	8	2	-3	2	11	39	1	-9	5	11	6	-3	0	7	11	12	1
-6	9	10	3	-6	-1	12	10	11	2	-2	2	11	10	1	-8	5	11	12	2	1	7	11	8	2
-5	9	10	3	-6	0	12	10	6	-3	-1	2	11	4	-4	-7	5	11	12	1	-8	8	11	8	2
-4	9	10	15	1	-4	13	10	3	-6	0	2	11	6	-3	-6	5	11	3	-6	-7	8	11	11	2
-3	9	10	7	2	-3	13	10	9	2	1	2	11	17	1	-5	5	11	8	2	-6	8	11	15	1
-2	9	10	5	-4	-2	13	10	3	-6	2	2	11	7	2	-4	5	11	18	1	-5	8	11	17	1
-1	9	10	7	3	-10	0	11	3	-6	3	2	11	3	-6	-3	5	11	3	-5	-4	8	11	18	1
0	9	10	12	2	-8	0	11	19	1	-10	3	11	3	-6	-2	5	11	3	-5	-3	8	11	6	-3
1	9	10	3	-6	-6	0	11	41	1	-9	3	11	9	2	-1	5	11	24	1	-2	8	11	3	-6
2	9	10	9	2	-4	0	11	5	-3	-8	3	11	13	1	0	5	11	15	1	-1	8	11	3	-6
-8	10	10	3	-6	-2	0	11	3	-5	-7	3	11	3	-5	1	5	11	3	-6	0	8	11	3	-6
-7	10	10	3	-6	0	0	11	13	1	-6	3	11	16	1	2	5	11	8	2	1	8	11	3	-6
-6	10	10	6	-3	2	0	11	3	-6	-5	3	11	5	-3	3	5	11	6	-3	2	8	11	16	1
-5	10	10	3	-6	-10	1	11	12	2	-4	3	11	4	-3	-9	6	11	3	-6	-7	9	11	8	2
-4	10	10	7	-3	-9	1	11	7	2	-3	3	11	32	1	-8	6	11	12	2	-6	9	11	9	2
-3	10	10	4	-4	-8	1	11	5	-3	-2	3	11	5	-3	-7	6	11	3	-6	-5	9	11	9	2
-2	10	10	5	-4	-7	1	11	5	-3	-1	3	11	14	1	-6	6	11	10	2	-4	9	11	3	-6

Table 21. (Continued)

F(obs) and sigma(F) (-sigma = unobserved): Trichlorobenzene Thiourea Adduct

h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s
-3	9	11	8	2	-1	1	12	3	-6	-3	4	12	4	-3	0	7	12	7	-3	1	1	13	12	2
-2	9	11	11	2	0	1	12	3	-6	-2	4	12	17	1	1	7	12	3	-6	-8	2	13	6	-3
-1	9	11	5	-4	1	1	12	7	2	-1	4	12	22	1	-7	8	12	8	2	-7	2	13	15	1
0	9	11	3	-6	2	1	12	12	2	0	4	12	7	2	-6	8	12	12	2	-6	2	13	3	-6
1	9	11	3	-6	-9	2	12	18	1	1	4	12	8	2	-5	8	12	8	2	-5	2	13	19	1
-7	10	11	3	-6	-8	2	12	14	1	2	4	12	3	-6	-4	8	12	9	2	-4	2	13	3	-6
-6	10	11	8	2	-7	2	12	13	1	-8	5	12	5	-4	-3	8	12	5	-4	-3	2	13	11	1
-5	10	11	5	-4	-6	2	12	22	1	-7	5	12	8	2	-2	8	12	9	2	-2	2	13	22	1
-4	10	11	11	2	-5	2	12	6	-3	-6	5	12	18	1	-1	8	12	3	-6	-1	2	13	3	-6
-3	10	11	6	-3	-4	2	12	14	1	-5	5	12	3	-6	0	8	12	3	-6	0	2	13	10	2
-2	10	11	13	1	-3	2	12	10	2	-4	5	12	22	1	-6	9	12	20	1	-8	3	13	6	-3
-1	10	11	3	-6	-2	2	12	3	-6	-3	5	12	13	1	-5	9	12	3	-6	-7	3	13	9	2
0	10	11	3	-6	-1	2	12	32	1	-2	5	12	3	-6	-4	9	12	6	-3	-6	3	13	7	2
-6	11	11	9	2	0	2	12	3	-6	-1	5	12	18	1	-3	9	12	13	2	-5	3	13	19	1
-5	11	11	3	-6	1	2	12	10	2	0	5	12	3	-6	-2	9	12	23	1	-4	3	13	8	2
-4	11	11	3	-6	2	2	12	12	2	1	5	12	6	-3	-1	9	12	8	2	-3	3	13	7	2
-3	11	11	9	2	-9	3	12	9	2	-8	6	12	12	2	-5	10	12	5	-4	-2	3	13	8	2
-2	11	11	11	2	-8	3	12	10	2	-7	6	12	6	-3	-4	10	12	8	2	-1	3	13	9	2
-1	11	11	20	1	-7	3	12	3	-6	-6	6	12	3	-6	-3	10	12	10	2	0	3	13	14	1
-3	12	11	3	-6	-6	3	12	8	2	-5	6	12	6	-3	-2	10	12	12	2	-8	4	13	3	-6
-8	0	12	10	2	-5	3	12	4	-4	-4	6	12	5	-3	-8	0	13	3	-6	-7	4	13	11	2
-6	0	12	13	1	-4	3	12	9	2	-3	6	12	3	-6	-6	0	13	4	-4	-6	4	13	7	3
-4	0	12	3	-6	-3	3	12	3	-5	-2	6	12	5	-4	-4	0	13	14	1	-5	4	13	12	1
-2	0	12	10	2	-2	3	12	16	1	-1	6	12	8	2	-2	0	13	32	1	-4	4	13	14	1
0	0	12	14	1	-1	3	12	25	1	0	6	12	7	3	0	0	13	5	-3	-3	4	13	12	1
2	0	12	14	1	0	3	12	8	2	1	6	12	30	1	-8	1	13	3	-6	-2	4	13	7	2
-9	1	12	3	-6	1	3	12	9	2	-8	7	12	6	-3	-7	1	13	8	2	-1	4	13	10	2
-8	1	12	6	-3	2	3	12	3	-6	-7	7	12	8	2	-6	1	13	5	-3	0	4	13	3	-6
-7	1	12	10	2	-9	4	12	3	-6	-6	7	12	8	2	-5	1	13	5	-4	-7	5	13	19	1
-6	1	12	14	1	-8	4	12	5	-3	-5	7	12	3	-6	-4	1	13	11	2	-6	5	13	10	2
-5	1	12	6	-3	-7	4	12	7	2	-4	7	12	3	-6	-3	1	13	7	2	-5	5	13	12	2
-4	1	12	48	1	-6	4	12	16	1	-3	7	12	13	1	-2	1	13	15	1	-4	5	13	3	-6
-3	1	12	9	2	-5	4	12	8	2	-2	7	12	14	1	-1	1	13	3	-6	-3	5	13	9	2
-2	1	12	3	-6	-4	4	12	11	2	-1	7	12	6	-3	0	1	13	3	-6	-2	5	13	10	2

Table 21. (Continued)

F(obs) and sigma(F) (-sigma = unobserved): Trichlorobenzene Thiourea Adduct

h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s	h	k	l	Fo	s
-1	5	13	3	-6	-6	7	13	10	2	-4	0	14	3	-6	-6	2	14	8	2	-3	3	14	23	1
0	5	13	14	1	-5	7	13	6	-3	-2	0	14	8	2	-5	2	14	8	2	-2	3	14	13	1
-7	6	13	3	-6	-4	7	13	7	2	-7	1	14	3	-6	-4	2	14	11	2	-6	4	14	3	-6
-6	6	13	3	-6	-3	7	13	8	2	-6	1	14	3	-6	-3	2	14	3	-6	-5	4	14	9	2
-5	6	13	7	2	-2	7	13	3	-6	-5	1	14	12	2	-2	2	14	8	2	-4	4	14	4	-4
-4	6	13	10	2	-5	8	13	3	-6	-4	1	14	3	-6	-6	3	14	3	-6	-3	4	14	7	3
-3	6	13	17	1	-4	8	13	9	2	-3	1	14	14	1	-5	3	14	12	1	-5	5	14	9	2
-2	6	13	17	1	-3	8	13	10	2	-2	1	14	7	3	-4	3	14	7	-3	-4	5	14	3	-6
-1	6	13	8	2	-6	0	14	14	1	-7	2	14	11	2										

Table 22. Observed and calculated structure factors for the 1,2,4 TCB-thiourea adduct structure.

Observed and calculated structure factors: Trichlorobenzene Thiourea Adduct

h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc
2	0	0	45	54	1	4	0	84	85	6	7	0	5	6	5	12	0	3	3	-8	1	1	37	37
4	0	0	21	23	2	4	0	52	54	7	7	0	9	9	6	12	0	8	10	-6	1	1	25	24
6	0	0	18	17	3	4	0	14	15	8	7	0	8	8	7	12	0	5	3	-5	1	1	23	25
8	0	0	7	8	4	4	0	3	4	0	8	0	53	42	10	12	0	4	2	-4	1	1	14	13
10	0	0	12	11	5	4	0	3	3	2	8	0	56	56	2	13	0	3	2	-3	1	1	29	26
1	1	0	8	8	7	4	0	20	21	3	8	0	8	8	3	13	0	6	2	-2	1	1	7	6
2	1	0	33	33	8	4	0	17	17	4	8	0	17	17	4	13	0	3	4	-1	1	1	11	16
3	1	0	59	56	10	4	0	8	8	5	8	0	3	3	5	13	0	12	12	0	1	1	2	4
4	1	0	19	20	1	5	0	19	17	6	8	0	3	1	0	14	0	16	17	1	1	1	11	9
5	1	0	19	20	2	5	0	47	46	7	8	0	8	8	1	14	0	10	10	2	1	1	117	119
6	1	0	13	14	3	5	0	13	13	8	8	0	12	12	2	14	0	7	8	3	1	1	4	4
7	1	0	15	15	4	5	0	35	37	9	8	0	5	5	5	14	0	5	5	4	1	1	16	16
8	1	0	6	4	5	5	0	35	36	10	8	0	4	5	1	15	0	5	4	5	1	1	20	20
10	1	0	5	4	6	5	0	4	6	1	9	0	9	8	2	15	0	6	6	6	1	1	9	9
0	2	0	15	17	7	5	0	3	3	2	9	0	44	41	3	15	0	12	13	7	1	1	4	4
1	2	0	2	2	8	5	0	7	9	3	9	0	4	4	4	15	0	4	2	8	1	1	5	4
2	2	0	7	4	9	5	0	4	5	5	9	0	9	10	5	15	0	3	1	9	1	1	11	11
3	2	0	47	48	10	5	0	6	5	6	9	0	4	1	6	15	0	4	2	10	1	1	4	1
4	2	0	5	5	11	5	0	4	5	9	9	0	4	4	0	16	0	3	6	11	1	1	4	4
5	2	0	3	2	0	6	0	23	20	0	10	0	17	17	1	16	0	3	0	-11	2	1	7	8
7	2	0	32	31	1	6	0	14	14	1	10	0	11	13	2	16	0	3	0	-8	2	1	5	7
9	2	0	4	5	2	6	0	24	21	2	10	0	35	35	3	16	0	5	5	-7	2	1	3	7
10	2	0	3	5	3	6	0	6	6	5	10	0	6	5	3	17	0	5	4	-5	2	1	37	38
1	3	0	6	8	4	6	0	22	26	7	10	0	3	2	0	18	0	10	9	-4	2	1	38	38
2	3	0	35	30	5	6	0	23	22	8	10	0	8	7	-8	0	1	5	5	-3	2	1	37	38
3	3	0	77	76	7	6	0	5	4	1	11	0	13	13	-6	0	1	9	10	-2	2	1	37	35
4	3	0	4	3	8	6	0	5	5	2	11	0	16	17	-4	0	1	82	85	-1	2	1	40	49
5	3	0	9	10	9	6	0	9	9	3	11	0	9	8	-2	0	1	14	15	0	2	1	2	3
6	3	0	3	4	10	6	0	8	6	4	11	0	7	5	2	0	1	69	74	1	2	1	10	9
7	3	0	19	20	1	7	0	4	6	5	11	0	23	24	4	0	1	43	41	2	2	1	37	35
9	3	0	5	4	2	7	0	10	8	0	12	0	21	19	6	0	1	30	32	3	2	1	49	48
11	3	0	4	2	3	7	0	10	11	1	12	0	13	12	12	0	1	5	5	4	2	1	13	12
12	3	0	5	3	4	7	0	8	7	2	12	0	3	1	-10	1	1	4	6	5	2	1	42	42
0	4	0	30	29	5	7	0	51	50	3	12	0	4	3	-9	1	1	5	4	6	2	1	7	6

Table 22. (Continued)

Observed and calculated structure factors: Trichlorobenzene Thiourea Adduct

h	k	l	F _o	F _c	h	k	l	F _o	F _c	h	k	l	F _o	F _c	h	k	l	F _o	F _c	h	k	l	F _o	F _c
7	2	1	15	15	5	4	1	31	32	4	6	1	6	9	7	8	1	18	18	7	11	1	8	9
12	2	1	4	3	6	4	1	24	24	6	6	1	14	14	11	8	1	4	2	8	11	1	5	4
-10	3	1	5	4	7	4	1	5	4	7	6	1	18	18	-6	9	1	25	25	-8	12	1	4	2
-9	3	1	9	7	-9	4	1	5	5	9	6	1	5	4	-5	9	1	14	15	-5	12	1	5	5
-7	3	1	10	9	-10	5	1	8	7	10	6	1	5	2	-2	9	1	9	9	-4	12	1	5	6
-6	3	1	38	36	-8	5	1	17	17	-9	7	1	6	6	-1	9	1	8	7	-3	12	1	27	28
-5	3	1	9	11	-7	5	1	5	4	-8	7	1	9	9	0	9	1	46	46	-2	12	1	4	2
-4	3	1	14	14	-6	5	1	30	30	-6	7	1	17	17	1	9	1	3	1	-1	12	1	4	7
-3	3	1	35	31	-5	5	1	6	4	-4	7	1	4	1	2	9	1	6	7	0	12	1	6	6
-2	3	1	70	67	-4	5	1	10	9	-3	7	1	30	30	3	9	1	11	12	2	12	1	3	3
-1	3	1	170	171	-2	5	1	10	8	-2	7	1	20	18	4	9	1	23	24	5	12	1	5	4
0	3	1	15	16	-1	5	1	25	28	-1	7	1	17	16	5	9	1	6	7	6	12	1	4	4
1	3	1	16	13	0	5	1	75	71	0	7	1	29	30	6	9	1	4	0	7	12	1	6	5
2	3	1	13	15	1	5	1	57	51	1	7	1	56	59	9	9	1	4	1	-7	13	1	6	5
3	3	1	21	21	2	5	1	52	51	2	7	1	6	7	10	9	1	5	4	-4	13	1	6	5
4	3	1	13	15	3	5	1	7	4	3	7	1	4	4	11	9	1	5	0	-2	13	1	8	8
5	3	1	6	3	5	5	1	6	3	5	7	1	6	8	-7	10	1	5	3	0	13	1	4	4
8	3	1	3	4	7	5	1	19	18	6	7	1	14	15	-6	10	1	19	19	1	13	1	18	17
9	3	1	18	16	8	5	1	3	4	7	7	1	16	15	-3	10	1	13	14	2	13	1	14	13
11	3	1	5	4	10	5	1	4	2	9	7	1	7	8	-2	10	1	6	7	4	13	1	9	8
-10	4	1	7	7	12	5	1	5	2	10	7	1	4	2	-1	10	1	16	15	5	13	1	8	6
-9	4	1	4	4	-10	6	1	4	1	-8	8	1	7	6	1	10	1	10	11	6	13	1	5	4
-8	4	1	4	6	-9	6	1	6	5	-6	8	1	14	16	3	10	1	13	13	7	13	1	7	7
-6	4	1	20	21	-8	6	1	4	5	-5	8	1	5	9	4	10	1	35	35	-7	14	1	5	4
-5	4	1	12	11	-6	6	1	16	16	-3	8	1	46	48	5	10	1	5	5	-6	14	1	3	0
-4	4	1	23	21	-5	6	1	18	18	-2	8	1	28	23	-6	11	1	9	9	-5	14	1	4	4
-3	4	1	25	27	-4	6	1	12	10	-1	8	1	3	4	-4	11	1	10	9	-4	14	1	6	6
-2	4	1	32	26	-3	6	1	80	79	0	8	1	19	21	-2	11	1	7	11	-3	14	1	9	9
-1	4	1	174	158	-2	6	1	11	14	1	8	1	19	18	-1	11	1	16	18	-1	14	1	12	12
0	4	1	40	39	-1	6	1	15	9	2	8	1	4	5	0	11	1	9	12	1	14	1	5	4
1	4	1	12	11	0	6	1	37	36	3	8	1	13	13	1	11	1	23	23	2	14	1	5	3
2	4	1	28	28	1	6	1	8	6	4	8	1	39	40	2	11	1	6	5	4	14	1	8	8
3	4	1	15	12	2	6	1	15	14	5	8	1	7	6	4	11	1	7	6	5	14	1	3	4
4	4	1	29	31	3	6	1	34	35	6	8	1	3	2	6	11	1	4	0	6	14	1	4	4

Table 22. (Continued)

Observed and calculated structure factors: Trichlorobenzene Thiourea Adduct

h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc
-6	15	1	5	6	-4	1	2	12	10	-7	3	2	12	14	-9	5	2	10	10	-1	7	2	77	78
-5	15	1	6	5	-3	1	2	57	53	-6	3	2	22	23	-7	5	2	14	15	0	7	2	28	29
-4	15	1	5	3	-2	1	2	123	111	-5	3	2	12	12	-6	5	2	14	16	1	7	2	4	3
-2	15	1	5	4	-1	1	2	4	4	-4	3	2	35	35	-4	5	2	60	60	2	7	2	7	8
-1	15	1	11	9	0	1	2	15	12	-3	3	2	59	61	-3	5	2	25	21	3	7	2	28	27
0	15	1	7	8	1	1	2	13	15	-2	3	2	174	159	-2	5	2	19	8	4	7	2	9	9
2	15	1	7	7	2	1	2	10	11	-1	3	2	2	4	-1	5	2	62	65	5	7	2	7	6
3	15	1	5	5	3	1	2	9	9	0	3	2	23	26	0	5	2	7	9	6	7	2	11	13
5	15	1	4	5	4	1	2	73	71	1	3	2	23	26	1	5	2	16	15	9	7	2	6	5
-5	16	1	4	6	5	1	2	15	14	2	3	2	40	37	3	5	2	9	11	-9	8	2	4	4
-1	16	1	9	8	7	1	2	6	5	3	3	2	14	13	4	5	2	19	18	-8	8	2	11	11
2	16	1	7	7	8	1	2	13	13	4	3	2	13	13	5	5	2	3	0	-7	8	2	16	16
-4	17	1	6	5	9	1	2	3	1	5	3	2	16	17	6	5	2	26	27	-5	8	2	3	4
-3	17	1	4	1	11	1	2	4	2	6	3	2	22	22	8	5	2	9	10	-4	8	2	19	20
-2	17	1	4	3	-9	2	2	19	18	7	3	2	7	6	-9	6	2	5	5	-3	8	2	6	4
-1	17	1	6	7	-8	2	2	9	10	9	3	2	3	4	-7	6	2	30	31	-2	8	2	12	8
2	17	1	5	4	-7	2	2	11	13	-11	4	2	4	4	-6	6	2	27	27	-1	8	2	28	27
1	18	1	4	1	-6	2	2	21	21	-9	4	2	7	8	-3	6	2	6	7	0	8	2	27	25
-8	0	2	7	6	-5	2	2	17	14	-8	4	2	7	7	-1	6	2	75	72	1	8	2	15	14
-6	0	2	37	37	-4	2	2	34	35	-7	4	2	7	8	0	6	2	14	13	2	8	2	3	2
-4	0	2	3	2	-3	2	2	41	42	-6	4	2	25	25	1	6	2	14	14	3	8	2	27	27
-2	0	2	120	133	-2	2	2	58	55	-5	4	2	22	23	2	6	2	4	7	4	8	2	4	2
0	0	2	10	10	-1	2	2	19	19	-4	4	2	26	25	3	6	2	20	19	6	8	2	9	9
2	0	2	15	16	0	2	2	47	52	-3	4	2	42	42	4	6	2	16	15	7	8	2	4	2
4	0	2	48	46	1	2	2	138	140	-2	4	2	42	28	5	6	2	17	18	-7	9	2	8	8
6	0	2	8	9	2	2	2	77	74	-1	4	2	3	5	6	6	2	7	8	-6	9	2	4	1
8	0	2	22	24	3	2	2	46	45	0	4	2	5	4	8	6	2	8	9	-5	9	2	4	1
10	0	2	4	4	4	2	2	32	31	1	4	2	79	79	9	6	2	8	7	-4	9	2	41	41
-11	1	2	4	6	8	2	2	13	14	2	4	2	38	38	-10	7	2	6	5	-2	9	2	3	5
-9	1	2	9	8	9	2	2	7	8	3	4	2	5	7	-6	7	2	3	3	-1	9	2	24	24
-8	1	2	4	6	11	2	2	7	7	4	4	2	20	23	-5	7	2	4	3	0	9	2	23	23
-7	1	2	5	6	12	2	2	5	0	6	4	2	5	5	-4	7	2	4	3	1	9	2	10	10
-6	1	2	20	20	-11	3	2	5	6	8	4	2	5	5	-3	7	2	4	7	2	9	2	4	3
-5	1	2	15	14	-9	3	2	17	17	11	4	2	5	5	-2	7	2	46	37	4	9	2	6	7

Table 22. (Continued)

Observed and calculated structure factors: Trichlorobenzene Thiourea Adduct

h	k	l	F _o	F _c	h	k	l	F _o	F _c	h	k	l	F _o	F _c	h	k	l	F _o	F _c	h	k	l	F _o	F _c
6	9	2	30	30	-6	13	2	4	5	-4	0	3	87	90	0	2	3	48	47	-3	4	3	43	32
8	9	2	8	7	-4	13	2	9	10	-2	0	3	77	78	1	2	3	2	5	-2	4	3	120	112
-9	10	2	5	7	-3	13	2	5	4	0	0	3	108	117	2	2	3	13	12	0	4	3	49	46
-8	10	2	6	6	-2	13	2	17	18	2	0	3	9	10	3	2	3	25	26	1	4	3	9	8
-7	10	2	5	4	-1	13	2	18	17	4	0	3	22	25	4	2	3	11	10	2	4	3	7	7
-6	10	2	4	2	0	13	2	11	12	6	0	3	19	20	5	2	3	13	14	4	4	3	8	8
-5	10	2	6	5	2	13	2	6	5	8	0	3	11	12	6	2	3	5	3	5	4	3	10	11
-4	10	2	20	21	3	13	2	10	10	-9	1	3	4	7	7	2	3	24	25	6	4	3	13	14
-3	10	2	4	1	4	13	2	9	8	-8	1	3	7	7	11	2	3	5	1	7	4	3	15	15
-2	10	2	24	23	5	13	2	4	1	-7	1	3	29	28	-10	3	3	4	3	8	4	3	11	11
-1	10	2	22	20	-6	14	2	8	7	-6	1	3	6	5	-9	3	3	7	6	-11	5	3	4	4
0	10	2	20	22	-5	14	2	9	9	-5	1	3	35	38	-8	3	3	6	4	-8	5	3	15	15
1	10	2	8	6	-3	14	2	7	7	-4	1	3	67	66	-7	3	3	44	44	-7	5	3	10	12
2	10	2	29	29	-1	14	2	4	5	-3	1	3	73	63	-6	3	3	5	4	-6	5	3	5	3
3	10	2	18	17	1	14	2	12	11	-2	1	3	14	15	-5	3	3	5	3	-5	5	3	35	37
4	10	2	9	9	2	14	2	6	5	-1	1	3	32	28	-4	3	3	42	44	-4	5	3	24	23
-9	11	2	4	2	3	14	2	4	2	0	1	3	93	95	-3	3	3	15	21	-3	5	3	27	12
-8	11	2	5	6	4	14	2	9	9	1	1	3	12	11	-2	3	3	41	39	-2	5	3	28	27
-4	11	2	15	14	-4	15	2	6	6	2	1	3	4	3	0	3	3	5	7	-1	5	3	12	13
-3	11	2	3	1	-3	15	2	6	6	3	1	3	30	30	1	3	3	9	10	0	5	3	63	61
-1	11	2	12	12	-1	15	2	4	1	4	1	3	13	13	2	3	3	45	44	1	5	3	3	5
1	11	2	11	11	3	15	2	5	6	5	1	3	11	12	3	3	3	94	91	2	5	3	12	13
2	11	2	3	4	4	15	2	4	2	6	1	3	6	6	4	3	3	11	11	3	5	3	9	8
3	11	2	13	13	5	15	2	4	3	8	1	3	4	6	5	3	3	6	6	5	5	3	7	8
4	11	2	6	7	-5	16	2	4	4	-11	2	3	5	2	7	3	3	9	10	7	5	3	11	12
6	11	2	14	13	-4	16	2	4	4	-10	2	3	7	5	8	3	3	6	5	9	5	3	4	4
-7	12	2	6	8	-2	16	2	4	4	-9	2	3	4	6	-11	4	3	4	4	-10	6	3	5	5
-6	12	2	7	7	-1	16	2	4	4	-8	2	3	3	3	-10	4	3	6	7	-9	6	3	13	12
-3	12	2	4	3	1	16	2	14	14	-7	2	3	11	11	-9	4	3	5	5	-8	6	3	7	7
-1	12	2	19	20	-2	17	2	8	9	-5	2	3	13	13	-8	4	3	7	7	-7	6	3	15	13
0	12	2	7	9	0	17	2	4	1	-4	2	3	22	19	-7	4	3	12	12	-6	6	3	8	9
1	12	2	3	4	-10	0	3	15	15	-3	2	3	8	10	-6	4	3	8	6	-5	6	3	18	17
3	12	2	23	23	-8	0	3	3	3	-2	2	3	83	80	-5	4	3	30	26	-4	6	3	15	16
7	12	2	5	1	-6	0	3	6	6	-1	2	3	4	7	-4	4	3	20	19	-3	6	3	57	43

Table 22. (Continued)

Observed and calculated structure factors: Trichlorobenzene Thiourea Adduct

h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc
-2	6	3	34	35	1	8	3	22	21	1	11	3	24	25	-3	15	3	5	5	6	1	4	20	20
-1	6	3	3	4	2	8	3	5	3	2	11	3	19	18	0	15	3	5	5	7	1	4	11	9
0	6	3	45	44	3	8	3	6	5	3	11	3	4	1	3	15	3	12	10	8	1	4	6	4
1	6	3	17	20	4	8	3	9	11	4	11	3	8	7	4	15	3	4	1	9	1	4	5	6
2	6	3	6	7	5	8	3	21	21	5	11	3	14	15	-3	16	3	6	6	-10	2	4	8	8
4	6	3	5	6	8	8	3	6	5	6	11	3	3	2	0	16	3	3	1	-8	2	4	5	5
5	6	3	35	36	-10	9	3	4	4	-6	12	3	6	6	1	16	3	5	4	-7	2	4	13	15
6	6	3	10	8	-8	9	3	4	3	-5	12	3	7	7	3	16	3	5	2	-6	2	4	15	14
8	6	3	7	6	-6	9	3	9	8	-4	12	3	12	11	-4	17	3	5	3	-5	2	4	52	49
9	6	3	4	3	-5	9	3	5	6	-2	12	3	7	6	2	17	3	4	1	-4	2	4	22	15
-9	7	3	8	6	-4	9	3	6	5	-1	12	3	8	8	-10	0	4	8	7	-3	2	4	3	8
-8	7	3	4	4	-3	9	3	18	14	0	12	3	16	17	-8	0	4	26	26	-2	2	4	29	30
-7	7	3	9	13	-1	9	3	13	14	1	12	3	9	10	-6	0	4	25	24	-1	2	4	12	12
-5	7	3	31	31	1	9	3	3	4	2	12	3	13	14	-4	0	4	34	27	0	2	4	21	22
-4	7	3	10	9	2	9	3	41	42	5	12	3	15	15	-2	0	4	28	29	2	2	4	22	21
-3	7	3	58	43	3	9	3	5	6	6	12	3	4	4	0	0	4	63	63	4	2	4	8	8
-1	7	3	14	14	5	9	3	4	2	-5	13	3	10	11	2	0	4	49	50	5	2	4	26	25
0	7	3	16	15	8	9	3	8	7	-3	13	3	12	11	4	0	4	12	12	7	2	4	4	2
1	7	3	47	49	-8	10	3	4	2	-2	13	3	3	3	6	0	4	8	9	8	2	4	5	3
2	7	3	3	4	-6	10	3	4	2	-1	13	3	3	4	-11	1	4	4	3	9	2	4	4	6
3	7	3	16	17	-5	10	3	7	7	0	13	3	8	9	-9	1	4	5	5	-11	3	4	5	5
4	7	3	17	17	-4	10	3	5	0	1	13	3	6	6	-8	1	4	36	36	-10	3	4	10	10
5	7	3	17	16	-2	10	3	44	46	2	13	3	10	9	-7	1	4	5	7	-9	3	4	5	5
7	7	3	5	1	-1	10	3	7	8	5	13	3	5	5	-6	1	4	7	7	-8	3	4	14	13
8	7	3	4	5	0	10	3	9	8	-7	14	3	4	3	-5	1	4	26	25	-6	3	4	10	9
-10	8	3	5	3	1	10	3	5	6	-4	14	3	7	6	-4	1	4	12	11	-4	3	4	22	22
-9	8	3	6	7	2	10	3	6	7	-3	14	3	6	6	-3	1	4	22	20	-3	3	4	32	32
-8	8	3	10	10	5	10	3	8	6	-2	14	3	13	13	-2	1	4	56	56	-2	3	4	3	4
-5	8	3	15	17	7	10	3	4	4	0	14	3	9	8	-1	1	4	70	63	-1	3	4	103	99
-4	8	3	4	2	-7	11	3	7	9	1	14	3	7	7	0	1	4	41	38	0	3	4	50	51
-3	8	3	4	14	-6	11	3	8	9	2	14	3	5	5	1	1	4	8	8	1	3	4	22	21
-2	8	3	57	55	-5	11	3	20	21	3	14	3	5	5	2	1	4	17	17	2	3	4	8	8
-1	8	3	14	11	-2	11	3	9	11	5	14	3	5	5	3	1	4	3	3	3	3	4	4	2
0	8	3	6	4	0	11	3	8	8	-4	15	3	5	4	5	1	4	16	16	4	3	4	9	10

Table 22. (Continued)

Observed and calculated structure factors: Trichlorobenzene Thiourea Adduct

h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc
5	3	4	24	25	4	5	4	14	14	-5	8	4	3	5	-5	11	4	7	8	-1	14	4	6	7
7	3	4	8	9	5	5	4	5	6	-4	8	4	15	7	-4	11	4	9	7	0	14	4	11	11
9	3	4	7	8	6	5	4	4	5	-3	8	4	22	21	-3	11	4	21	21	2	14	4	9	8
-8	4	4	14	17	7	5	4	12	12	-1	8	4	9	10	-1	11	4	5	7	3	14	4	4	2
-6	4	4	27	26	-8	6	4	9	7	1	8	4	35	35	0	11	4	27	29	4	14	4	7	7
-5	4	4	56	58	-7	6	4	8	8	2	8	4	6	5	1	11	4	16	17	-3	15	4	4	4
-4	4	4	27	21	-5	6	4	6	7	3	8	4	25	25	3	11	4	6	6	-1	15	4	12	12
-3	4	4	43	44	-4	6	4	11	4	4	8	4	24	24	4	11	4	9	10	0	15	4	4	5
-2	4	4	21	20	-3	6	4	45	47	-10	9	4	11	10	-7	12	4	4	5	3	15	4	4	3
-1	4	4	14	14	-2	6	4	6	5	-9	9	4	5	5	-5	12	4	5	4	-5	16	4	9	8
0	4	4	18	18	-1	6	4	4	4	-8	9	4	4	2	-4	12	4	11	8	-4	16	4	6	5
1	4	4	37	37	0	6	4	3	3	-6	9	4	9	9	-3	12	4	23	21	1	16	4	5	4
2	4	4	66	65	1	6	4	18	18	-4	9	4	6	6	-2	12	4	6	6	-3	17	4	5	0
3	4	4	19	21	2	6	4	52	52	-3	9	4	12	12	-1	12	4	6	6	-1	17	4	5	7
4	4	4	24	25	3	6	4	17	16	-1	9	4	6	3	0	12	4	12	12	-8	0	5	13	13
5	4	4	12	13	4	6	4	9	10	0	9	4	34	37	1	12	4	10	10	-6	0	5	18	19
6	4	4	7	8	6	6	4	4	3	3	9	4	13	13	2	12	4	10	11	-2	0	5	48	48
7	4	4	9	10	-10	7	4	5	4	4	9	4	8	9	3	12	4	11	11	0	0	5	45	45
8	4	4	4	1	-8	7	4	5	7	-9	10	4	4	4	5	12	4	5	5	2	0	5	5	7
11	4	4	5	1	-6	7	4	13	13	-8	10	4	6	5	6	12	4	4	5	4	0	5	8	9
-10	5	4	12	13	-5	7	4	4	6	-6	10	4	20	22	-8	13	4	5	7	8	0	5	14	13
-9	5	4	4	2	-4	7	4	32	21	-5	10	4	9	8	-7	13	4	6	7	-11	1	5	4	2
-8	5	4	14	12	-3	7	4	55	51	-4	10	4	3	6	-5	13	4	4	5	-10	1	5	4	3
-7	5	4	4	3	-2	7	4	5	3	-3	10	4	10	12	-3	13	4	12	12	-8	1	5	13	11
-6	5	4	7	6	-1	7	4	12	9	-2	10	4	5	5	-2	13	4	4	3	-7	1	5	5	6
-5	5	4	23	23	0	7	4	4	3	-1	10	4	4	4	-1	13	4	7	7	-6	1	5	38	38
-4	5	4	5	5	1	7	4	20	18	0	10	4	20	18	0	13	4	7	7	-5	1	5	20	18
-3	5	4	27	28	2	7	4	3	1	1	10	4	5	2	2	13	4	5	3	-4	1	5	36	36
-2	5	4	15	16	4	7	4	3	3	2	10	4	8	7	3	13	4	4	0	-3	1	5	26	26
-1	5	4	23	23	5	7	4	6	9	4	10	4	22	23	5	13	4	5	6	-2	1	5	25	25
0	5	4	10	9	7	7	4	18	18	5	10	4	3	5	-6	14	4	3	5	-1	1	5	25	24
1	5	4	29	31	-8	8	4	7	5	-9	11	4	4	2	-4	14	4	4	5	0	1	5	3	4
2	5	4	26	25	-7	8	4	10	9	-8	11	4	5	5	-3	14	4	7	8	1	1	5	16	16
3	5	4	8	9	-6	8	4	17	19	-6	11	4	4	2	-2	14	4	4	0	3	1	5	12	13

Table 22. (Continued)

Observed and calculated structure factors: Trichlorobenzene Thiourea Adduct

h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc
4	1	5	52	54	-11	4	5	4	2	-10	6	5	6	4	-3	8	5	7	7	2	10	5	22	23
5	1	5	9	10	-9	4	5	13	15	-8	6	5	3	3	-2	8	5	4	6	3	10	5	9	10
7	1	5	6	6	-8	4	5	13	13	-7	6	5	14	14	-1	8	5	40	39	5	10	5	5	2
-11	2	5	11	11	-7	4	5	17	18	-6	6	5	13	12	0	8	5	6	7	6	10	5	13	13
-9	2	5	19	18	-6	4	5	3	3	-4	6	5	31	30	1	8	5	4	3	-7	11	5	4	3
-8	2	5	5	4	-5	4	5	24	22	-3	6	5	13	12	2	8	5	10	10	-5	11	5	8	4
-7	2	5	6	8	-4	4	5	24	26	-2	6	5	17	19	3	8	5	3	2	-4	11	5	14	14
-6	2	5	23	21	-3	4	5	13	15	-1	6	5	55	59	4	8	5	4	3	-3	11	5	7	7
-5	2	5	20	16	-2	4	5	28	25	1	6	5	21	21	5	8	5	5	6	-2	11	5	6	7
-4	2	5	12	11	-1	4	5	9	11	2	6	5	5	5	6	8	5	12	12	-1	11	5	6	7
-3	2	5	49	50	0	4	5	15	14	3	6	5	7	6	7	8	5	5	3	0	11	5	5	6
-2	2	5	24	25	1	4	5	36	35	4	6	5	8	9	-8	9	5	7	6	2	11	5	7	9
-1	2	5	21	18	2	4	5	7	7	5	6	5	3	2	-7	9	5	4	6	3	11	5	16	14
0	2	5	55	54	4	4	5	5	5	6	6	5	5	4	-6	9	5	17	17	4	11	5	3	3
1	2	5	60	62	5	4	5	8	6	7	6	5	5	4	-5	9	5	19	16	6	11	5	4	4
2	2	5	11	12	6	4	5	19	19	8	6	5	4	5	-4	9	5	38	39	-7	12	5	7	6
4	2	5	6	5	7	4	5	7	6	-10	7	5	4	4	-2	9	5	3	1	-5	12	5	7	3
5	2	5	4	5	8	4	5	5	5	-9	7	5	6	6	0	9	5	6	6	-2	12	5	9	10
6	2	5	13	14	-11	5	5	9	7	-7	7	5	13	14	1	9	5	4	6	-1	12	5	27	28
7	2	5	9	9	-9	5	5	6	6	-5	7	5	5	10	2	9	5	24	24	0	12	5	5	3
8	2	5	7	7	-8	5	5	5	5	-4	7	5	25	24	3	9	5	7	7	2	12	5	8	8
-7	3	5	7	5	-7	5	5	4	4	-3	7	5	6	7	5	9	5	5	2	4	12	5	4	4
-5	3	5	26	24	-6	5	5	30	32	-2	7	5	12	9	6	9	5	11	11	5	12	5	3	4
-4	3	5	24	21	-5	5	5	18	21	-1	7	5	17	18	7	9	5	5	2	-6	13	5	5	6
-3	3	5	55	52	-4	5	5	17	15	0	7	5	27	28	-9	10	5	7	7	-5	13	5	5	7
-2	3	5	8	10	-3	5	5	38	38	1	7	5	7	9	-8	10	5	11	11	-4	13	5	7	8
-1	3	5	12	11	-2	5	5	15	16	2	7	5	5	5	-7	10	5	8	8	-2	13	5	6	6
0	3	5	12	10	-1	5	5	14	13	3	7	5	25	25	-6	10	5	5	4	-1	13	5	4	3
1	3	5	64	63	0	5	5	4	6	4	7	5	11	11	-5	10	5	17	12	2	13	5	8	9
2	3	5	22	22	1	5	5	5	4	5	7	5	5	3	-4	10	5	5	3	3	13	5	6	8
3	3	5	8	8	2	5	5	11	14	-9	8	5	4	4	-2	10	5	5	7	4	13	5	8	9
4	3	5	5	7	3	5	5	14	14	-8	8	5	7	7	-1	10	5	26	24	-5	14	5	3	5
6	3	5	7	8	4	5	5	27	26	-6	8	5	6	8	0	10	5	12	11	-4	14	5	4	2
8	3	5	5	5	6	5	5	17	16	-5	8	5	5	0	1	10	5	4	2	-2	14	5	6	8

Table 22. (Continued)

Observed and calculated structure factors: Trichlorobenzene Thiourea Adduct

h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc
-1	14	5	6	6	5	1	6	4	4	-6	4	6	20	17	-1	6	6	22	23	-6	9	6	13	11
1	14	5	7	6	6	1	6	7	7	-4	4	6	17	18	0	6	6	8	8	-5	9	6	8	11
4	14	5	5	1	7	1	6	4	4	-3	4	6	3	3	1	6	6	4	3	-4	9	6	13	13
-6	15	5	4	3	-11	2	6	5	4	-2	4	6	32	35	2	6	6	9	9	-3	9	6	5	4
-5	15	5	4	3	-9	2	6	6	5	-1	4	6	11	12	5	6	6	27	29	-2	9	6	39	40
-4	15	5	5	5	-7	2	6	19	20	0	4	6	9	12	6	6	6	6	6	1	9	6	9	9
-3	15	5	6	4	-5	2	6	30	28	1	4	6	4	6	-10	7	6	4	3	2	9	6	16	17
-2	15	5	7	7	-4	2	6	45	46	2	4	6	8	9	-9	7	6	14	15	3	9	6	3	2
-1	15	5	4	3	-3	2	6	24	25	3	4	6	33	33	-8	7	6	5	6	5	9	6	4	5
0	15	5	4	1	-2	2	6	24	22	5	4	6	4	3	-7	7	6	11	12	-9	10	6	4	2
1	15	5	6	6	-1	2	6	18	18	6	4	6	8	8	-6	7	6	3	1	-6	10	6	6	8
-3	16	5	5	4	1	2	6	16	17	-10	5	6	6	4	-4	7	6	10	13	-5	10	6	6	8
-1	16	5	4	0	2	2	6	5	7	-9	5	6	11	10	-2	7	6	7	8	-4	10	6	4	4
1	16	5	9	11	3	2	6	51	53	-7	5	6	6	8	-1	7	6	13	12	-3	10	6	6	6
-2	17	5	7	7	4	2	6	12	12	-6	5	6	13	16	1	7	6	35	35	-2	10	6	28	27
-8	0	6	5	6	5	2	6	4	3	-5	5	6	8	11	2	7	6	7	6	-1	10	6	8	7
-6	0	6	8	10	7	2	6	9	7	-4	5	6	4	5	4	7	6	7	7	0	10	6	5	7
-4	0	6	85	84	-9	3	6	7	8	-2	5	6	13	13	5	7	6	4	4	1	10	6	8	8
-2	0	6	10	9	-8	3	6	12	11	-1	5	6	10	10	7	7	6	4	0	2	10	6	8	8
0	0	6	15	14	-7	3	6	30	30	0	5	6	35	34	-9	8	6	5	4	3	10	6	7	7
2	0	6	7	6	-6	3	6	15	15	1	5	6	15	16	-8	8	6	8	8	4	10	6	7	7
6	0	6	21	19	-4	3	6	14	14	2	5	6	10	11	-7	8	6	6	6	5	10	6	5	7
-10	1	6	8	6	-3	3	6	8	10	3	5	6	4	5	-6	8	6	3	4	6	10	6	4	3
-9	1	6	10	10	-2	3	6	37	40	4	5	6	4	5	-5	8	6	15	16	-9	11	6	8	6
-7	1	6	10	11	-1	3	6	25	24	5	5	6	5	5	-2	8	6	35	34	-7	11	6	4	4
-6	1	6	23	22	0	3	6	17	16	6	5	6	10	11	-1	8	6	7	7	-5	11	6	12	10
-5	1	6	4	6	1	3	6	8	8	7	5	6	5	3	1	8	6	8	9	-4	11	6	5	5
-4	1	6	4	4	2	3	6	14	13	-9	6	6	8	7	2	8	6	3	3	-2	11	6	21	20
-2	1	6	14	16	3	3	6	24	24	-8	6	6	6	5	3	8	6	4	4	-1	11	6	5	4
-1	1	6	3	7	5	3	6	4	1	-7	6	6	14	14	4	8	6	11	12	0	11	6	11	11
0	1	6	86	85	7	3	6	8	9	-6	6	6	3	5	5	8	6	15	14	1	11	6	22	22
1	1	6	15	15	-11	4	6	5	7	-5	6	6	21	21	-10	9	6	7	6	4	11	6	5	4
2	1	6	11	11	-9	4	6	7	7	-4	6	6	26	26	-9	9	6	4	2	-7	12	6	5	5
3	1	6	19	18	-7	4	6	6	5	-2	6	6	7	10	-8	9	6	4	4	-5	12	6	13	13

Table 22. (Continued)

Observed and calculated structure factors: Trichlorobenzene Thiourea Adduct

h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc
-4	12	6	8	8	4	0	7	5	3	0	3	7	6	8	5	5	7	6	5	-2	8	7	12	12
-3	12	6	4	0	-10	1	7	4	4	1	3	7	3	3	-10	6	7	4	4	-1	8	7	11	11
-2	12	6	7	8	-7	1	7	6	4	2	3	7	3	3	-9	6	7	3	1	0	8	7	32	33
-1	12	6	3	1	-6	1	7	6	6	4	3	7	7	7	-8	6	7	14	14	1	8	7	6	5
1	12	6	7	8	-5	1	7	29	30	5	3	7	23	24	-7	6	7	14	13	3	8	7	11	12
2	12	6	4	2	-4	1	7	7	6	6	3	7	4	2	-6	6	7	6	6	4	8	7	13	13
4	12	6	3	2	-3	1	7	11	11	7	3	7	5	4	-5	6	7	11	10	-8	9	7	6	5
5	12	6	10	9	-2	1	7	19	20	-10	4	7	6	8	-4	6	7	4	3	-6	9	7	10	9
-6	13	6	6	4	-1	1	7	32	34	-8	4	7	13	14	-3	6	7	7	3	-4	9	7	4	3
-3	13	6	6	4	2	1	7	23	24	-7	4	7	5	5	-2	6	7	5	5	0	9	7	10	10
-2	13	6	8	7	3	1	7	5	1	-6	4	7	12	13	-1	6	7	5	5	1	9	7	5	3
0	13	6	10	10	4	1	7	4	0	-5	4	7	23	25	0	6	7	9	8	4	9	7	13	12
1	13	6	11	12	5	1	7	19	20	-4	4	7	11	9	1	6	7	10	11	-6	10	7	7	8
2	13	6	4	4	6	1	7	5	4	-2	4	7	27	26	2	6	7	14	13	-3	10	7	6	8
4	13	6	5	4	-11	2	7	4	1	-1	4	7	28	28	3	6	7	13	13	-2	10	7	4	1
-6	14	6	6	3	-9	2	7	3	2	0	4	7	22	23	4	6	7	4	3	-1	10	7	5	4
-4	14	6	8	7	-8	2	7	11	13	1	4	7	16	15	6	6	7	4	4	0	10	7	32	33
-3	14	6	10	10	-7	2	7	13	16	2	4	7	19	19	-10	7	7	4	4	1	10	7	7	6
-2	14	6	7	8	-6	2	7	8	9	3	4	7	6	6	-8	7	7	5	5	5	10	7	4	0
-1	14	6	4	2	-5	2	7	26	27	5	4	7	5	6	-7	7	7	6	6	-8	11	7	3	2
1	14	6	4	4	-4	2	7	8	9	-11	5	7	3	2	-5	7	7	13	15	-6	11	7	7	7
-6	15	6	5	3	-3	2	7	20	19	-10	5	7	7	6	-4	7	7	4	3	-5	11	7	8	10
-1	15	6	5	4	-2	2	7	9	10	-9	5	7	6	6	-3	7	7	56	57	-4	11	7	3	5
0	15	6	3	4	-1	2	7	34	34	-1	5	7	10	9	-2	7	7	20	21	-3	11	7	17	18
1	15	6	4	3	1	2	7	12	12	-6	5	7	7	8	-1	7	7	9	11	-1	11	7	5	5
-3	16	6	5	4	2	2	7	24	23	-4	5	7	10	9	0	7	7	7	7	0	11	7	5	5
0	16	6	5	6	6	2	7	4	4	-3	5	7	40	39	1	7	7	4	3	1	11	7	3	0
-10	0	7	13	14	-10	3	7	11	11	-2	5	7	22	21	3	7	7	13	12	3	11	7	9	8
-8	0	7	24	23	-8	3	7	3	0	-1	5	7	16	13	4	7	7	6	5	4	11	7	5	5
-6	0	7	6	5	-7	3	7	12	14	0	5	7	7	6	5	7	7	4	3	-8	12	7	7	7
-4	0	7	12	12	-5	3	7	36	35	1	5	7	11	10	-7	8	7	13	13	-7	12	7	9	7
-2	0	7	13	14	-3	3	7	11	10	2	5	7	6	7	-6	8	7	16	16	-5	12	7	3	1
0	0	7	27	27	-2	3	7	20	19	3	5	7	12	13	-5	8	7	6	6	-4	12	7	10	9
2	0	7	62	65	-1	3	7	26	28	4	5	7	15	15	-3	8	7	19	16	2	12	7	8	7

Table 22. (Continued)

Observed and calculated structure factors: Trichlorobenzene Thiourea Adduct

h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	
3	12	7	5	4	5	1	8	5	3	-5	4	8	5	7	-7	7	8	8	9	-3	10	8	3	1	
4	12	7	4	1	6	1	8	3	1	-4	4	8	27	28	-6	7	8	10	11	-1	10	8	10	9	
-5	13	7	4	2	-11	2	8	4	6	-3	4	8	25	24	-5	7	8	14	15	2	10	8	4	2	
-3	13	7	10	11	-10	2	8	5	3	-1	4	8	11	10	-4	7	8	16	20	-6	11	8	4	4	
-2	13	7	8	8	-9	2	8	9	9	0	4	8	5	5	-3	7	8	6	6	-3	11	8	4	3	
-1	13	7	7	6	-8	2	8	4	1	1	4	8	9	11	-2	7	8	10	11	-2	11	8	6	7	
2	13	7	4	4	-7	2	8	3	3	2	4	8	5	3	-1	7	8	27	26	-1	11	8	12	13	
3	13	7	6	7	-6	2	8	4	2	3	4	8	7	8	0	7	8	7	5	1	11	8	5	6	
-5	14	7	7	8	-5	2	8	8	6	4	4	8	7	7	1	7	8	7	7	2	11	8	10	9	
-3	14	7	5	4	-4	2	8	6	6	6	4	8	9	10	2	7	8	9	7	3	11	8	5	6	
0	14	7	7	6	-3	2	8	48	49	-10	5	8	5	6	3	7	8	8	10	-5	12	8	6	6	
2	14	7	5	7	-2	2	8	13	13	-8	5	8	13	13	4	7	8	4	3	-3	12	8	3	4	
-5	15	7	6	5	-1	2	8	9	9	-7	5	8	15	14	-8	8	8	7	7	-2	12	8	7	9	
-4	15	7	4	3	0	2	8	7	6	-6	5	8	24	25	-6	8	8	9	9	-1	12	8	13	14	
-1	15	7	8	10	1	2	8	6	5	-5	5	8	11	10	-4	8	8	14	15	0	12	8	4	1	
-10	0	8	4	3	2	2	8	7	4	-4	5	8	4	2	-3	8	8	13	13	3	12	8	5	2	
-6	0	8	19	18	4	2	8	16	15	-3	5	8	13	13	-1	8	8	19	20	-6	13	8	11	10	
-4	0	8	10	11	-11	3	8	6	5	-1	5	8	12	11	0	8	8	12	13	-5	13	8	8	7	
-2	0	8	31	32	-10	3	8	4	1	0	5	8	8	11	2	8	8	9	10	-2	13	8	6	4	
0	0	8	11	12	-9	3	8	9	9	1	5	8	4	3	3	8	8	5	1	-3	14	8	8	6	6
2	0	8	5	5	-8	3	8	12	11	2	5	8	25	25	-9	9	8	5	2	-1	14	8	4	6	6
4	0	8	39	39	-7	3	8	5	6	3	5	8	7	6	-8	9	8	8	7	-4	15	8	6	6	6
-9	1	8	3	6	-6	3	8	5	6	4	5	8	5	6	-7	9	8	3	1	-2	15	8	6	4	4
-8	1	8	14	15	-4	3	8	23	25	6	5	8	4	1	-6	9	8	3	3	-8	0	9	5	3	3
-7	1	8	4	2	-1	3	8	6	7	-10	6	8	6	5	-5	9	8	5	5	-4	0	9	41	40	40
-6	1	8	25	24	0	3	8	8	7	-7	6	8	7	8	-4	9	8	11	9	-2	0	9	15	14	14
-5	1	8	4	5	1	3	8	32	31	-5	6	8	7	8	-2	9	8	4	3	0	0	9	26	25	25
-4	1	8	11	11	2	3	8	13	13	-4	6	8	13	13	-1	9	8	7	8	2	0	9	6	5	5
-2	1	8	4	4	3	3	8	4	4	-3	6	8	3	3	0	9	8	4	5	-11	1	9	4	4	4
-1	1	8	12	13	-10	4	8	3	1	-1	6	8	38	38	2	9	8	24	25	-9	1	9	5	5	5
0	1	8	17	19	-9	4	8	8	8	0	6	8	13	12	-3	9	8	5	6	-8	1	9	10	10	10
1	1	8	27	28	-8	4	8	4	2	4	6	8	7	8	-6	10	8	8	7	-6	1	9	7	7	7
2	1	8	9	10	-7	4	8	9	8	5	6	8	4	5	-5	10	8	6	5	-5	1	9	4	5	5
4	1	8	23	22	-6	4	8	8	9	-9	7	8	4	2	-4	10	8	15	14	-4	1	9	31	32	32

Table 22. (Continued)

Observed and calculated structure factors: Trichlorobenzene Thiourea Adduct

h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc
-2	1	9	12	11	3	4	9	17	16	-1	7	9	6	6	-3	13	9	3	3	-7	3	10	12	12
-1	1	9	13	13	4	4	9	7	7	0	7	9	4	0	-2	13	9	4	4	-6	3	10	5	4
0	1	9	17	17	5	4	9	4	2	1	7	9	12	12	0	13	9	5	6	-5	3	10	32	32
1	1	9	5	5	-10	5	9	4	2	4	7	9	4	3	-4	14	9	5	4	-3	3	10	7	7
3	1	9	6	6	-9	5	9	9	8	-9	8	9	6	5	-3	14	9	9	8	-2	3	10	9	9
-9	2	9	9	9	-7	5	9	5	6	-7	8	9	5	5	-10	0	10	7	6	0	3	10	3	2
-8	2	9	4	1	-6	5	9	8	8	-6	8	9	12	11	-8	0	10	11	12	1	3	10	9	9
-7	2	9	21	21	-5	5	9	6	3	-4	8	9	10	9	-6	0	10	5	3	2	3	10	8	7
-4	2	9	17	18	-4	5	9	21	21	1	8	9	18	16	-4	0	10	6	3	4	3	10	4	4
-2	2	9	13	15	-3	5	9	7	6	2	8	9	9	10	-2	0	10	34	33	-10	4	10	9	10
-1	2	9	14	16	-2	5	9	29	29	-8	9	9	4	2	2	0	10	6	6	-9	4	10	6	5
1	2	9	8	8	-1	5	9	11	12	-5	9	9	4	5	-10	1	10	5	5	-7	4	10	7	7
2	2	9	6	5	0	5	9	12	11	-2	9	9	28	27	-8	1	10	4	5	-5	4	10	6	6
3	2	9	31	31	1	5	9	14	14	1	9	9	4	5	-7	1	10	8	8	-4	4	10	4	4
4	2	9	3	1	4	5	9	3	3	-8	10	9	3	3	-6	1	10	4	1	-2	4	10	17	18
-9	3	9	5	3	5	5	9	6	5	-7	10	9	6	6	-5	1	10	21	21	-1	4	10	9	9
-8	3	9	8	10	-9	6	9	6	6	-6	10	9	11	11	-4	1	10	10	11	0	4	10	19	20
-7	3	9	4	6	-7	6	9	6	5	-5	10	9	6	8	-2	1	10	10	11	1	4	10	12	11
-5	3	9	10	12	-6	6	9	6	4	-3	10	9	4	2	-1	1	10	5	6	2	4	10	6	5
-4	3	9	10	10	-5	6	9	22	21	-2	10	9	3	2	1	1	10	11	12	-8	5	10	5	5
-3	3	9	6	6	-4	6	9	17	18	-1	10	9	3	1	2	1	10	19	19	-7	5	10	7	7
-2	3	9	32	32	-3	6	9	5	5	0	10	9	4	3	-10	2	10	4	3	-6	5	10	4	4
-1	3	9	26	27	-2	6	9	8	7	1	10	9	5	4	-9	2	10	4	3	-5	5	10	16	16
1	3	9	5	6	-1	6	9	7	6	3	10	9	4	3	-8	2	10	8	8	-3	5	10	23	23
2	3	9	5	7	1	6	9	28	30	-3	11	9	3	3	-6	2	10	10	8	0	5	10	18	17
3	3	9	6	6	2	6	9	4	5	-2	11	9	9	10	-5	2	10	8	7	2	5	10	10	10
-9	4	9	7	5	4	6	9	6	4	0	11	9	5	5	-4	2	10	5	6	-3	5	10	8	8
-7	4	9	10	11	5	6	9	6	6	1	11	9	7	7	-3	2	10	10	11	-8	6	10	4	4
-6	4	9	16	17	-9	7	9	9	8	-7	12	9	5	4	-2	2	10	12	13	-7	6	10	10	9
-4	4	9	4	3	-8	7	9	5	5	-6	12	9	4	4	-1	2	10	12	11	-6	6	10	7	8
-2	4	9	6	6	-6	7	9	4	3	-4	12	9	9	10	0	2	10	12	13	-5	6	10	8	9
0	4	9	9	8	-5	7	9	6	4	-1	12	9	4	3	1	2	10	6	7	-4	6	10	7	6
1	4	9	4	4	-4	7	9	7	8	1	12	9	10	10	2	2	10	6	4	-3	6	10	17	17
2	4	9	3	3	-2	7	9	11	10	-4	13	9	8	8	-8	3	10	5	4	-2	6	10	15	15

Table 22. (Continued)

Observed and calculated structure factors: Trichlorobenzene Thiourea Adduct

h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc
0	6	10	5	6	-1	12	10	5	3	-4	4	11	11	11	-5	9	11	5	2	-2	3	12	8	7
1	6	10	4	4	-3	13	10	4	5	-3	4	11	22	24	-3	9	11	4	1	-1	3	12	13	12
2	6	10	5	7	-8	0	11	10	9	-1	4	11	12	13	-2	9	11	6	6	0	3	12	4	3
-7	7	10	13	12	-6	0	11	21	21	0	4	11	5	6	-6	10	11	4	5	1	3	12	4	5
-6	7	10	4	5	0	0	11	7	8	2	4	11	12	12	-4	10	11	6	4	-7	4	12	3	5
-4	7	10	4	5	-10	1	11	6	4	-8	5	11	6	6	-2	10	11	7	6	-6	4	12	8	9
-3	7	10	14	14	-9	1	11	3	2	-7	5	11	6	6	-6	11	11	5	4	-5	4	12	4	4
-2	7	10	7	6	-6	1	11	14	14	-5	5	11	4	3	-3	11	11	5	4	-4	4	12	6	6
1	7	10	4	2	-4	1	11	4	4	-4	5	11	9	9	-2	11	11	6	5	-2	4	12	9	8
2	7	10	6	4	-3	1	11	12	13	-1	5	11	12	13	-1	11	11	10	10	-1	4	12	11	12
3	7	10	14	16	-2	1	11	4	2	0	5	11	8	8	-8	0	12	5	7	0	4	12	4	5
-9	8	10	4	4	-1	1	11	10	11	2	5	11	4	5	-6	0	12	6	5	1	4	12	4	4
-5	8	10	4	3	0	1	11	23	24	-8	6	11	6	7	-2	0	12	5	7	-7	5	12	4	3
-4	8	10	5	5	1	1	11	5	7	-6	6	11	5	4	0	0	12	7	7	-6	5	12	9	9
-3	8	10	13	14	2	1	11	5	3	-5	6	11	14	13	2	0	12	7	7	-4	5	12	11	11
-2	8	10	4	1	-8	2	11	5	4	-4	6	11	4	2	-7	1	12	5	3	-3	5	12	7	6
-1	8	10	4	2	-6	2	11	7	6	-3	6	11	4	4	-6	1	12	7	6	-1	5	12	9	10
0	8	10	17	18	-5	2	11	6	8	-2	6	11	3	3	-4	1	12	25	25	-8	6	12	6	5
2	8	10	4	1	-4	2	11	6	6	-1	6	11	6	4	-3	1	12	4	4	-1	6	12	4	2
-4	9	10	8	6	-3	2	11	20	19	2	6	11	4	5	1	1	12	3	3	0	6	12	3	3
-3	9	10	4	3	-2	2	11	5	4	-8	7	11	3	5	2	1	12	6	3	1	6	12	15	15
-1	9	10	3	4	1	2	11	9	8	-4	7	11	8	8	-9	2	12	9	8	-7	7	12	4	4
0	9	10	6	6	2	2	11	4	4	-3	7	11	6	7	-8	2	12	7	4	-6	7	12	4	3
2	9	10	5	2	-9	3	11	4	5	-1	7	11	16	15	-7	2	12	7	6	-3	7	12	7	6
-1	10	10	4	3	-8	3	11	7	8	0	7	11	6	5	-6	2	12	11	10	-2	7	12	7	8
0	10	10	16	16	-5	3	11	8	8	1	7	11	4	3	-4	2	12	7	6	-7	8	12	4	2
2	10	10	4	3	-3	3	11	16	16	-8	8	11	4	1	-3	2	12	5	3	-6	8	12	6	6
-7	11	10	4	4	-1	3	11	7	8	-7	8	11	5	4	-1	2	12	16	17	-5	8	12	4	4
-5	11	10	9	8	0	3	11	8	7	-6	8	11	8	6	1	2	12	5	3	-4	8	12	5	5
-4	11	10	9	9	1	3	11	10	10	-5	8	11	8	8	2	2	12	6	5	-2	8	12	5	5
-3	11	10	6	7	2	3	11	8	9	-4	8	11	9	10	-9	3	12	5	5	-6	9	12	10	8
-5	12	10	7	5	3	3	11	4	2	2	8	11	8	8	-8	3	12	5	4	-3	9	12	6	5
-3	12	10	6	4	-8	4	11	7	7	-7	9	11	4	4	-6	3	12	4	5	-2	9	12	12	11
-2	12	10	4	4	-6	4	11	7	7	-6	9	11	5	1	-4	3	12	5	4	-1	9	12	4	1

Table 22. (Continued)

Observed and calculated structure factors: Trichlorobenzene Thiourea Adduct

h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc
2	0	0	45	54	1	4	0	84	85	6	7	0	5	6	5	12	0	3	3	-8	1	1	37	37
4	0	0	21	23	2	4	0	52	54	7	7	0	9	9	6	12	0	8	10	-6	1	1	25	24
6	0	0	18	17	3	4	0	14	15	8	7	0	8	8	7	12	0	5	3	-5	1	1	23	25
8	0	0	7	8	4	4	0	3	4	0	8	0	53	42	10	12	0	4	2	-4	1	1	14	13
10	0	0	12	11	5	4	0	3	3	2	8	0	56	56	2	13	0	3	2	-3	1	1	29	26
1	1	0	8	8	7	4	0	20	21	3	8	0	8	8	3	13	0	6	2	-2	1	1	7	6
2	1	0	33	33	8	4	0	17	17	4	8	0	17	17	4	13	0	3	4	-1	1	1	11	16
3	1	0	59	56	10	4	0	8	8	5	8	0	3	3	5	13	0	12	12	0	1	1	2	4
4	1	0	19	20	1	5	0	19	17	6	8	0	3	1	0	14	0	16	17	1	1	1	11	9
5	1	0	19	20	2	5	0	47	46	7	8	0	8	8	1	14	0	10	10	2	1	1	117	119
6	1	0	13	14	3	5	0	13	13	8	8	0	12	12	2	14	0	7	8	3	1	1	4	4
7	1	0	15	15	4	5	0	35	37	9	8	0	5	5	5	14	0	5	5	4	1	1	16	16
8	1	0	6	4	5	5	0	35	36	10	8	0	4	5	1	15	0	5	4	5	1	1	20	20
10	1	0	5	4	6	5	0	4	6	1	9	0	9	8	2	15	0	6	6	6	1	1	9	9
0	2	0	15	17	7	5	0	3	3	2	9	0	44	41	3	15	0	12	13	7	1	1	4	4
1	2	0	2	2	8	5	0	7	9	3	9	0	4	4	4	15	0	4	2	8	1	1	5	4
2	2	0	7	4	9	5	0	4	5	5	9	0	9	10	5	15	0	3	1	9	1	1	11	11
3	2	0	47	48	10	5	0	6	5	6	9	0	4	1	6	15	0	4	2	10	1	1	4	1
4	2	0	5	5	11	5	0	4	5	6	9	0	4	4	0	16	0	3	6	11	1	1	4	4
5	2	0	3	2	0	6	0	23	20	0	10	0	17	17	1	16	0	3	0	-11	2	1	7	8
7	2	0	32	31	1	6	0	14	14	1	10	0	11	13	2	16	0	3	0	-8	2	1	5	7
9	2	0	4	5	2	6	0	24	21	2	10	0	35	35	3	16	0	5	5	-7	2	1	3	7
10	2	0	3	5	3	6	0	6	6	5	10	0	6	5	3	17	0	5	4	-5	2	1	37	38
1	3	0	6	8	4	6	0	22	26	7	10	0	3	2	0	18	0	10	9	-4	2	1	38	38
2	3	0	35	30	5	6	0	23	22	8	10	0	8	7	-8	0	1	5	5	-3	2	1	37	38
3	3	0	77	76	7	6	0	5	4	1	11	0	13	13	-6	0	1	9	10	-2	2	1	37	35
4	3	0	4	3	8	6	0	5	5	2	11	0	16	17	-4	0	1	82	85	-1	2	1	40	49
5	3	0	9	10	9	6	0	9	9	3	11	0	9	8	-2	0	1	14	15	0	2	1	2	3
6	3	0	3	4	10	6	0	8	6	4	11	0	7	5	2	0	1	69	74	1	2	1	10	9
7	3	0	19	20	1	7	0	4	6	5	11	0	23	24	4	0	1	43	41	2	2	1	37	35
9	3	0	5	4	2	7	0	10	8	0	12	0	21	19	6	0	1	30	32	3	2	1	49	48
11	3	0	4	2	3	7	0	10	11	1	12	0	13	12	12	0	1	5	5	4	2	1	13	12
12	3	0	5	3	4	7	0	8	7	2	12	0	3	1	-10	1	1	4	6	5	2	1	42	42
0	4	0	30	29	5	7	0	51	50	3	12	0	4	3	-9	1	1	5	4	6	2	1	7	6

APPENDIX D

TABLES FOR PUBLICATION FOR THE 1,2,4
TMB-THIOUREA ADDUCT STRUCTURE

APPENDIX D

Table 23. Atomic coordinates and isotropic thermal parameters for the 1,2,4 TMB-thiourea adduct structure.

	Atomic coordinates ($\times 10^4$) and isotropic thermal parameters ($\text{\AA}^2 \times 10^3$)			
	x	y	z	U
F(1)	3250(77)	476(49)	2178(61)	1035(152)
F(2)	1812	272	1496	210(38)
F(3)	990	-204	1981	199(41)
F(4)	1605	-477	3150	95(18)
F(5)	3042	-274	3832	148(30)
F(6)	3865	202	3347	164(30)
T(3)	3855(72)	340(52)	2991(37)	137(49)
T(4)	2934	-296	3137	222(67)
T(5)	1650	-510	2203	146(36)
T(6)	1287	-87	1124	227(49)
T(1)	2208	548	977	117(13)
T(2)	3492	762	1911	253(33)
B(1)	4202(31)	627(16)	3056(27)	107(13)
B(2)	4816	315	4207	102(11)
B(3)	4069	-293	4608	102(12)
B(4)	2708	-589	3860	122(15)
B(5)	2094	-277	2709	94(12)
B(6)	2841	331	2307	212(23)
B(21)	2954(27)	255(25)	2412(26)	80
B(22)	2604	613	1296	175(25)
B(23)	1279	416	399	62(12)
B(24)	304	-140	618	69(11)
B(25)	653	-499	1734	81(14)
B(26)	1978	-301	2631	575(114)
S(1)	4007(3)	6507(2)	4393(2)	73(1)*
S(2)	-29(3)	6405(2)	1403(2)	67(1)*
S(3)	3134(3)	3000(2)	2035(2)	71(1)*
C(1)	2875(10)	6892(5)	4995(8)	69(4)*
C(2)	934(10)	7101(6)	932(8)	70(4)*
C(3)	2719(10)	4067(6)	2226(8)	70(4)*
N(11)	3295(9)	7129(5)	6101(6)	86(4)*
N(12)	1430(8)	6974(5)	4342(7)	82(4)*
N(21)	332(9)	7506(5)	-142(6)	86(4)*
N(22)	2337(8)	7275(5)	1558(7)	88(4)*
N(31)	1762(8)	4527(5)	1350(6)	92(4)*
N(32)	3305(8)	4449(5)	3264(6)	87(4)*
B(10)	2048(58)	-672(33)	4014(48)	50
B(12)	372(338)	-2335(207)	-86(271)	50
B(13)	4326(70)	-583(38)	5573(53)	50
T(8)	243(54)	457(30)	-1008(44)	50
Fh(1)	3390(71)	-630(41)	4658(51)	50
Fh(2)	576(43)	157(28)	65(42)	50
Fh(3)	2203(70)	-922(43)	3357(56)	50
Fm(1)	4758(85)	802(50)	2808(64)	50
Tm(1)	4750(58)	533(33)	3644(44)	50
Fm(2)	4597(194)	2501(108)	7788(145)	50
Tm(3)	523(57)	-842(36)	2196(46)	50
Tm(2)	3314(229)	794(139)	221(181)	50
Bm(1)	1132(91)	510(50)	-178(80)	50

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

Table 24. Anisotropic thermal parameters for the 1,2,4 TMB-thiourea adduct structure.

Anisotropic thermal parameters ($\text{\AA}^2 \times 10^3$)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S(1)	58(2)	85(2)	61(2)	-15(1)	8(1)	4(2)
S(2)	60(2)	67(2)	61(2)	9(1)	8(1)	-3(1)
S(3)	81(2)	66(2)	51(1)	-2(1)	11(1)	10(2)
C(1)	63(6)	57(6)	74(7)	10(5)	13(6)	0(5)
C(2)	66(7)	71(6)	70(6)	-13(5)	24(5)	8(5)
C(3)	68(7)	70(6)	71(6)	-13(5)	26(5)	-2(5)
N(11)	79(6)	107(7)	62(5)	-24(5)	17(5)	1(5)
N(12)	60(5)	104(7)	83(6)	-5(5)	31(5)	4(5)
N(21)	119(8)	71(5)	58(5)	19(4)	22(5)	18(5)
N(22)	69(6)	93(6)	90(6)	14(5)	16(5)	-17(5)
N(31)	105(7)	62(5)	74(5)	-5(4)	-3(5)	24(5)
N(32)	103(7)	60(5)	78(5)	-17(4)	14(5)	11(5)

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

Table 25. H-atom coordinates and isotropic thermal parameters for the 1,2,4 TMB-thiourea adduct structure.

H-Atom coordinates ($\times 10^4$) and isotropic thermal parameters ($\text{\AA}^2 \times 10^3$)

	x	y	z	U
H(11a)	2619	7336	6421	116
H(11b)	4304	7091	6592	116
H(12a)	803	7186	4708	98
H(12b)	1037	6813	3527	98
H(21a)	862	6963	-20	102
H(21b)	-71	7764	-911	102
H(22a)	2763	7806	1412	107
H(22b)	2908	6873	2159	107
H(31a)	1500	5119	1463	110
H(31b)	1335	4254	592	110
H(32a)	3035	5041	3367	103
H(32b)	3997	4136	3915	103

Table 26. Bond lengths for the 1,2,4 TMB-thiourea adduct structure.

Bond lengths (Å)			
S(1)-C(1)	1.684(11)	S(2)-C(2)	1.679(11)
S(3)-C(3)	1.709(10)	C(1)-N(11)	1.315(11)
C(1)-N(12)	1.365(11)	C(2)-N(21)	1.372(11)
C(2)-N(22)	1.345(11)	C(3)-N(31)	1.332(10)
C(3)-N(32)	1.319(11)		

Table 27. Bond angles for the 1,2,4 TMB-thiourea adduct structure.

Table 3. Bond angles (°)

S(1)-C(1)-N(11)	123.6(7)	S(1)-C(1)-N(12)	121.0(7)
N(11)-C(1)-N(12)	115.4(10)	S(2)-C(2)-N(21)	121.3(7)
S(2)-C(2)-N(22)	122.6(7)	N(21)-C(2)-N(22)	118.1(9)
S(3)-C(3)-N(31)	121.4(7)	S(3)-C(3)-N(32)	120.6(6)
N(31)-C(3)-N(32)	118.0(8)	C(2)-H(21a)-N(21)	79.6(6)

Table 28. F(Obs) and sigma (F) for the 1,2,4 TMB-thiourea adduct structure.

F(obs) and sigma(F) (-sigma = unobserved): Trimethylbenzene Thiourea Adduct

h	k	l	10Fo	10s	h	k	l	10Fo	10s	h	k	l	10Fo	10s	h	k	l	10Fo	10s	h	k	l	10Fo	10s
-6	3	10	117	22	-8	6	10	38	-76	-2	9	10	105	26	-5	3	11	74	-35	0	6	11	36	-52
-5	3	10	468	8	-7	6	10	85	33	-1	9	10	58	-36	-4	3	11	36	-71	-7	7	11	38	-75
-4	3	10	35	-70	-6	6	10	113	24	0	9	10	90	24	-3	3	11	345	9	-6	7	11	38	-75
-3	3	10	104	24	-5	6	10	120	22	-5	10	10	38	-76	-2	3	11	36	-72	-5	7	11	37	-75
-2	3	10	187	15	-4	6	10	36	-71	-4	10	10	97	29	-1	3	11	160	11	-4	7	11	106	26
-1	3	10	58	-32	-3	6	10	324	10	-3	10	10	37	-74	0	3	11	161	12	-3	7	11	108	25
0	3	10	35	-49	-2	6	10	247	11	-2	10	10	101	27	1	3	11	173	14	-2	7	11	86	31
1	3	10	146	16	-1	6	10	35	-49	-1	10	10	37	-52	-8	4	11	132	23	-1	7	11	296	13
2	3	10	108	25	0	6	10	120	16	-9	1	11	53	-41	-7	4	11	37	-74	0	7	11	105	21
3	3	10	117	23	1	6	10	107	19	-8	1	11	54	-39	-6	4	11	72	-38	-6	8	11	80	-37
-9	4	10	111	26	2	6	10	98	28	-7	1	11	36	-51	-5	4	11	86	31	-5	8	11	172	17
-8	4	10	53	-52	-8	7	10	38	-76	-6	1	11	128	31	-4	4	11	171	16	-4	8	11	148	20
-7	4	10	150	18	-7	7	10	237	13	-5	1	11	36	-50	-3	4	11	362	9	-3	8	11	37	-74
-6	4	10	51	-50	-6	7	10	112	24	-4	1	11	109	17	-2	4	11	36	-71	-2	8	11	37	-74
-5	4	10	63	-42	-5	7	10	36	-73	-3	1	11	217	21	-1	4	11	203	10	-1	8	11	61	-32
-4	4	10	90	28	-4	7	10	36	-72	-2	1	11	35	-50	0	4	11	93	24	-4	9	11	38	-75
-3	4	10	35	-70	-3	7	10	211	13	-1	1	11	146	9	1	4	11	78	29	-3	9	11	37	-74
-2	4	10	254	11	-2	7	10	66	-39	0	1	11	428	4	-8	5	11	88	33	-8	0	12	58	-50
-1	4	10	160	18	-1	7	10	83	28	1	1	11	116	12	-7	5	11	121	24	-7	0	12	37	-75
0	4	10	332	15	0	7	10	75	25	2	1	11	98	28	-6	5	11	65	-41	-6	0	12	103	27
1	4	10	205	9	1	7	10	68	-28	-8	2	11	70	-40	-5	5	11	79	-34	-5	0	12	37	-73
2	4	10	127	21	-7	8	10	68	-42	-7	2	11	95	28	-4	5	11	150	18	-4	0	12	37	-73
-9	5	10	79	-37	-6	8	10	87	31	-6	2	11	123	22	-3	5	11	67	-39	-3	0	12	36	-72
-8	5	10	134	21	-5	8	10	94	29	-5	2	11	112	23	-2	5	11	36	-72	-2	0	12	101	26
-7	5	10	94	29	-4	8	10	109	24	-4	2	11	91	28	-1	5	11	164	11	-1	0	12	64	-29
-6	5	10	102	26	-3	8	10	268	11	-3	2	11	278	10	0	5	11	135	14	0	0	12	161	12
-5	5	10	275	11	-2	8	10	100	26	-2	2	11	67	-38	1	5	11	91	27	-8	1	12	67	-34
-4	5	10	36	-71	-1	8	10	101	25	-1	2	11	35	-50	-7	6	11	33	-75	-7	1	12	37	-53
-3	5	10	338	9	0	8	10	248	18	0	2	11	93	22	-6	6	11	109	26	-6	1	12	69	-28
-2	5	10	77	-33	1	8	10	37	-52	1	2	11	161	12	-5	6	11	232	13	-5	1	12	92	21
-1	5	10	80	21	-6	9	10	94	30	2	2	11	65	-43	-4	6	11	80	-32	-4	1	12	441	9
0	5	10	309	7	-5	9	10	37	-74	-8	3	11	118	24	-3	6	11	117	23	-3	1	12	48	-40
1	5	10	82	23	-4	9	10	145	19	-7	3	11	37	-74	-2	6	11	100	26	-2	1	12	36	-51
2	5	10	167	17	-3	9	10	81	-33	-6	3	11	96	28	-1	6	11	81	30	-1	1	12	65	24

Table 28. (Continued)

F(obs) and sigma(F) (-sigma = unobserved): Trimethylbenzene Thiourea Adduct

h	k	l	10Fo	10s	h	k	l	10Fo	10s	h	k	l	10Fo	10s	h	k	l	10Fo	10s	h	k	l	10Fo	10s
-6	1	9	84	21	-1	3	9	426	6	-8	6	9	37	-74	2	8	9	161	18	-1	0	10	34	-49
-5	1	9	75	25	0	3	9	34	-48	-7	6	9	53	-49	-7	9	9	38	-75	0	0	10	35	-49
-4	1	9	624	6	1	3	9	120	28	-6	6	9	59	-44	-6	9	9	72	-39	1	0	10	35	-49
-3	1	9	65	25	2	3	9	65	-39	-5	6	9	338	9	-5	9	9	98	27	2	0	10	183	15
-2	1	9	209	9	3	3	9	142	19	-4	6	9	209	13	-4	9	9	36	-72	3	0	10	37	-74
-1	1	9	219	9	4	3	9	37	-74	-3	6	9	60	-42	-3	9	9	63	-40	-9	1	10	37	-52
0	1	9	279	7	-9	4	9	65	-43	-2	6	9	163	16	-2	9	9	479	8	-8	1	10	114	17
1	1	9	72	23	-8	4	9	36	-72	-1	6	9	35	-49	-1	9	9	102	21	-7	1	10	90	27
2	1	9	35	-50	-7	4	9	203	13	0	6	9	77	23	0	9	9	71	-30	-6	1	10	62	-33
3	1	9	130	15	-6	4	9	231	12	1	6	9	461	7	1	9	9	123	16	-5	1	10	301	26
4	1	9	37	-52	-5	4	9	35	-71	2	6	9	36	-72	2	9	9	37	-74	-4	1	10	140	13
-10	2	9	38	-76	-4	4	9	35	-70	3	6	9	99	27	-6	10	9	213	14	-3	1	10	58	-33
-9	2	9	149	19	-3	4	9	79	30	-8	7	9	110	25	-5	10	9	37	-74	-2	1	10	156	12
-8	2	9	92	28	-2	4	9	35	-70	-7	7	9	37	-73	-4	10	9	67	-40	-1	1	10	109	13
-7	2	9	275	11	-1	4	9	34	-48	-6	7	9	36	-72	-3	10	9	59	-44	0	1	10	85	16
-6	2	9	64	-40	0	4	9	163	11	-5	7	9	160	17	-2	10	9	56	-48	1	1	10	205	7
-5	2	9	35	-69	1	4	9	70	25	-4	7	9	205	13	-1	10	9	36	-50	2	1	10	318	9
-4	2	9	281	10	2	4	9	61	-41	-3	7	9	35	-70	0	10	9	70	-31	3	1	10	37	-52
-3	2	9	60	-38	3	4	9	296	10	-2	7	9	95	27	1	10	9	92	28	-9	2	10	37	-75
-2	2	9	168	14	4	4	9	118	24	-1	7	9	35	-49	-5	11	9	68	-42	-8	2	10	89	30
-1	2	9	256	7	-9	5	9	105	28	0	7	9	110	26	-4	11	9	76	-37	-7	2	10	100	26
0	2	9	95	20	-8	5	9	37	-74	1	7	9	203	10	-3	11	9	36	-73	-6	2	10	156	17
1	2	9	141	14	-7	5	9	36	-72	2	7	9	36	-73	-2	11	9	225	13	-5	2	10	175	15
2	2	9	84	30	-6	5	9	155	17	3	7	9	86	32	-1	11	9	36	-51	-4	2	10	90	38
3	2	9	506	8	-5	5	9	65	-40	-8	8	9	38	-75	0	11	9	105	24	-3	2	10	200	14
4	2	9	52	-52	-4	5	9	326	9	-7	8	9	80	-35	-3	12	9	93	29	-2	2	10	263	11
-9	3	9	57	-49	-3	5	9	126	19	-6	8	9	178	16	-9	0	10	37	-74	-1	2	10	216	8
-8	3	9	134	20	-2	5	9	504	8	-5	8	9	36	-72	-8	0	10	37	-74	0	2	10	189	10
-7	3	9	36	-72	-1	5	9	222	13	-4	8	9	166	16	-7	0	10	35	-71	1	2	10	121	15
-6	3	9	35	-71	0	5	9	188	11	-3	8	9	58	-43	-6	0	10	60	-42	2	2	10	87	30
-5	3	9	152	17	1	5	9	235	13	-2	8	9	92	28	-5	0	10	53	-48	3	2	10	37	-74
-4	3	9	59	-41	2	5	9	36	-71	-1	8	9	57	-34	-4	0	10	58	-43	-9	3	10	76	-38
-3	3	9	90	26	3	5	9	36	-73	0	8	9	35	-50	-3	0	10	35	-70	-8	3	10	37	-74
-2	3	9	544	8	-9	6	9	126	23	1	8	9	355	12	-2	0	10	568	8	-7	3	10	135	20

Table 28. (Continued)

F(obs) and sigma(F) (-sigma = unobserved): Trimethylbenzene Thiourea Adduct

h	k	l	10Fo	10s	h	k	l	10Fo	10s	h	k	l	10Fo	10s	h	k	l	10Fo	10s	h	k	l	10Fo	10s
-4	0	8	93	23	-2	2	8	195	12	0	4	8	33	-47	-9	7	8	96	30	0	9	8	91	21
-3	0	8	93	22	-1	2	8	131	14	1	4	8	174	12	-8	7	8	37	-73	1	9	8	78	28
-2	0	8	516	7	0	2	8	116	14	2	4	8	90	28	-7	7	8	151	18	2	9	8	371	9
-1	0	8	32	-45	1	2	8	161	18	3	4	8	129	20	-6	7	8	197	14	3	9	8	113	23
0	0	8	158	12	2	2	8	89	28	4	4	8	123	22	-5	7	8	214	13	-7	10	8	77	-37
1	0	8	86	22	3	2	8	57	-43	5	4	8	38	-75	-4	7	8	237	12	-6	10	8	123	23
2	0	8	120	20	4	2	8	296	10	-9	5	8	37	-74	-3	7	8	129	20	-5	10	8	36	-73
3	0	8	35	-70	5	2	8	62	-44	-8	5	8	211	13	-2	7	8	181	15	-4	10	8	282	10
4	0	8	663	8	-10	3	8	37	-75	-7	5	8	233	12	-1	7	8	496	14	-3	10	8	63	-39
5	0	8	37	-74	-9	3	8	222	13	-6	5	8	337	9	0	7	8	91	19	-2	10	8	36	-71
-10	1	8	38	-53	-8	3	8	110	24	-5	5	8	156	16	1	7	8	132	13	-1	10	8	73	26
-9	1	8	102	20	-7	3	8	36	-71	-4	5	8	35	-69	2	7	8	134	19	0	10	8	35	-50
-8	1	8	183	20	-6	3	8	58	-42	-3	5	8	170	14	3	7	8	162	17	1	10	8	36	-50
-7	1	8	51	-36	-5	3	8	68	-34	-2	5	8	34	-67	4	7	8	97	28	2	10	8	57	-48
-6	1	8	303	38	-4	3	8	216	11	-1	5	8	198	9	-8	8	8	74	-38	-6	11	8	75	-38
-5	1	8	65	-29	-3	3	8	156	15	0	5	8	164	16	-7	8	8	84	32	-5	11	8	37	-75
-4	1	8	219	10	-2	3	8	33	-65	1	5	8	94	21	-6	8	8	96	28	-4	11	8	37	-73
-3	1	8	32	-45	-1	3	8	141	13	2	5	8	438	8	-5	8	8	107	24	-3	11	8	53	-49
-2	1	8	95	16	0	3	8	90	25	3	5	8	35	-71	-4	8	8	232	13	-2	11	8	87	31
-1	1	8	173	7	1	3	8	538	16	4	5	8	74	-36	-3	8	8	147	18	-1	11	8	193	10
0	1	8	295	5	2	3	8	273	11	-9	6	8	69	-41	-2	8	8	78	-32	0	11	8	36	-51
1	1	8	468	7	3	3	8	108	23	-8	6	8	37	-73	-1	8	8	381	9	1	11	8	117	18
2	1	8	179	11	4	3	8	36	-73	-7	6	8	116	23	0	8	8	206	10	-5	12	8	109	27
3	1	8	75	29	5	3	8	38	-75	-6	6	8	80	-33	1	8	8	35	-49	-4	12	8	37	-75
4	1	8	471	7	-10	4	8	38	-76	-5	6	8	128	20	2	8	8	181	15	-3	12	8	92	29
5	1	8	53	-40	-9	4	8	124	22	-4	6	8	291	10	3	8	8	37	-73	-2	12	8	103	27
-10	2	8	37	-75	-8	4	8	75	-35	-3	6	8	34	-68	-8	9	8	148	20	-1	12	8	221	17
-9	2	8	58	-46	-7	4	8	83	32	-2	6	8	34	-68	-7	9	8	37	-74	0	12	8	89	28
-8	2	8	103	25	-6	4	8	170	16	-1	6	8	579	21	-6	9	8	36	-73	-3	13	8	38	-75
-7	2	8	35	-70	-5	4	8	66	-36	0	6	8	200	12	-5	9	8	95	27	-2	13	8	122	23
-6	2	8	35	-69	-4	4	8	426	8	1	6	8	50	-37	-4	9	8	193	14	-10	1	9	99	21
-5	2	8	34	-67	-3	4	8	462	7	2	6	8	60	-42	-3	9	8	36	-71	-9	1	9	37	-52
-4	2	8	119	18	-2	4	8	71	-31	3	6	8	36	-72	-2	9	8	65	-39	-8	1	9	140	21
-3	2	8	704	7	-1	4	8	159	13	4	6	8	154	18	-1	9	8	203	9	-7	1	9	73	-29

Table 28. (Continued)

F(obs) and sigma(F) (-sigma = unobserved): Trimethylbenzene Thiourea Adduct

h	k	l	10Fo	10s	h	k	l	10Fo	10s	h	k	l	10Fo	10s	h	k	l	10Fo	10s	h	k	l	10Fo	10s
4	1	7	74	29	4	3	7	73	-35	5	5	7	125	23	-6	8	7	193	14	2	10	7	36	-71
5	1	7	364	15	5	3	7	462	8	-9	6	7	37	-75	-5	8	7	36	-71	3	10	7	36	-73
6	1	7	54	-40	6	3	7	38	-76	-8	6	7	227	13	-4	8	7	35	-70	-7	11	7	120	24
-10	2	7	73	-38	-10	4	7	203	15	-7	6	7	157	17	-3	8	7	404	9	-6	11	7	143	20
-9	2	7	36	-72	-9	4	7	66	-41	-6	6	7	75	-34	-2	8	7	144	17	-5	11	7	158	18
-8	2	7	198	14	-8	4	7	176	16	-5	6	7	214	12	-1	8	7	164	10	-4	11	7	36	-72
-7	2	7	138	18	-7	4	7	158	16	-4	6	7	61	-37	0	8	7	447	6	-3	11	7	247	11
-6	2	7	136	18	-6	4	7	170	15	-3	6	7	34	-67	1	8	7	127	15	-2	11	7	35	-70
-5	2	7	214	11	-5	4	7	323	9	-2	6	7	184	13	2	8	7	35	-70	-1	11	7	112	16
-4	2	7	32	-64	-4	4	7	122	17	-1	6	7	90	17	3	8	7	235	12	0	11	7	36	-50
-3	2	7	287	8	-3	4	7	31	-63	0	6	7	226	12	4	8	7	255	12	1	11	7	73	29
-2	2	7	134	15	-2	4	7	433	7	1	6	7	207	8	-8	9	7	112	25	2	11	7	36	-72
-1	2	7	589	5	-1	4	7	520	13	2	6	7	254	11	-7	9	7	91	30	3	11	7	155	18
0	2	7	31	-43	0	4	7	373	6	3	6	7	223	12	-6	9	7	197	14	-6	12	7	38	-76
1	2	7	230	7	1	4	7	209	11	4	6	7	36	-72	-5	9	7	36	-72	-5	12	7	37	-74
2	2	7	438	8	2	4	7	307	10	5	6	7	37	-74	-4	9	7	36	-71	-4	12	7	167	17
3	2	7	35	-69	3	4	7	99	26	-9	7	7	37	-75	-3	9	7	127	20	-3	12	7	36	-72
4	2	7	35	-70	4	4	7	81	32	-8	7	7	37	-73	-2	9	7	66	-37	-2	12	7	99	29
5	2	7	120	23	5	4	7	112	24	-7	7	7	101	26	-1	9	7	73	24	-1	12	7	85	21
6	2	7	38	-76	-10	5	7	94	31	-6	7	7	36	-72	0	9	7	146	12	0	12	7	71	-30
-10	3	7	158	18	-9	5	7	37	-74	-5	7	7	198	14	1	9	7	72	24	1	12	7	99	20
-9	3	7	65	-41	-8	5	7	36	-72	-4	7	7	112	21	2	9	7	35	-70	2	12	7	141	20
-8	3	7	77	-33	-7	5	7	79	-33	-3	7	7	886	2	3	9	7	36	-72	-5	13	7	38	-76
-7	3	7	123	20	-6	5	7	150	17	-2	7	7	379	8	4	9	7	168	17	-4	13	7	76	-37
-6	3	7	34	-68	-5	5	7	139	18	-1	7	7	121	26	-8	10	7	95	30	-3	13	7	235	12
-5	3	7	600	7	-4	5	7	172	14	0	7	7	58	-32	-7	10	7	70	-40	-2	13	7	116	24
-4	3	7	31	-62	-3	5	7	659	7	1	7	7	121	22	-6	10	7	95	29	-1	13	7	107	21
-3	3	7	144	14	-2	5	7	306	9	2	7	7	35	-70	-5	10	7	36	-72	0	13	7	102	27
-2	3	7	265	9	-1	5	7	289	10	3	7	7	271	11	-4	10	7	80	32	-10	0	8	90	31
-1	3	7	460	9	0	5	7	160	14	4	7	7	115	23	-3	10	7	35	-70	-9	0	8	36	-72
0	3	7	85	23	1	5	7	180	10	5	7	7	38	-75	-2	10	7	35	-71	-8	0	8	61	-41
1	3	7	83	18	2	5	7	147	17	-9	8	7	69	-42	-1	10	7	58	-33	-7	0	8	35	-70
2	3	7	92	25	3	5	7	187	14	-8	8	7	37	-74	0	10	7	594	8	-6	0	8	303	9
3	3	7	35	-70	4	5	7	254	11	-7	8	7	205	14	1	10	7	102	25	-5	0	8	33	-66

Table 28. (Continued)

F(obs) and sigma(F) (-sigma = unobserved): Trimethylbenzene Thiourea Adduct

h	k	l	10Fo	10s	h	k	l	10Fo	10s	h	k	l	10Fo	10s	h	k	l	10Fo	10s	h	k	l	10Fo	10s
-7	3	6	350	9	-7	5	6	145	18	-6	7	6	35	-71	-1	9	6	94	24	-3	12	6	95	26
-6	3	6	251	10	-6	5	6	140	17	-5	7	6	35	-69	0	9	6	34	-48	-2	12	6	167	16
-5	3	6	51	-39	-5	5	6	79	29	-4	7	6	157	16	1	9	6	233	9	-1	12	6	35	-71
-4	3	6	167	12	-4	5	6	121	18	-3	7	6	34	-68	2	9	6	286	10	0	12	6	63	-28
-3	3	6	165	11	-3	5	6	30	-61	-2	7	6	96	24	3	9	6	72	-34	1	12	6	107	18
-2	3	6	538	6	-2	5	6	388	7	-1	7	6	221	8	4	9	6	36	-72	2	12	6	36	-73
-1	3	6	430	6	-1	5	6	151	22	0	7	6	33	-46	5	9	6	153	19	3	12	6	99	27
0	3	6	347	5	0	5	6	561	6	1	7	6	588	11	-8	10	6	56	-52	-5	13	6	38	-75
1	3	6	138	17	1	5	6	229	8	2	7	6	77	30	-7	10	6	37	-74	-4	13	6	37	-74
2	3	6	241	11	2	5	6	183	13	3	7	6	65	-38	-6	10	6	149	18	-3	13	6	113	23
3	3	6	477	8	3	5	6	98	25	4	7	6	117	22	-5	10	6	114	23	-2	13	6	36	-73
4	3	6	35	-70	4	5	6	86	29	5	7	6	84	33	-4	10	6	82	31	-1	13	6	77	29
5	3	6	36	-72	5	5	6	36	-73	-9	8	6	38	-76	-3	10	6	116	22	0	13	6	149	13
6	3	6	96	28	6	5	6	152	19	-8	8	6	63	-44	-2	10	6	448	8	1	13	6	213	10
-10	4	6	88	32	-10	6	6	72	-41	-7	8	6	150	18	-1	10	6	118	15	2	13	6	102	27
-9	4	6	120	22	-9	6	6	75	-37	-6	8	6	36	-72	0	10	6	122	16	-4	14	6	127	23
-8	4	6	36	-72	-8	6	6	65	-41	-5	8	6	309	10	1	10	6	110	16	-3	14	6	157	18
-7	4	6	186	15	-7	6	6	196	14	-4	8	6	69	-35	2	10	6	139	18	-2	14	6	96	29
-6	4	6	279	9	-6	6	6	86	28	-3	8	6	34	-67	3	10	6	128	20	-1	14	6	78	27
-5	4	6	32	-65	-5	6	6	359	8	-2	8	6	565	7	4	10	6	152	18	0	14	6	74	-31
-4	4	6	199	10	-4	6	6	429	7	-1	8	6	84	24	-7	11	6	38	-75	-10	1	7	130	16
-3	4	6	29	-59	-3	6	6	32	-63	0	8	6	71	22	-6	11	6	37	-74	-9	1	7	36	-51
-2	4	6	499	6	-2	6	6	78	25	1	8	6	164	11	-5	11	6	145	18	-8	1	7	96	27
-1	4	6	145	10	-1	6	6	405	5	2	8	6	35	-70	-4	11	6	36	-71	-7	1	7	134	23
0	4	6	183	8	0	6	6	161	10	3	8	6	111	22	-3	11	6	35	-70	-6	1	7	136	13
1	4	6	57	-24	1	6	6	97	25	4	8	6	176	15	-2	11	6	440	8	-5	1	7	417	57
2	4	6	93	24	2	6	6	120	20	5	8	6	301	11	-1	11	6	108	22	-4	1	7	158	9
3	4	6	570	7	3	6	6	35	-70	-8	9	6	98	29	0	11	6	144	13	-3	1	7	67	23
4	4	6	35	-70	4	6	6	103	24	-7	9	6	123	22	1	11	6	292	8	-2	1	7	268	10
5	4	6	93	28	5	6	6	471	8	-6	9	6	133	20	2	11	6	36	-71	-1	1	7	483	8
6	4	6	163	18	6	6	6	120	24	-5	9	6	127	21	3	11	6	36	-72	0	1	7	60	19
-10	5	6	122	24	-9	7	6	238	13	-4	9	6	246	11	-6	12	6	140	20	1	1	7	76	18
-9	5	6	170	17	-8	7	6	37	-73	-3	9	6	91	26	-5	12	6	243	12	2	1	7	443	7
-8	5	6	70	-37	-7	7	6	75	-36	-2	9	6	697	8	-4	12	6	64	-42	3	1	7	74	23

Table 28. (Continued)

F(obs) and sigma(F) (-sigma = unobserved): Trimethylbenzene Thiourea Adduct

h	k	l	10Fo	10s	h	k	l	10Fo	10s	h	k	l	10Fo	10s	h	k	l	10Fo	10s	h	k	l	10Fo	10s
-4	6	5	481	7	-2	8	5	108	20	2	10	5	397	9	0	13	5	60	-33	-6	1	6	278	45
-3	6	5	141	14	-1	8	5	780	6	3	10	5	177	15	1	13	5	82	23	-5	1	6	90	19
-2	6	5	293	8	0	8	5	108	14	4	10	5	36	-72	2	13	5	130	21	-4	1	6	84	15
-1	6	5	813	10	1	8	5	97	21	5	10	5	71	-39	3	13	5	125	22	-3	1	6	73	20
0	6	5	45	-31	2	8	5	169	15	-7	11	5	37	-75	-5	14	5	38	-76	-2	1	6	179	7
1	6	5	314	6	3	8	5	59	-42	-6	11	5	111	24	-4	14	5	63	-44	-1	1	6	49	-20
2	6	5	150	15	4	8	5	35	-71	-5	11	5	90	29	-3	14	5	62	-42	0	1	6	1531	18
3	6	5	142	17	5	8	5	36	-72	-4	11	5	328	9	-2	14	5	160	18	1	1	6	289	4
4	6	5	124	20	6	8	5	184	16	-3	11	5	68	-37	-1	14	5	177	11	2	1	6	183	9
5	6	5	74	-35	-9	9	5	38	-76	-2	11	5	102	24	0	14	5	79	29	3	1	6	384	6
6	6	5	98	29	-8	9	5	119	24	-1	11	5	158	11	1	14	5	53	-39	4	1	6	35	-49
-9	7	5	123	23	-7	9	5	154	18	0	11	5	68	-30	-2	15	5	109	25	5	1	6	62	-33
-8	7	5	36	-73	-6	9	5	201	14	1	11	5	56	-34	-1	15	5	67	-32	6	1	6	148	24
-7	7	5	245	12	-5	9	5	317	10	2	11	5	185	14	-10	0	6	37	-74	7	1	6	49	-44
-6	7	5	77	-32	-4	9	5	591	8	3	11	5	202	13	-9	0	6	70	-36	-10	2	6	37	-74
-5	7	5	115	20	-3	9	5	34	-68	4	11	5	54	-50	-8	0	6	78	-32	-9	2	6	102	26
-4	7	5	272	10	-2	9	5	70	-32	-7	12	5	129	23	-7	0	6	34	-67	-8	2	6	35	-71
-3	7	5	181	12	-1	9	5	76	21	-6	12	5	100	27	-6	0	6	119	18	-7	2	6	296	10
-2	7	5	166	13	0	9	5	141	12	-5	12	5	36	-73	-5	0	6	30	-60	-6	2	6	108	20
-1	7	5	223	8	1	9	5	68	-28	-4	12	5	36	-72	-3	0	6	28	-56	-5	2	6	431	7
0	7	5	469	9	2	9	5	408	8	-3	12	5	35	-70	-2	0	6	73	22	-4	2	6	716	6
1	7	5	120	26	3	9	5	181	14	-2	12	5	154	17	-1	0	6	27	-39	-3	2	6	344	7
2	7	5	33	-66	4	9	5	35	-71	-1	12	5	479	13	0	0	6	320	15	-2	2	6	223	8
3	7	5	438	8	5	9	5	37	-74	0	12	5	47	-38	1	0	6	38	-34	-1	2	6	300	10
4	7	5	212	13	-8	10	5	121	24	1	12	5	83	26	2	0	6	65	-32	0	2	6	184	26
5	7	5	36	-72	-7	10	5	139	20	2	12	5	139	19	3	0	6	140	18	1	2	6	206	13
6	7	5	55	-52	-6	10	5	107	25	3	12	5	63	-42	4	0	6	35	-70	2	2	6	103	20
-9	8	5	126	22	-5	10	5	190	15	4	12	5	37	-75	5	0	6	36	-72	3	2	6	868	9
-8	8	5	77	-35	-4	10	5	108	24	-6	13	5	114	25	6	0	6	409	9	4	2	6	177	15
-7	8	5	36	-72	-3	10	5	49	-48	-5	13	5	63	-44	7	0	6	67	-43	5	2	6	58	-45
-6	8	5	154	17	-2	10	5	34	-68	-4	13	5	74	-37	-10	1	6	139	15	6	2	6	120	23
-5	8	5	35	-69	-1	10	5	231	8	-3	13	5	35	-71	-9	1	6	138	15	-10	3	6	37	-74
-4	8	5	34	-67	0	10	5	249	8	-2	13	5	134	20	-8	1	6	35	-50	-9	3	6	112	23
-3	8	5	177	13	1	10	5	102	20	-1	13	5	35	-50	-7	1	6	61	-28	-8	3	6	158	17

Table 28. (Continued)

F(obs) and sigma(F) (-sigma = unobserved): Trimethylbenzene Thiourea Adduct

h	k	l	10Fo	10s	h	k	l	10Fo	10s	h	k	l	10Fo	10s	h	k	l	10Fo	10s	h	k	l	10Fo	10s
0	1	12	52	-29	-6	3	12	141	20	-4	4	12	129	21	-6	6	12	38	-76	-4	1	13	126	21
-7	2	12	83	-34	-5	3	12	37	-74	-3	4	12	37	-73	-5	6	12	105	27	-3	1	13	37	-53
-6	2	12	174	16	-4	3	12	144	19	-2	4	12	153	18	-4	6	12	38	-75	-2	1	13	165	15
-5	2	12	37	-73	-3	3	12	37	-73	-1	4	12	219	10	-3	6	12	54	-51	-5	2	13	186	16
-4	2	12	97	28	-2	3	12	125	23	-6	5	12	152	20	-2	6	12	87	33	-4	2	13	38	-75
-3	2	12	36	-72	-1	3	12	201	10	-5	5	12	38	-76	-4	7	12	80	-36	-3	2	13	93	29
-2	2	12	37	-73	0	3	12	96	20	-4	5	12	174	17	-3	7	12	80	-36	-5	3	13	60	-49
-1	2	12	296	7	-7	4	12	95	31	-3	5	12	115	24	-6	1	13	38	-53	-4	3	13	38	-76
0	2	12	36	-52	-6	4	12	145	20	-2	5	12	37	-74	-5	1	13	73	-33	-3	3	13	38	-76
-7	3	12	68	-42	-5	4	12	38	-75	-1	5	12	178	12										

Table 28. (Continued)

F(obs) and sigma(F) (-sigma = unobserved): Trimethylbenzene Thiourea Adduct

h	k	l	10Fo	10s	h	k	l	10Fo	10s	h	k	l	10Fo	10s	h	k	l	10Fo	10s	h	k	l	10Fo	10s
0	7	2	492	4	0	9	2	371	5	3	11	2	132	19	0	14	2	69	27	-9	2	3	64	-41
1	7	2	67	22	1	9	2	184	8	4	11	2	85	31	1	14	2	126	17	-8	2	3	111	23
2	7	2	122	15	2	9	2	122	19	5	11	2	36	-72	2	14	2	97	26	-7	2	3	109	22
3	7	2	391	7	3	9	2	136	17	6	11	2	301	11	3	14	2	36	-72	-6	2	3	74	26
4	7	2	121	20	4	9	2	75	-32	-7	12	2	127	23	4	14	2	145	20	-5	2	3	289	7
5	7	2	95	26	5	9	2	36	-72	-6	12	2	100	27	-4	15	2	137	21	-4	2	3	448	5
6	7	2	136	20	6	9	2	543	8	-5	12	2	36	-72	-3	15	2	104	26	-3	2	3	372	6
7	7	2	37	-73	7	9	2	38	-75	-4	12	2	84	30	-2	15	2	36	-73	-1	2	3	70	16
8	7	2	38	-76	-8	10	2	38	-76	-3	12	2	35	-70	-1	15	2	71	-30	0	2	3	888	5
-9	8	2	80	-37	-7	10	2	37	-73	-2	12	2	67	-37	0	15	2	108	26	1	2	3	96	12
-8	8	2	144	19	-6	10	2	36	-72	-1	12	2	345	9	1	15	2	56	-36	2	2	3	236	8
-7	8	2	309	10	-5	10	2	112	23	0	12	2	177	10	2	15	2	36	-73	3	2	3	357	7
-6	8	2	87	30	-4	10	2	307	9	1	12	2	147	27	3	15	2	128	21	4	2	3	208	10
-5	8	2	34	-69	-3	10	2	82	27	2	12	2	86	29	-2	16	2	73	-38	5	2	3	221	11
-4	8	2	189	12	-2	10	2	398	8	3	12	2	414	8	-1	16	2	63	-34	6	2	3	92	27
-3	8	2	31	-62	-1	10	2	273	7	4	12	2	36	-71	0	16	2	37	-52	7	2	3	410	9
-2	8	2	157	12	0	10	2	356	5	5	12	2	37	-74	-10	1	3	104	22	8	2	3	81	-34
-1	8	2	546	6	1	10	2	135	28	-6	13	2	73	-38	-9	1	3	101	26	-10	3	3	74	-37
0	8	2	342	5	2	10	2	489	8	-5	13	2	96	28	-8	1	3	144	13	-9	3	3	121	22
1	8	2	248	7	3	10	2	224	12	-4	13	2	107	24	-7	1	3	482	13	-8	3	3	141	19
2	8	2	31	-62	4	10	2	122	21	-3	13	2	35	-70	-6	1	3	78	23	-7	3	3	779	7
3	8	2	568	8	5	10	2	61	-42	-2	13	2	293	10	-5	1	3	504	34	-6	3	3	32	-64
4	8	2	34	-68	6	10	2	94	30	-1	13	2	269	9	-3	1	3	710	12	-5	3	3	29	-58
5	8	2	35	-71	7	10	2	87	33	0	13	2	172	10	-2	1	3	140	11	-2	3	3	518	6
6	8	2	111	24	-7	11	2	37	-74	1	13	2	35	-49	-1	1	3	476	12	-1	3	3	69	20
7	8	2	97	28	-6	11	2	36	-72	2	13	2	108	23	1	1	3	563	8	0	3	3	121	9
-8	9	2	78	-35	-5	11	2	36	-72	3	13	2	140	19	2	1	3	27	-38	2	3	3	789	6
-7	9	2	197	14	-4	11	2	372	9	4	13	2	161	17	3	1	3	534	7	4	3	3	196	11
-6	9	2	71	-37	-3	11	2	73	-32	5	13	2	90	31	4	1	3	261	7	5	3	3	102	24
-5	9	2	35	-70	-2	11	2	119	20	-5	14	2	157	18	5	1	3	220	8	6	3	3	35	-70
-4	9	2	677	7	-1	11	2	110	14	-4	14	2	37	-74	6	1	3	167	12	7	3	3	83	32
-3	9	2	32	-64	0	11	2	57	-28	-3	14	2	124	21	7	1	3	121	26	8	3	3	95	30
-2	9	2	209	11	1	11	2	172	10	-2	14	2	74	-34	8	1	3	92	28	-10	4	3	79	-37
-1	9	2	499	6	2	11	2	93	26	-1	14	2	120	21	-10	2	3	142	21	-9	4	3	64	-41

Table 28. (Continued)

F(obs) and sigma(F) (-sigma = unobserved): Trimethylbenzene Thiourea Adduct

h	k	l	10Fo	10s	h	k	l	10Fo	10s	h	k	l	10Fo	10s	h	k	l	10Fo	10s	h	k	l	10Fo	10s
-8	4	3	87	30	-9	6	3	203	14	7	7	3	68	-40	-8	10	3	79	-36	-2	12	3	223	13
-7	4	3	127	19	-8	6	3	151	18	-9	8	3	116	25	-7	10	3	36	-73	-1	12	3	133	25
-6	4	3	97	22	-7	6	3	244	12	-8	8	3	163	17	-6	10	3	36	-72	0	12	3	247	11
-5	4	3	376	7	-6	6	3	104	23	-7	8	3	97	27	-5	10	3	128	20	1	12	3	150	12
-4	4	3	221	9	-5	6	3	313	9	-6	8	3	35	-70	-4	10	3	35	-69	2	12	3	221	12
-3	4	3	462	5	-4	6	3	220	9	-5	8	3	317	9	-3	10	3	101	22	3	12	3	35	-70
-1	4	3	80	18	-3	6	3	844	7	-4	8	3	107	21	-2	10	3	864	7	4	12	3	68	-38
0	4	3	781	14	-2	6	3	701	7	-3	8	3	57	-34	-1	10	3	147	10	5	12	3	215	14
1	4	3	160	7	-1	6	3	81	17	-2	8	3	786	7	0	10	3	94	18	-6	13	3	81	-35
2	4	3	202	9	0	6	3	769	14	-1	8	3	105	13	1	10	3	152	20	-5	13	3	182	16
3	4	3	128	15	1	6	3	272	6	0	8	3	133	10	2	10	3	86	27	-4	13	3	62	-41
4	4	3	165	13	2	6	3	64	-27	1	8	3	411	5	3	10	3	101	24	-3	13	3	89	28
5	4	3	110	22	3	6	3	113	18	2	8	3	83	25	4	10	3	87	29	-2	13	3	79	32
6	4	3	255	11	4	6	3	112	21	3	8	3	134	17	5	10	3	83	32	-1	13	3	57	-33
7	4	3	328	10	5	6	3	542	8	4	8	3	158	17	6	10	3	37	-75	0	13	3	168	18
8	4	3	241	13	6	6	3	194	14	5	8	3	390	9	-7	11	3	129	22	1	13	3	184	10
-10	5	3	75	-39	7	6	3	87	31	6	8	3	36	-72	-6	11	3	193	14	2	13	3	52	-48
-9	5	3	97	28	8	6	3	184	16	7	8	3	38	-75	-5	11	3	296	10	3	13	3	112	23
-8	5	3	295	11	-9	7	3	206	14	-8	9	3	128	22	-4	11	3	63	-39	4	13	3	109	25
-7	5	3	237	12	-8	7	3	99	27	-7	9	3	106	24	-3	11	3	34	-69	-5	14	3	118	24
-6	5	3	125	18	-7	7	3	158	17	-6	9	3	113	23	-2	11	3	123	20	-4	14	3	61	-45
-5	5	3	452	7	-6	7	3	35	-69	-5	9	3	160	16	-1	11	3	120	14	-3	14	3	91	28
-3	5	3	153	10	-5	7	3	489	7	-4	9	3	34	-67	0	11	3	103	21	-2	14	3	193	14
-2	5	3	543	6	-4	7	3	146	15	-3	9	3	238	10	1	11	3	364	8	-1	14	3	35	-49
-1	5	3	127	8	-3	7	3	620	6	-2	9	3	32	-64	2	11	3	378	9	0	14	3	188	10
0	5	3	1019	10	-2	7	3	30	-59	-1	9	3	206	18	3	11	3	35	-69	1	14	3	124	16
1	5	3	132	8	-1	7	3	205	7	0	9	3	43	-34	4	11	3	134	19	2	14	3	136	20
2	5	3	269	8	0	7	3	298	5	1	9	3	230	7	5	11	3	283	11	3	14	3	62	-44
3	5	3	255	9	1	7	3	640	12	2	9	3	659	7	6	11	3	89	32	-4	15	3	38	-75
4	5	3	49	-43	2	7	3	81	25	3	9	3	81	28	-7	12	3	74	-39	-3	15	3	107	25
5	5	3	173	14	3	7	3	296	9	4	9	3	35	-71	-6	12	3	37	-74	-2	15	3	36	-73
6	5	3	76	-34	4	7	3	270	10	5	9	3	118	22	-5	12	3	181	15	-1	15	3	106	17
7	5	3	136	20	5	7	3	365	9	6	9	3	37	-73	-4	12	3	175	15	0	15	3	150	14
8	5	3	73	-39	6	7	3	36	-71	7	9	3	38	-76	-3	12	3	115	22	1	15	3	36	-51

Table 28. (Continued)

F(obs) and sigma(F) (-sigma = unobserved): Trimethylbenzene Thiourea Adduct

h	k	l	10Fo	10s	h	k	l	10Fo	10s	h	k	l	10Fo	10s	h	k	l	10Fo	10s	h	k	l	10Fo	10s
2	15	3	37	-74	4	1	4	32	-45	1	3	4	377	4	-2	5	4	170	10	-3	7	4	993	7
-10	0	4	161	18	5	1	4	275	13	2	3	4	117	15	-1	5	4	524	4	-2	7	4	115	15
-9	0	4	64	-40	6	1	4	283	14	3	3	4	52	-35	0	5	4	384	5	-1	7	4	233	6
-8	0	4	607	7	7	1	4	158	14	4	3	4	132	18	1	5	4	461	4	0	7	4	54	-26
-7	0	4	33	-66	8	1	4	87	25	5	3	4	425	9	2	5	4	502	6	1	7	4	392	11
-6	0	4	300	8	-10	2	4	158	18	6	3	4	151	17	3	5	4	80	27	2	7	4	68	-31
-5	0	4	28	-56	-9	2	4	96	27	7	3	4	149	19	4	5	4	184	14	3	7	4	83	27
-4	0	4	135	11	-8	2	4	232	12	8	3	4	38	-76	5	5	4	151	17	4	7	4	66	-37
-3	0	4	26	-53	-7	2	4	190	13	-10	4	4	38	-76	6	5	4	36	-72	5	7	4	107	25
-2	0	4	300	7	-6	2	4	168	13	-9	4	4	88	30	7	5	4	211	14	6	7	4	86	31
-1	0	4	55	19	-5	2	4	584	6	-8	4	4	228	12	-10	6	4	86	34	7	7	4	338	11
0	0	4	824	9	-4	2	4	41	-37	-7	4	4	34	-69	-9	6	4	95	29	-9	8	4	71	-40
1	0	4	26	-37	-3	2	4	43	-34	-6	4	4	382	8	-8	6	4	186	15	-8	8	4	37	-73
2	0	4	882	8	-2	2	4	462	6	-5	4	4	786	7	-7	6	4	108	24	-7	8	4	171	16
3	0	4	29	-58	-1	2	4	285	10	-4	4	4	247	8	-6	6	4	98	24	-6	8	4	272	11
4	0	4	237	10	0	2	4	182	9	-3	4	4	707	6	-5	6	4	32	-65	-5	8	4	81	39
5	0	4	109	22	1	2	4	26	-37	-2	4	4	433	6	-4	6	4	30	-61	-4	8	4	33	-66
6	0	4	253	12	2	2	4	433	6	-1	4	4	359	14	-3	6	4	680	7	-3	8	4	366	8
7	0	4	36	-73	3	2	4	51	-35	0	4	4	278	5	-2	6	4	90	19	-2	8	4	57	-34
8	0	4	38	-76	4	2	4	137	16	1	4	4	630	4	-1	6	4	72	16	-1	8	4	138	10
-10	1	4	83	30	5	2	4	529	8	2	4	4	1074	8	0	6	4	55	-23	0	8	4	106	14
-9	1	4	97	19	6	2	4	36	-72	3	4	4	348	7	1	6	4	260	7	1	8	4	605	12
-8	1	4	544	15	7	2	4	36	-73	4	4	4	424	8	2	6	4	868	8	2	8	4	33	-66
-7	1	4	73	23	8	2	4	38	-75	5	4	4	316	10	3	6	4	297	9	3	8	4	453	8
-6	1	4	32	-45	-10	3	4	211	14	6	4	4	147	18	4	6	4	244	11	4	8	4	358	9
-5	1	4	404	44	-9	3	4	121	22	7	4	4	163	18	5	6	4	63	-40	5	8	4	36	-72
-4	1	4	319	9	-8	3	4	229	13	-10	5	4	167	18	6	6	4	81	32	6	8	4	81	-34
-3	1	4	296	7	-7	3	4	34	-68	-9	5	4	36	-73	7	6	4	81	-35	-9	9	4	131	23
-2	1	4	971	7	-6	3	4	134	17	-8	5	4	122	22	-9	7	4	53	-53	-8	9	4	37	-74
-1	1	4	1111	6	-5	3	4	149	13	-7	5	4	35	-70	-8	7	4	131	20	-7	9	4	36	-72
0	1	4	585	4	-4	3	4	466	6	-6	5	4	218	11	-7	7	4	36	-71	-6	9	4	36	-73
1	1	4	127	6	-3	3	4	531	6	-5	5	4	192	12	-6	7	4	148	17	-5	9	4	82	30
2	1	4	345	6	-1	3	4	1753	6	-4	5	4	76	23	-5	7	4	109	21	-4	9	4	34	-68
3	1	4	73	22	0	3	4	502	11	-3	5	4	439	6	-4	7	4	462	7	-3	9	4	279	10

Table 28. (Continued)

F(obs) and sigma(F) (-sigma = unobserved): Trimethylbenzene Thiourea Adduct

h	k	l	10Fo	10s	h	k	l	10Fo	10s	h	k	l	10Fo	10s	h	k	l	10Fo	10s	h	k	l	10Fo	10s
-2	9	4	47	-45	2	11	4	53	-46	2	14	4	197	15	0	2	5	843	9	-2	4	5	470	6
-1	9	4	94	20	3	11	4	107	23	-3	15	4	37	-73	1	2	5	975	15	-1	4	5	43	-28
0	9	4	614	6	4	11	4	167	16	-2	15	4	37	-74	2	2	5	151	12	0	4	5	278	5
1	9	4	86	25	5	11	4	77	-36	-1	15	4	198	10	3	2	5	118	17	1	4	5	703	6
2	9	4	62	-38	-7	12	4	113	25	0	15	4	67	-34	4	2	5	54	-44	2	4	5	127	16
3	9	4	247	11	-6	12	4	65	-42	1	15	4	56	-37	5	2	5	74	-34	3	4	5	54	-40
4	9	4	69	-37	-5	12	4	117	22	-10	1	5	37	-52	6	2	5	220	13	4	4	5	35	-69
5	9	4	36	-72	-4	12	4	214	13	-9	1	5	36	-51	7	2	5	170	17	5	4	5	57	-45
6	9	4	37	-75	-3	12	4	328	9	-8	1	5	173	11	-10	3	5	78	-36	6	4	5	292	11
-8	10	4	143	20	-2	12	4	76	-33	-7	1	5	103	16	-9	3	5	37	-73	7	4	5	144	20
-7	10	4	37	-73	-1	12	4	120	23	-6	1	5	619	83	-8	3	5	79	-32	-10	5	5	38	-76
-6	10	4	403	8	0	12	4	149	12	-5	1	5	219	19	-7	3	5	88	27	-9	5	5	37	-73
-5	10	4	75	-34	1	12	4	153	22	-4	1	5	542	27	-6	3	5	33	-65	-8	5	5	123	21
-4	10	4	35	-69	2	12	4	63	-40	-3	1	5	325	6	-5	3	5	372	7	-7	5	5	77	-33
-3	10	4	34	-68	3	12	4	188	14	-2	1	5	386	9	-4	3	5	271	8	-6	5	5	456	7
-2	10	4	60	-38	4	12	4	37	-74	-1	1	5	386	5	-3	3	5	811	7	-5	5	5	236	10
-1	10	4	81	20	-6	13	4	38	-75	0	1	5	95	14	-2	3	5	131	12	-4	5	5	227	9
0	10	4	355	6	-5	13	4	112	24	1	1	5	287	4	-1	3	5	215	7	-3	5	5	641	7
1	10	4	128	13	-4	13	4	36	-72	2	1	5	50	-24	0	3	5	182	11	-2	5	5	207	9
2	10	4	90	27	-3	13	4	279	10	3	1	5	173	10	1	3	5	1112	17	-1	5	5	237	8
3	10	4	35	-70	-2	13	4	36	-71	4	1	5	990	3	2	3	5	365	7	0	5	5	59	23
4	10	4	432	8	-1	13	4	35	-49	5	1	5	122	15	3	3	5	144	16	1	5	5	191	7
5	10	4	37	-73	0	13	4	35	-49	6	1	5	36	-51	4	3	5	91	26	2	5	5	217	11
6	10	4	96	30	1	13	4	93	24	7	1	5	130	15	5	3	5	60	-42	3	5	5	197	12
-8	11	4	87	34	2	13	4	55	-47	-10	2	5	37	-74	6	3	5	146	19	4	5	5	466	8
-7	11	4	37	-75	3	13	4	36	-73	-9	2	5	323	10	7	3	5	117	24	5	5	5	36	-72
-6	11	4	36	-73	4	13	4	38	-75	-8	2	5	74	-35	-10	4	5	80	-35	6	5	5	355	9
-5	11	4	175	15	-5	14	4	38	-75	-7	2	5	34	-68	-9	4	5	263	11	7	5	5	38	-75
-4	11	4	167	16	-4	14	4	113	24	-6	2	5	255	9	-8	4	5	143	19	-10	6	5	77	-38
-3	11	4	291	10	-3	14	4	111	24	-5	2	5	152	12	-7	4	5	235	12	-9	6	5	37	-74
-2	11	4	78	31	-2	14	4	36	-71	-4	2	5	183	10	-6	4	5	34	-68	-8	6	5	56	-46
-1	11	4	159	11	-1	14	4	137	17	-3	2	5	777	7	-5	4	5	125	17	-7	6	5	193	14
0	11	4	490	6	0	14	4	179	11	-2	2	5	427	6	-4	4	5	416	6	-6	6	5	165	15
1	11	4	267	7	1	14	4	66	-27	-1	2	5	561	4	-3	4	5	375	6	-5	6	5	34	-68

Table 28. (Continued)

F(obs) and sigma(F) (-sigma = unobserved): Trimethylbenzene Thiourea Adduct

h	k	l	10Fo	10s	h	k	l	10Fo	10s	h	k	l	10Fo	10s	h	k	l	10Fo	10s	h	k	l	10Fo	10s
-4	13	1	115	22	-8	0	2	112	23	8	1	2	364	7	5	3	2	230	11	2	5	2	182	9
-3	13	1	107	23	-7	0	2	77	29	9	1	2	90	23	6	3	2	406	8	3	5	2	169	11
-2	13	1	175	15	-6	0	2	655	7	-10	2	2	69	-41	7	3	2	170	16	4	5	2	286	9
-1	13	1	99	18	-5	0	2	27	-55	-9	2	2	422	9	8	3	2	69	-39	5	5	2	35	-69
0	13	1	34	-49	-4	0	2	88	16	-7	2	2	187	14	9	3	2	85	-35	6	5	2	469	8
1	13	1	282	7	-3	0	2	54	-26	-6	2	2	294	8	-10	4	2	38	-76	7	5	2	62	-42
2	13	1	253	11	-1	0	2	18	-25	-5	2	2	256	8	-9	4	2	253	12	8	5	2	197	15
3	13	1	83	30	0	0	2	229	4	-4	2	2	583	6	-8	4	2	61	-43	-9	6	2	37	-74
4	13	1	158	17	1	0	2	162	5	-3	2	2	653	6	-7	4	2	36	-72	-8	6	2	36	-72
5	13	1	140	20	2	0	2	570	6	-1	2	2	313	5	-6	4	2	283	9	-7	6	2	580	7
-5	14	1	55	-51	3	0	2	27	-54	0	2	2	787	4	-5	4	2	350	7	-6	6	2	369	8
-4	14	1	141	20	4	0	2	979	8	1	2	2	2594	5	-4	4	2	312	6	-5	6	2	33	-66
-3	14	1	189	14	5	0	2	31	-63	2	2	2	1161	6	-3	4	2	522	6	-4	6	2	88	22
-2	14	1	35	-71	6	0	2	163	16	3	2	2	766	6	-2	4	2	492	6	-3	6	2	144	12
-1	14	1	158	11	7	0	2	66	-39	4	2	2	708	7	-1	4	2	69	19	-2	6	2	124	13
0	14	1	62	-32	8	0	2	350	10	5	2	2	32	-64	0	4	2	73	17	-1	6	2	1316	9
1	14	1	35	-49	9	0	2	38	-77	6	2	2	34	-69	1	4	2	1513	7	0	6	2	262	7
2	14	1	70	-36	-10	1	2	72	28	7	2	2	36	-71	2	4	2	679	6	1	6	2	155	16
3	14	1	36	-71	-9	1	2	136	14	8	2	2	259	12	3	4	2	53	-30	2	6	2	264	8
4	14	1	97	28	-8	1	2	103	26	9	2	2	154	20	4	4	2	383	7	3	6	2	314	8
-4	15	1	99	29	-7	1	2	137	12	-10	3	2	83	-35	5	4	2	402	22	4	6	2	362	8
-3	15	1	87	31	-6	1	2	411	16	-9	3	2	228	13	6	4	2	68	-36	5	6	2	341	9
-2	15	1	54	-49	-5	1	2	298	13	-8	3	2	78	-33	7	4	2	36	-72	6	6	2	181	15
-1	15	1	197	10	-4	1	2	163	7	-7	3	2	259	11	8	4	2	37	-74	7	6	2	36	-72
0	15	1	150	13	-3	1	2	861	6	-6	3	2	285	9	-10	5	2	77	-38	8	6	2	150	19
1	15	1	67	-32	-1	1	2	40	11	-5	3	2	307	7	-9	5	2	190	15	-9	7	2	107	27
2	15	1	176	16	0	1	2	300	5	-4	3	2	558	6	-8	5	2	61	-43	-8	7	2	59	-44
3	15	1	97	28	1	1	2	445	3	-3	3	2	916	7	-7	5	2	186	15	-7	7	2	69	-38
-2	16	1	37	-74	2	1	2	248	6	-1	3	2	72	14	-6	5	2	366	8	-6	7	2	35	-70
-1	16	1	178	11	3	1	2	64	17	0	3	2	306	5	-5	5	2	31	-61	-5	7	2	33	-67
0	16	1	54	-38	4	1	2	1289	13	1	3	2	404	5	-3	5	2	445	6	-4	7	2	32	-64
1	16	1	37	-52	5	1	2	223	8	2	3	2	384	6	-2	5	2	156	11	-3	7	2	205	9
-10	0	2	126	22	6	1	2	34	-48	3	3	2	241	7	-1	5	2	927	14	-2	7	2	901	7
-9	0	2	36	-72	7	1	2	136	14	4	3	2	221	9	1	5	2	294	5	-1	7	2	1331	7

Table 28. (Continued)

F(obs) and sigma(F) (-sigma = unobserved): Trimethylbenzene Thiourea Adduct

h	k	l	10Fo	10s	h	k	l	10Fo	10s	h	k	l	10Fo	10s	h	k	l	10Fo	10s	h	k	l	10Fo	10s
-9	3	1	181	16	7	4	1	59	-44	5	6	1	63	-37	4	8	1	546	7	5	10	1	70	-36
-8	3	1	36	-72	8	4	1	52	-50	6	6	1	262	12	5	8	1	131	19	6	10	1	36	-73
-7	3	1	134	19	9	4	1	89	32	7	6	1	396	9	6	8	1	65	-40	7	10	1	38	-75
-6	3	1	588	7	-9	5	1	37	-75	8	6	1	37	-74	7	8	1	394	9	-7	11	1	54	-52
-5	3	1	148	13	-8	5	1	303	10	-9	7	1	168	18	8	8	1	86	34	-6	11	1	144	19
-4	3	1	199	9	-7	5	1	35	-71	-8	7	1	214	14	-8	9	1	37	-75	-5	11	1	67	-39
-3	3	1	539	6	-6	5	1	490	7	-7	7	1	70	-37	-7	9	1	77	-35	-4	11	1	127	20
-1	3	1	3020	45	-5	5	1	168	13	-6	7	1	215	13	-6	9	1	380	9	-3	11	1	34	-68
0	3	1	246	4	-4	5	1	81	20	-5	7	1	57	-39	-5	9	1	183	15	-2	11	1	148	17
1	3	1	312	5	-3	5	1	104	15	-4	7	1	51	-40	-4	9	1	50	-45	-1	11	1	231	13
2	3	1	92	18	-2	5	1	114	14	-3	7	1	571	6	-3	9	1	59	-36	0	11	1	286	7
3	3	1	407	6	0	5	1	1290	5	-2	7	1	315	7	-2	9	1	167	13	1	11	1	335	6
4	3	1	297	7	1	5	1	761	10	-1	7	1	88	19	-1	9	1	30	-42	2	11	1	34	-68
5	3	1	210	11	2	5	1	927	7	0	7	1	382	12	0	9	1	743	9	3	11	1	35	-69
6	3	1	34	-68	3	5	1	29	-57	1	7	1	1065	24	1	9	1	154	10	4	11	1	217	13
7	3	1	129	20	4	5	1	48	-38	2	7	1	184	10	2	9	1	157	14	5	11	1	63	-41
8	3	1	71	-38	5	5	1	99	22	3	7	1	108	17	3	9	1	237	11	6	11	1	55	-49
9	3	1	348	10	6	5	1	35	-70	4	7	1	72	-31	4	9	1	446	8	7	11	1	111	27
-9	4	1	69	-40	7	5	1	305	10	5	7	1	86	27	5	9	1	125	20	-7	12	1	64	-46
-8	4	1	157	17	8	5	1	37	-74	6	7	1	231	12	6	9	1	36	-72	-6	12	1	87	32
-7	4	1	35	-69	9	5	1	125	24	7	7	1	251	12	7	9	1	62	-45	-5	12	1	100	26
-6	4	1	497	7	-9	6	1	130	22	8	7	1	37	-75	-8	10	1	96	30	-4	12	1	112	32
-5	4	1	272	8	-8	6	1	67	-39	-8	8	1	100	27	-7	10	1	70	-39	-3	12	1	444	8
-4	4	1	321	6	-7	6	1	111	23	-7	8	1	36	-72	-6	10	1	413	9	-2	12	1	117	21
-3	4	1	259	7	-6	6	1	301	10	-6	8	1	274	11	-5	10	1	36	-71	-1	12	1	45	-38
-2	4	1	363	6	-5	6	1	275	9	-5	8	1	85	28	-4	10	1	34	-69	0	12	1	88	19
-1	4	1	2598	5	-4	6	1	259	9	-4	8	1	92	23	-3	10	1	89	25	1	12	1	110	17
0	4	1	710	4	-2	6	1	121	13	-3	8	1	934	8	-2	10	1	117	19	2	12	1	74	-33
1	4	1	247	6	-1	6	1	26	-37	-2	8	1	402	7	-1	10	1	85	26	3	12	1	35	-70
2	4	1	380	6	0	6	1	655	5	-1	8	1	115	11	0	10	1	65	-26	4	12	1	147	18
3	4	1	510	6	1	6	1	157	12	0	8	1	416	5	1	10	1	218	8	5	12	1	131	21
4	4	1	439	7	2	6	1	277	7	1	8	1	237	6	2	10	1	83	27	6	12	1	37	-75
5	4	1	614	7	3	6	1	520	7	2	8	1	77	23	3	10	1	161	15	-6	13	1	38	-75
6	4	1	389	8	4	6	1	221	10	3	8	1	258	10	4	10	1	600	8	-5	13	1	37	-74

Table 28. (Continued)

F(obs) and sigma(F) (-sigma = unobserved): Trimethylbenzene Thiourea Adduct

h	k	l	10Fo	10s	h	k	l	10Fo	10s	h	k	l	10Fo	10s	h	k	l	10Fo	10s	h	k	l	10Fo	10s
2	0	0	800	5	8	3	0	53	-49	4	7	0	193	12	4	11	0	78	-32	-5	1	1	176	10
3	0	0	54	-27	9	3	0	67	-42	5	7	0	941	7	5	11	0	369	9	-4	1	1	91	21
4	0	0	188	9	0	4	0	938	6	6	7	0	78	-32	6	11	0	37	-73	-3	1	1	380	6
5	0	0	29	-57	1	4	0	1537	20	7	7	0	166	16	7	11	0	38	-76	-2	1	1	59	11
6	0	0	375	8	2	4	0	963	7	8	7	0	99	28	0	12	0	427	8	-1	1	1	564	19
7	0	0	35	-69	3	4	0	328	7	9	7	0	38	-76	1	12	0	160	18	1	1	1	268	3
8	0	0	143	18	4	4	0	68	24	0	8	0	595	6	2	12	0	156	16	2	1	1	2262	5
9	0	0	37	-73	5	4	0	31	-62	1	8	0	109	11	3	12	0	85	29	4	1	1	396	5
1	1	0	130	5	6	4	0	56	-43	2	8	0	897	7	4	12	0	35	-70	5	1	1	255	7
2	1	0	479	5	7	4	0	331	10	3	8	0	139	15	5	12	0	36	-73	6	1	1	85	19
3	1	0	983	17	8	4	0	339	9	4	8	0	352	8	6	12	0	156	18	7	1	1	35	-50
4	1	0	388	9	9	4	0	67	-42	5	8	0	35	-69	1	13	0	35	-49	8	1	1	128	15
5	1	0	267	6	1	5	0	314	5	6	8	0	92	28	2	13	0	35	-70	9	1	1	188	16
6	1	0	313	12	2	5	0	731	6	7	8	0	136	20	3	13	0	35	-70	-10	2	1	102	28
7	1	0	338	7	3	5	0	254	7	8	8	0	208	14	4	13	0	36	-72	-9	2	1	36	-72
8	1	0	151	13	4	5	0	403	6	1	9	0	100	13	5	13	0	237	13	-8	2	1	71	-36
9	1	0	72	27	5	5	0	561	7	2	9	0	572	7	6	13	0	69	-42	-7	2	1	78	31
0	2	0	669	4	6	5	0	34	-68	3	9	0	60	-36	0	14	0	246	11	-6	2	1	190	12
1	2	0	18	-26	7	5	0	36	-72	4	9	0	103	23	1	14	0	172	11	-5	2	1	629	6
2	2	0	147	9	8	5	0	180	16	5	9	0	268	11	2	14	0	136	19	-4	2	1	690	6
3	2	0	986	7	9	5	0	126	22	6	9	0	36	-72	3	14	0	58	-43	-3	2	1	465	6
4	2	0	27	-55	0	6	0	289	6	7	9	0	84	31	4	14	0	37	-73	-2	2	1	540	5
5	2	0	56	-31	1	6	0	230	8	8	9	0	38	-76	5	14	0	38	-76	-1	2	1	1377	4
6	2	0	33	-66	2	6	0	420	6	0	10	0	328	8	1	15	0	36	-50	0	2	1	18	-25
7	2	0	481	8	3	6	0	72	23	1	10	0	168	9	2	15	0	86	30	1	2	1	169	5
8	2	0	36	-72	4	6	0	226	9	2	10	0	629	7	3	15	0	207	14	2	2	1	537	6
9	2	0	94	29	5	6	0	256	11	3	10	0	33	-66	0	16	0	37	-73	3	2	1	546	6
1	3	0	48	19	6	6	0	53	-46	4	10	0	71	-34	1	16	0	37	-52	4	2	1	244	8
2	3	0	658	7	7	6	0	134	20	5	10	0	36	-72	2	16	0	37	-74	5	2	1	808	8
3	3	0	1369	7	8	6	0	118	23	6	10	0	80	-33	-10	1	1	69	-30	6	2	1	115	21
4	3	0	161	10	9	6	0	140	22	7	10	0	37	-74	-9	1	1	62	-31	7	2	1	296	10
5	3	0	213	10	1	7	0	169	7	1	11	0	216	8	-8	1	1	699	16	8	2	1	36	-72
6	3	0	34	-68	2	7	0	74	23	2	11	0	347	9	-7	1	1	34	-48	9	2	1	139	21
7	3	0	467	8	3	7	0	141	13	3	11	0	165	15	-6	1	1	458	12	-10	3	1	150	20

Table 29. Observed and calculated structure factors for the 1,2,4 TMB-thiourea adduct structure.

Observed and calculated structure factors: Trimethylbenzene Thiourea Adduct

h	k	l	10Fo	10Fc	h	k	l	10Fo	10Fc	h	k	l	10Fo	10Fc	h	k	l	10Fo	10Fc	h	k	l	10Fo	10Fc
-1	6	3	48	38	5	8	3	234	249	-3	12	3	69	51	-10	1	4	50	7	-4	3	4	279	326
0	6	3	461	429	-8	9	3	77	42	-2	12	3	134	139	-9	1	4	58	49	-3	3	4	319	332
1	6	3	163	177	-7	9	3	64	45	-1	12	3	80	80	-8	1	4	326	294	-1	3	4	1052	947
3	6	3	68	46	-6	9	3	68	55	0	12	3	148	153	-7	1	4	44	51	0	3	4	301	293
4	6	3	67	42	-5	9	3	96	87	1	12	3	90	87	-5	1	4	242	243	1	3	4	226	227
5	6	3	325	345	-3	9	3	143	147	2	12	3	132	148	-4	1	4	192	174	2	3	4	70	82
6	6	3	116	131	-1	9	3	124	117	5	12	3	129	124	-3	1	4	178	184	4	3	4	79	90
7	6	3	52	4	1	9	3	138	130	-5	13	3	109	121	-2	1	4	583	605	5	3	4	255	252
8	6	3	111	104	2	9	3	396	405	-3	13	3	53	54	-1	1	4	667	625	6	3	4	91	39
-9	7	3	124	115	3	9	3	49	32	-2	13	3	48	47	0	1	4	351	340	7	3	4	89	84
-8	7	3	59	19	5	9	3	71	60	0	13	3	101	99	1	1	4	76	76	-9	4	4	53	48
-7	7	3	95	81	-5	10	3	77	43	1	13	3	110	101	2	1	4	207	202	-8	4	4	137	138
-5	7	3	294	334	-3	10	3	60	11	3	13	3	67	53	3	1	4	44	19	-6	4	4	229	265
-4	7	3	88	80	-2	10	3	518	509	4	13	3	66	26	5	1	4	165	147	-5	4	4	472	569
-3	7	3	372	365	-1	10	3	88	79	-5	14	3	71	38	6	1	4	170	177	-4	4	4	148	157
-1	7	3	123	129	0	10	3	56	48	-3	14	3	54	43	7	1	4	95	106	-3	4	4	425	428
0	7	3	179	173	1	10	3	91	89	-2	14	3	116	106	8	1	4	52	54	-2	4	4	260	239
1	7	3	384	407	2	10	3	52	32	0	14	3	113	116	-10	2	4	95	59	-1	4	4	215	204
2	7	3	49	59	3	10	3	60	28	1	14	3	74	76	-9	2	4	57	35	0	4	4	167	170
3	7	3	177	190	4	10	3	52	37	2	14	3	81	85	-8	2	4	139	141	1	4	4	378	353
4	7	3	162	155	5	10	3	50	5	-3	15	3	64	59	-7	2	4	114	125	2	4	4	644	636
5	7	3	219	221	-7	11	3	77	77	-1	15	3	64	61	-6	2	4	101	143	3	4	4	209	208
-9	8	3	69	46	-6	11	3	116	88	0	15	3	90	93	-5	2	4	351	423	4	4	4	254	273
-8	8	3	98	102	-5	11	3	178	174	-10	0	4	95	65	-2	2	4	277	291	5	4	4	190	177
-7	8	3	58	27	-2	11	3	74	104	-8	0	4	364	359	-1	2	4	171	134	6	4	4	88	72
-5	8	3	191	184	-1	11	3	72	79	-6	0	4	180	200	0	2	4	109	101	7	4	4	98	86
-4	8	3	64	66	0	11	3	62	46	-4	0	4	81	100	2	2	4	260	274	-10	5	4	100	103
-2	8	3	471	463	1	11	3	219	236	-2	0	4	180	192	4	2	4	82	85	-8	5	4	73	73
-1	8	3	63	85	2	11	3	227	233	-1	0	4	33	0	5	2	4	317	331	-6	5	4	131	142
0	8	3	80	63	4	11	3	80	70	0	0	4	494	456	-10	3	4	127	106	-5	5	4	115	137
1	8	3	246	252	5	11	3	170	155	2	0	4	529	521	-9	3	4	72	41	-4	5	4	46	9
2	8	3	50	46	6	11	3	53	17	4	0	4	142	161	-8	3	4	137	147	-3	5	4	264	259
3	8	3	80	58	-5	12	3	108	111	5	0	4	66	0	-6	3	4	80	99	-2	5	4	102	95
4	8	3	95	118	-4	12	3	105	107	6	0	4	152	157	-5	3	4	89	113	-1	5	4	315	310

Table 29. (Continued)

Observed and calculated structure factors: Trimethylbenzene Thiourea Adduct

h	k	l	10Fo	10Fc	h	k	l	10Fo	10Fc	h	k	l	10Fo	10Fc	h	k	l	10Fo	10Fc	h	k	l	10Fo	10Fc
-2	6	2	74	73	-2	9	2	125	109	3	12	2	249	248	6	1	3	100	89	-4	4	3	133	167
-1	6	2	790	769	-1	9	2	299	287	-5	13	2	58	13	7	1	3	73	43	-3	4	3	277	271
0	6	2	157	179	0	9	2	222	213	-4	13	2	64	63	8	1	3	55	27	-1	4	3	48	28
1	6	2	93	79	1	9	2	110	102	-2	13	2	176	172	-10	2	3	85	67	0	4	3	469	444
2	6	2	158	153	2	9	2	73	77	-1	13	2	161	173	-8	2	3	67	51	1	4	3	96	109
3	6	2	188	192	3	9	2	82	74	0	13	2	103	115	-7	2	3	65	30	2	4	3	121	126
4	6	2	217	201	6	9	2	326	324	2	13	2	65	56	-6	2	3	45	20	3	4	3	77	32
5	6	2	205	214	-5	10	2	67	75	3	13	2	84	101	-5	2	3	173	198	4	4	3	99	92
6	6	2	109	96	-4	10	2	184	204	4	13	2	96	92	-4	2	3	269	288	5	4	3	66	53
8	6	2	90	89	-3	10	2	49	36	5	13	2	54	1	-3	2	3	223	246	6	4	3	153	152
-9	7	2	64	18	-2	10	2	239	247	-5	14	2	94	81	-1	2	3	42	91	7	4	3	197	198
-3	7	2	123	121	-1	10	2	164	155	-3	14	2	74	84	0	2	3	533	536	8	4	3	145	142
-2	7	2	541	490	0	10	2	213	212	-1	14	2	72	94	1	2	3	58	43	-9	5	3	58	46
-1	7	2	799	775	1	10	2	81	54	0	14	2	41	19	2	2	3	142	135	-8	5	3	177	171
0	7	2	296	284	2	10	2	294	300	1	14	2	76	76	3	2	3	214	208	-7	5	3	142	159
1	7	2	40	33	3	10	2	134	123	2	14	2	58	25	4	2	3	125	121	-6	5	3	75	45
2	7	2	73	80	4	10	2	73	102	4	14	2	87	107	5	2	3	132	135	-5	5	3	271	291
3	7	2	235	236	6	10	2	56	30	-4	15	2	82	79	6	2	3	55	53	-3	5	3	92	87
4	7	2	73	91	7	10	2	52	42	-3	15	2	62	47	7	2	3	246	243	-2	5	3	326	314
5	7	2	57	31	-4	11	2	223	214	0	15	2	65	40	-9	3	3	72	54	-1	5	3	76	80
6	7	2	82	71	-2	11	2	72	56	-3	15	2	77	71	-8	3	3	85	59	0	5	3	612	567
-8	8	2	87	72	-1	11	2	66	64	-10	1	3	63	68	-7	3	3	468	458	1	5	3	79	105
-7	8	2	185	201	1	11	2	103	96	-9	1	3	61	47	-2	3	3	311	284	2	5	3	161	189
-6	8	2	52	50	2	11	2	56	42	-8	1	3	87	89	-1	3	3	41	51	3	5	3	153	135
-4	8	2	113	112	3	11	2	79	69	-7	1	3	289	272	0	3	3	72	59	5	5	3	104	113
-2	8	2	94	100	4	11	2	51	43	-6	1	3	47	46	2	3	3	474	475	7	5	3	82	101
-1	8	2	328	325	6	11	2	180	177	-5	1	3	302	301	4	3	3	118	118	-9	6	3	122	93
0	8	2	206	205	-7	12	2	76	85	-3	1	3	426	403	5	3	3	61	105	-8	6	3	91	90
1	8	2	149	154	-6	12	2	60	50	-2	1	3	84	69	7	3	3	50	37	-7	6	3	146	111
3	8	2	341	349	-4	12	2	51	21	-1	1	3	286	199	8	3	3	57	56	-6	6	3	63	83
6	8	2	66	36	-1	12	2	207	216	1	1	3	338	336	-8	4	3	52	47	-5	6	3	188	211
7	8	2	58	24	0	12	2	106	110	3	1	3	320	324	-7	4	3	76	56	-4	6	3	132	131
-7	9	2	118	97	1	12	2	88	73	4	1	3	156	151	-6	4	3	58	46	-3	6	3	507	433
-4	9	2	406	408	2	12	2	52	46	-5	1	3	132	133	-5	4	3	225	246	-2	6	3	421	401

Table 29. (Continued)

Observed and calculated structure factors: Trimethylbenzene Thiourea Adduct

h	k	l	10Fo	10Fc	h	k	l	10Fo	10Fc	h	k	l	10Fo	10Fc	h	k	l	10Fo	10Fc	h	k	l	10Fo	10Fc
7	6	1	238	240	2	9	1	95	83	1	13	1	169	176	-3	1	2	516	507	2	3	2	231	231
-9	7	1	101	85	3	9	1	142	146	2	13	1	152	131	-1	1	2	24	4	3	3	2	145	143
-8	7	1	128	129	4	9	1	268	271	3	13	1	50	26	0	1	2	180	171	4	3	2	132	123
-6	7	1	129	128	5	9	1	75	67	4	13	1	95	80	1	1	2	267	232	5	3	2	138	167
-3	7	1	343	340	-8	10	1	58	31	5	13	1	84	75	2	1	2	149	155	6	3	2	244	243
-2	7	1	189	183	-6	10	1	248	243	-4	14	1	85	96	3	1	2	39	52	7	3	2	102	75
-1	7	1	53	6	-3	10	1	54	72	-3	14	1	113	134	4	1	2	774	693	-9	4	2	152	128
0	7	1	229	212	-2	10	1	70	67	-1	14	1	25	94	5	1	2	134	139	-6	4	2	170	188
1	7	1	639	615	-1	10	1	51	75	4	14	1	58	57	7	1	2	82	78	-5	4	2	210	198
2	7	1	110	117	1	10	1	131	130	-4	15	1	60	13	8	1	2	218	206	-4	4	2	187	187
3	7	1	65	28	2	10	1	50	28	-3	15	1	52	44	9	1	2	54	51	-3	4	2	313	293
5	7	1	52	69	3	10	1	96	85	-1	15	1	118	97	-9	2	2	253	238	-2	4	2	295	282
6	7	1	139	123	4	10	1	360	362	0	15	1	90	92	-7	2	2	112	82	-1	4	2	41	12
7	7	1	150	141	-6	11	1	86	101	2	15	1	105	105	-6	2	2	176	158	0	4	2	44	25
-8	8	1	60	42	-4	11	1	76	82	3	15	1	58	50	-5	2	2	153	162	1	4	2	908	866
-6	8	1	164	183	-2	11	1	89	97	-1	16	1	107	106	-4	2	2	350	348	2	4	2	407	389
-5	8	1	51	78	-1	11	1	139	159	-10	0	2	76	20	-3	2	2	392	408	4	4	2	230	234
-4	8	1	55	27	0	11	1	172	183	-8	0	2	67	77	-1	2	2	188	195	5	4	2	61	6
-3	8	1	561	539	1	11	1	201	177	-7	0	2	46	0	0	2	2	472	585	-9	5	2	114	93
-2	8	1	241	221	4	11	1	130	134	-6	0	2	393	362	1	2	2	1556	1404	-7	5	2	112	121
-1	8	1	69	61	7	11	1	66	73	-4	0	2	53	54	2	2	2	697	650	-6	5	2	220	227
0	8	1	250	265	-6	12	1	52	58	0	0	2	137	114	3	2	2	460	477	-3	5	2	267	270
1	8	1	142	136	-5	12	1	60	85	1	0	2	97	0	4	2	2	425	403	-2	5	2	94	153
2	8	1	46	38	-4	12	1	67	60	2	0	2	342	349	8	2	2	155	146	-1	5	2	556	544
3	8	1	155	172	-3	12	1	266	276	4	0	2	588	591	9	2	2	92	92	1	5	2	176	165
4	8	1	328	329	-2	12	1	70	11	6	0	2	98	99	-9	3	2	137	117	2	5	2	109	91
5	8	1	79	60	0	12	1	53	71	8	0	2	210	201	-7	3	2	155	149	3	5	2	101	100
7	8	1	237	224	1	12	1	66	72	-10	1	2	43	7	-6	3	2	171	185	4	5	2	172	171
8	8	1	52	24	4	12	1	88	74	-9	1	2	82	66	-5	3	2	184	172	6	5	2	281	303
-6	9	1	228	226	5	12	1	79	59	-8	1	2	62	38	-4	3	2	335	349	8	5	2	118	116
-5	9	1	110	118	-4	13	1	69	65	-7	1	2	82	75	-3	3	2	550	563	-7	6	2	348	334
-2	9	1	100	76	-3	13	1	64	14	-6	1	2	247	240	-1	3	2	43	29	-6	6	2	222	231
0	9	1	446	448	-2	13	1	105	114	-5	1	2	179	174	0	3	2	184	221	-4	6	2	53	60
1	9	1	93	112	-1	13	1	60	50	-4	1	2	98	93	1	3	2	242	212	-3	6	2	86	77

Table 29. (Continued)

Observed and calculated structure factors: Trimethylbenzene Thiourea Adduct

h	k	l	10Fo	10Fc	h	k	l	10Fo	10Fc	h	k	l	10Fo	10Fc	h	k	l	10Fo	10Fc	h	k	l	10Fo	10Fc
2	0	0	480	557	4	5	0	242	236	1	10	0	101	92	-5	2	1	378	368	-2	4	1	218	228
4	0	0	113	119	5	5	0	337	331	2	10	0	377	383	-4	2	1	414	446	-1	4	1	1559	1360
6	0	0	225	202	8	5	0	108	114	1	11	0	130	133	-3	2	1	279	311	0	4	1	426	383
8	0	0	86	54	9	5	0	75	35	2	11	0	208	198	-2	2	1	324	338	1	4	1	148	121
1	1	0	78	83	0	6	0	173	196	3	11	0	99	101	-1	2	1	827	830	2	4	1	228	211
2	1	0	287	314	1	6	0	138	135	5	11	0	221	229	1	2	1	102	97	3	4	1	306	293
3	1	0	590	521	2	6	0	252	251	0	12	0	256	245	2	2	1	322	291	4	4	1	264	270
4	1	0	233	234	3	6	0	43	15	1	12	0	96	81	3	2	1	328	295	5	4	1	368	375
5	1	0	160	154	4	6	0	135	159	2	12	0	94	96	4	2	1	147	138	6	4	1	234	227
6	1	0	188	175	5	6	0	153	151	3	12	0	51	35	5	2	1	485	454	9	4	1	54	6
7	1	0	203	198	7	6	0	80	81	6	12	0	94	107	6	2	1	69	69	-8	5	1	182	173
8	1	0	90	77	8	6	0	71	45	5	13	0	142	152	7	2	1	177	170	-6	5	1	294	289
9	1	0	43	11	9	6	0	84	97	0	14	0	148	155	9	2	1	83	76	-5	5	1	101	88
0	2	0	402	403	1	7	0	102	103	1	14	0	103	109	-10	3	1	90	58	-4	5	1	49	53
2	2	0	88	56	2	7	0	44	9	2	14	0	82	78	-9	3	1	109	84	-3	5	1	63	58
3	2	0	591	582	3	7	0	84	69	2	15	0	52	42	-7	3	1	80	86	-2	5	1	69	94
7	2	0	289	266	4	7	0	116	119	3	15	0	124	126	-6	3	1	353	343	0	5	1	774	737
9	2	0	57	25	5	7	0	565	567	-8	1	1	420	376	-5	3	1	89	86	1	5	1	457	427
1	3	0	29	36	7	7	0	100	94	-6	1	1	275	248	-4	3	1	119	104	2	5	1	556	564
2	3	0	395	322	8	7	0	59	80	-5	1	1	106	110	-3	3	1	324	301	5	5	1	59	28
3	3	0	822	765	0	8	0	357	367	-4	1	1	55	47	-1	3	1	1812	1666	7	5	1	183	160
4	3	0	96	98	1	8	0	65	63	-3	1	1	228	199	0	3	1	147	164	9	5	1	75	52
5	3	0	128	125	2	8	0	538	539	-2	1	1	35	39	1	3	1	187	119	-9	6	1	78	45
7	3	0	280	273	3	8	0	83	82	-1	1	1	338	341	2	3	1	55	24	-7	6	1	67	56
0	4	0	563	554	4	8	0	211	231	1	1	1	161	105	3	3	1	244	218	-6	6	1	181	169
1	4	0	922	878	6	8	0	55	48	2	1	1	1358	1240	4	3	1	178	185	-5	6	1	165	167
2	4	0	578	592	7	8	0	81	70	4	1	1	237	224	5	3	1	126	107	-4	6	1	155	162
3	4	0	197	218	8	8	0	125	132	5	1	1	153	154	7	3	1	78	6	-2	6	1	72	102
4	4	0	41	49	1	9	0	60	59	6	1	1	51	65	9	3	1	209	195	0	6	1	393	369
7	4	0	199	173	2	9	0	343	341	8	1	1	77	40	-8	4	1	94	87	1	6	1	94	73
8	4	0	203	168	4	9	0	62	52	9	1	1	113	104	-6	4	1	298	289	2	6	1	166	142
1	5	0	188	172	5	9	0	161	156	-10	2	1	61	47	-5	4	1	163	157	3	6	1	312	311
2	5	0	439	486	7	9	0	51	18	-7	2	1	47	52	-4	4	1	193	167	4	6	1	132	138
3	5	0	152	126	0	10	0	197	203	-6	2	1	114	88	-3	4	1	155	188	6	6	1	157	169

Table 29. (Continued)

Observed and calculated structure factors: Trimethylbenzene Thiourea Adduct

h	k	l	10Fo	10Fc	h	k	l	10Fo	10Fc	h	k	l	10Fo	10Fc	h	k	l	10Fo	10Fc	h	k	l	10Fo	10Fc
-4	3	8	130	152	-6	7	8	118	116	-3	12	8	55	67	-6	4	9	138	130	-2	9	9	287	273
-3	3	8	94	86	-5	7	8	129	116	-2	12	8	62	92	-3	4	9	48	23	-1	9	9	61	39
-1	3	8	84	88	-4	7	8	142	142	-1	12	8	133	130	0	4	9	98	83	1	9	9	74	60
0	3	8	54	32	-3	7	8	77	84	0	12	8	54	8	1	4	9	42	12	-6	10	9	128	92
1	3	8	323	330	-2	7	8	108	112	-2	13	8	73	54	3	4	9	178	190	1	10	9	55	21
2	3	8	164	155	-1	7	8	298	290	-10	1	9	59	42	4	4	9	71	93	-2	11	9	135	119
3	3	8	65	58	0	7	8	54	65	-8	1	9	84	77	-9	5	9	63	70	0	11	9	63	59
-9	4	8	74	70	1	7	8	79	75	-6	1	9	50	63	-6	5	9	93	66	-3	12	9	56	2
-7	4	8	50	55	2	7	8	80	63	-5	1	9	45	30	-4	5	9	196	183	-2	0	10	341	325
-6	4	8	102	115	3	7	8	97	107	-4	1	9	375	351	-3	5	9	76	60	2	0	10	110	71
-4	4	8	255	275	4	7	8	58	66	-3	1	9	39	23	-2	5	9	302	288	-8	1	10	69	87
-3	4	8	277	267	-7	8	8	50	18	-2	1	9	126	124	-1	5	9	133	127	-7	1	10	54	41
-1	4	8	95	86	-6	8	8	58	58	-1	1	9	132	134	0	5	9	113	129	-5	1	10	181	177
1	4	8	104	91	-5	8	8	64	55	0	1	9	168	158	1	5	9	141	153	-4	1	10	84	76
2	4	8	54	55	-4	8	8	139	141	1	1	9	43	33	-9	6	9	76	66	-2	1	10	94	83
3	4	8	78	94	-3	8	8	88	86	3	1	9	73	44	-5	6	9	203	211	-1	1	10	65	48
4	4	8	74	68	-1	8	8	229	222	-9	2	9	89	91	-4	6	9	125	135	0	1	10	51	49
-8	5	8	127	118	0	8	8	124	125	-8	2	9	55	34	-2	6	9	98	85	1	1	10	123	145
-7	5	8	140	154	2	8	8	109	96	-7	2	9	165	194	0	6	9	46	34	2	1	10	191	199
-6	5	8	202	198	-8	9	8	89	79	-4	2	9	169	182	1	6	9	277	283	-8	2	10	54	66
-5	5	8	94	89	-5	9	8	58	75	-2	2	9	101	117	3	6	9	60	16	-7	2	10	60	28
-3	5	8	102	100	-4	9	8	116	118	-1	2	9	154	167	-8	7	9	66	47	-6	2	10	94	53
-1	5	8	119	122	-1	9	8	122	111	0	2	9	57	41	-5	7	9	96	93	-5	2	10	105	95
0	5	8	99	114	0	9	8	55	50	1	2	9	85	90	-4	7	9	133	118	-4	2	10	54	48
1	5	8	56	51	1	9	8	47	31	2	2	9	50	28	-2	7	9	57	47	-3	2	10	120	106
2	5	8	263	310	2	9	8	223	224	3	2	9	303	314	0	7	9	66	15	-2	2	10	158	156
-7	6	8	69	29	3	9	8	68	47	-8	3	9	81	85	1	7	9	122	127	-1	2	10	130	118
-5	6	8	77	79	-6	10	8	74	79	-5	3	9	91	111	3	7	9	52	28	0	2	10	113	125
-4	6	8	175	160	-4	10	8	169	166	-3	3	9	54	45	-6	8	9	107	84	1	2	10	73	73
-1	6	8	347	372	-1	10	8	44	58	-2	3	9	327	322	-4	8	9	100	85	2	2	10	52	35
0	6	8	120	112	-2	11	8	52	57	-1	3	9	256	260	-2	8	9	55	33	-7	3	10	81	103
4	6	8	92	74	-1	11	8	116	110	1	3	9	72	35	1	8	9	213	237	-6	3	10	70	59
-9	7	8	58	27	1	11	8	70	66	3	3	9	85	41	2	8	9	96	113	-5	3	10	281	287
-7	7	8	91	97	-5	12	8	66	58	-7	4	9	122	121	-5	9	9	59	23	-3	3	10	62	70

Table 29. (Continued)

Observed and calculated structure factors: Trimethylbenzene Thiourea Adduct

h	k	l	10Fo	10Fc	h	k	l	10Fo	10Fc	h	k	l	10Fo	10Fc	h	k	l	10Fo	10Fc	h	k	l	10Fo	10Fc
4	10	6	91	91	4	1	7	44	24	4	4	7	48	67	-6	8	7	116	139	-2	13	7	69	73
-5	11	6	87	93	5	1	7	218	221	5	4	7	67	38	-3	8	7	243	232	-1	13	7	64	43
-2	11	6	264	251	-8	2	7	119	124	-10	5	7	57	37	-2	8	7	86	79	0	13	7	61	29
-1	11	6	65	58	-7	2	7	83	117	-6	5	7	90	82	-1	8	7	98	111	-10	0	8	54	15
0	11	6	87	83	-6	2	7	82	115	-5	5	7	84	61	0	8	7	268	274	-6	0	8	182	205
1	11	6	175	175	-5	2	7	128	163	-4	5	7	103	74	1	8	7	76	77	-4	0	8	56	56
-6	12	6	84	42	-3	2	7	172	175	-3	5	7	396	407	3	8	7	141	153	-3	0	8	56	0
-5	12	6	146	148	-2	2	7	81	81	-2	5	7	184	176	4	8	7	153	171	-2	0	8	310	298
-3	12	6	57	9	-1	2	7	354	345	-1	5	7	173	164	-8	9	7	67	43	0	0	8	95	93
-2	12	6	100	85	1	2	7	138	131	0	5	7	96	101	-7	9	7	55	7	1	0	8	52	0
1	12	6	64	92	2	2	7	263	267	1	5	7	108	112	-6	9	7	119	129	2	0	8	72	52
3	12	6	60	67	5	2	7	72	54	2	5	7	88	50	-3	9	7	77	59	4	0	8	398	412
-3	13	6	68	41	-10	3	7	95	72	3	5	7	112	110	-1	9	7	44	19	-9	1	8	61	54
-1	13	6	46	28	-7	3	7	74	113	4	5	7	152	162	0	9	7	88	84	-8	1	8	110	116
0	13	6	89	109	-5	3	7	360	379	5	5	7	75	106	1	9	7	43	29	-6	1	8	182	200
1	13	6	128	130	-3	3	7	87	86	-8	6	7	136	140	4	9	7	101	113	-4	1	8	131	143
2	13	6	61	36	-2	3	7	159	153	-7	6	7	94	96	-8	10	7	57	9	-2	1	8	57	67
-4	14	6	76	83	-1	3	7	276	256	-5	6	7	128	139	-6	10	7	57	65	-1	1	8	104	98
-3	14	6	94	88	0	3	7	51	47	-2	6	7	110	107	-4	10	7	48	21	0	1	8	177	175
-2	14	6	58	47	1	3	7	50	32	-1	6	7	54	47	0	10	7	357	372	1	1	8	281	275
-1	14	6	47	19	2	3	7	55	29	0	6	7	135	135	1	10	7	61	57	2	1	8	108	111
-10	1	7	78	61	5	3	7	277	305	1	6	7	124	131	-7	11	7	72	39	3	1	8	45	76
-8	1	7	57	44	-10	4	7	122	98	2	6	7	153	152	-6	11	7	86	85	4	1	8	283	299
-7	1	7	80	100	-8	4	7	106	102	3	6	7	134	147	-5	11	7	95	85	-3	2	8	62	33
-6	1	7	82	56	-7	4	7	95	51	-7	7	7	61	48	-3	11	7	148	128	-4	2	8	71	75
-5	1	7	250	278	-6	4	7	102	118	-5	7	7	119	115	-1	11	7	67	66	-3	2	8	422	441
-4	1	7	95	80	-5	4	7	194	201	-4	7	7	67	45	1	11	7	44	2	-2	2	8	117	125
-3	1	7	40	44	-4	4	7	73	75	-3	7	7	532	516	3	11	7	93	90	-1	2	8	79	70
-2	1	7	161	165	-2	4	7	260	253	-2	7	7	227	214	-4	12	7	100	91	0	2	8	70	70
-1	1	7	290	304	-1	4	7	312	293	-1	7	7	73	90	-2	12	7	54	33	1	2	8	97	64
0	1	7	36	6	0	4	7	224	228	1	7	7	72	45	-1	12	7	51	46	2	2	8	53	85
1	1	7	45	41	1	4	7	125	130	3	7	7	163	180	1	12	7	59	41	4	2	8	178	153
2	1	7	266	243	2	4	7	184	186	4	7	7	69	13	2	12	7	85	59	-9	3	8	133	122
3	1	7	44	37	3	4	7	59	51	-7	8	7	123	121	-3	13	7	141	139	-8	3	8	66	67

Table 29. (Continued)

Observed and calculated structure factors: Trimethylbenzene Thiourea Adduct

h	k	l	10Fo	10Fc	h	k	l	10Fo	10Fc	h	k	l	10Fo	10Fc	h	k	l	10Fo	10Fc	h	k	l	10Fo	10Fc
-9	8	5	76	40	3	11	5	121	122	-7	2	6	178	209	2	4	6	56	87	1	7	6	353	357
-6	8	5	92	65	-7	12	5	77	50	-6	2	6	65	63	3	4	6	342	357	2	7	6	46	50
-3	8	5	106	97	-6	12	5	60	35	-5	2	6	259	263	5	4	6	56	20	4	7	6	70	91
-2	8	5	65	23	-2	12	5	93	80	-4	2	6	479	449	6	4	6	98	99	5	7	6	50	19
-1	8	5	468	458	-1	12	5	287	274	-3	2	6	207	206	-10	5	6	73	65	-7	8	6	90	91
0	8	5	65	66	1	12	5	50	54	-2	2	6	134	162	-9	5	6	102	87	-5	8	6	185	173
1	8	5	58	52	2	12	5	83	106	-1	2	6	180	155	-7	5	6	87	103	-2	8	6	339	313
2	8	5	101	105	-6	13	5	68	50	0	2	6	110	24	-6	5	6	84	76	-1	8	6	51	43
6	8	5	111	83	-2	13	5	80	79	1	2	6	123	132	-5	5	6	47	86	0	8	6	43	13
-8	9	5	71	78	1	13	5	49	42	2	2	6	62	68	-4	5	6	73	92	1	8	6	99	88
-7	9	5	92	74	2	13	5	78	75	3	2	6	521	516	-2	5	6	233	225	3	8	6	67	49
-6	9	5	120	138	3	13	5	75	92	4	2	6	106	154	-1	5	6	90	59	4	8	6	106	124
-5	9	5	190	192	-2	14	5	96	103	6	2	6	72	60	0	5	6	336	339	5	8	6	181	181
-4	9	5	355	370	-1	14	5	106	105	-9	3	6	67	61	1	5	6	137	148	-8	9	6	59	67
-1	9	5	46	23	0	14	5	47	7	-8	3	6	95	110	2	5	6	110	112	-7	9	6	74	4
0	9	5	85	72	-2	15	5	65	49	-7	3	6	210	246	3	5	6	59	77	-6	9	6	80	66
2	9	5	245	258	-6	0	6	72	31	-6	3	6	151	178	4	5	6	52	60	-5	9	6	76	79
3	9	5	109	105	-2	0	6	44	67	-4	3	6	100	101	6	5	6	91	98	-4	9	6	147	125
-8	10	5	72	84	0	0	6	192	160	-3	3	6	99	115	-7	6	6	118	136	-3	9	6	55	50
-7	10	5	83	77	3	0	6	84	0	-2	3	6	323	323	-6	6	6	52	72	-2	9	6	419	413
-6	10	5	64	75	6	0	6	245	256	-1	3	6	258	277	-5	6	6	215	233	-1	9	6	56	10
-5	10	5	114	98	-10	1	6	83	66	0	3	6	209	201	-4	6	6	257	251	1	9	6	140	154
-4	10	5	65	83	-9	1	6	83	74	1	3	6	83	134	-2	6	6	47	50	2	9	6	172	196
-1	10	5	139	127	-6	1	6	167	176	2	3	6	144	158	-1	6	6	243	231	5	9	6	92	54
0	10	5	149	142	-5	1	6	54	35	3	3	6	286	296	0	6	6	97	94	-6	10	6	89	92
1	10	5	61	15	-4	1	6	51	62	6	3	6	58	12	1	6	6	58	63	-5	10	6	63	54
2	10	5	238	238	-3	1	6	44	48	-10	4	6	53	15	2	6	6	72	75	-4	10	6	49	7
3	10	5	106	110	-2	1	6	107	110	-9	4	6	72	72	4	6	6	62	7	-3	10	6	70	83
-6	11	5	67	37	0	1	6	919	870	-7	4	6	111	136	5	6	6	283	297	-2	10	6	269	256
-5	11	5	54	33	1	1	6	173	173	-6	4	6	167	186	6	6	6	72	81	-1	10	6	71	72
-4	11	5	197	185	2	1	6	110	118	-4	4	6	119	117	-9	7	6	143	127	0	10	6	73	77
-2	11	5	61	23	3	1	6	231	216	-2	4	6	299	308	-4	7	6	94	82	1	10	6	66	67
-1	11	5	95	93	6	1	6	89	96	-1	4	6	87	86	-2	7	6	58	29	2	10	6	83	80
2	11	5	111	121	-9	2	6	61	45	0	4	6	110	104	-1	7	6	133	110	3	10	6	77	73

Table 29. (Continued)

Observed and calculated structure factors: Trimethylbenzene Thiourea Adduct

h	k	l	10Fo	10Fc	h	k	l	10Fo	10Fc	h	k	l	10Fo	10Fc	h	k	l	10Fo	10Fc	h	k	l	10Fo	10Fc
0	5	4	230	230	-5	8	4	49	43	-4	12	4	129	114	-2	2	5	256	288	-6	5	5	274	277
1	5	4	277	293	-3	8	4	220	236	-3	12	4	197	191	-1	2	5	337	361	-5	5	5	142	172
2	5	4	301	281	-1	8	4	83	88	-1	12	4	72	62	0	2	5	506	516	-4	5	5	136	132
3	5	4	48	78	0	8	4	64	47	0	12	4	89	115	1	2	5	585	612	-3	5	5	385	405
4	5	4	110	128	1	8	4	363	368	1	12	4	92	87	2	2	5	91	105	-2	5	5	124	111
5	5	4	91	92	3	8	4	272	268	3	12	4	113	113	3	2	5	71	58	-1	5	5	142	126
7	5	4	126	148	4	8	4	215	211	-5	13	4	67	43	6	2	5	132	141	0	5	5	36	32
-10	6	4	51	33	-9	9	4	78	44	-3	13	4	167	172	7	2	5	102	103	1	5	5	114	89
-9	6	4	57	10	-5	9	4	49	12	1	13	4	56	36	-7	3	5	53	43	2	5	5	130	142
-8	6	4	112	115	-3	9	4	167	161	-4	14	4	68	48	-5	3	5	223	259	3	5	5	118	175
-7	6	4	65	57	-1	9	4	56	49	-3	14	4	67	70	-4	3	5	162	178	4	5	5	280	277
-6	6	4	59	44	0	9	4	368	379	-1	14	4	82	68	-3	3	5	487	470	6	5	5	213	242
-3	6	4	408	411	1	9	4	52	38	0	14	4	108	116	-2	3	5	78	78	-7	6	5	119	136
-2	6	4	54	48	3	9	4	148	149	2	14	4	118	112	-1	3	5	129	130	-6	6	5	99	111
-1	6	4	43	35	-8	10	4	86	46	-1	15	4	119	99	0	3	5	109	95	-4	6	5	288	287
1	6	4	156	172	-6	10	4	242	255	-8	1	5	104	115	1	3	5	668	639	-3	6	5	85	79
2	6	4	521	542	-1	10	4	48	44	-7	1	5	62	94	2	3	5	219	227	-2	6	5	176	156
3	6	4	178	194	0	10	4	213	220	-6	1	5	371	399	3	3	5	86	88	-1	6	5	488	483
4	6	4	147	161	1	10	4	77	94	-5	1	5	131	140	4	3	5	55	32	1	6	5	189	175
6	6	4	49	48	2	10	4	54	48	-4	1	5	325	348	6	3	5	87	101	2	6	5	90	102
-8	7	4	79	62	4	10	4	259	271	-3	1	5	195	193	7	3	5	70	32	3	6	5	85	91
-6	7	4	89	102	6	10	4	58	19	-2	1	5	232	235	-9	4	5	158	156	4	6	5	75	62
-5	7	4	66	112	-8	11	4	52	35	-1	1	5	231	223	-8	4	5	86	100	6	6	5	59	63
-4	7	4	277	282	-5	11	4	105	85	0	1	5	57	8	-7	4	5	141	156	-9	7	5	74	61
-3	7	4	596	569	-4	11	4	100	119	1	1	5	172	175	-5	4	5	75	87	-7	7	5	147	157
-2	7	4	69	49	-3	11	4	175	159	3	1	5	104	97	-4	4	5	250	268	-5	7	5	69	85
-1	7	4	140	143	-2	11	4	47	40	4	1	5	594	604	-3	4	5	225	210	-4	7	5	163	179
1	7	4	235	252	-1	11	4	95	90	5	1	5	73	54	-2	4	5	282	267	-3	7	5	109	102
3	7	4	50	26	0	11	4	294	313	7	1	5	78	87	0	4	5	167	167	-2	7	5	100	76
5	7	4	64	85	1	11	4	160	170	-9	2	5	194	175	1	4	5	422	416	-1	7	5	134	128
6	7	4	52	54	3	11	4	64	61	-6	2	5	153	173	2	4	5	76	76	0	7	5	281	274
7	7	4	203	208	4	11	4	100	104	-5	2	5	91	111	6	4	5	175	182	1	7	5	72	70
-7	8	4	102	98	-7	12	4	68	47	-4	2	5	110	132	7	4	5	87	85	3	7	5	263	277
-6	8	4	163	178	-5	12	4	70	29	-3	2	5	466	473	-8	5	5	74	61	4	7	5	127	136

Table 29. (Continued)

Observed and calculated structure factors: Trimethylbenzene Thiourea Adduct

h	k	l	10F _o	10F _c	h	k	l	10F _o	10F _c	h	k	l	10F _o	10F _c	h	k	l	10F _o	10F _c	h	k	l	10F _o	10F _c
-2	3	10	112	104	-2	6	10	148	157	-3	1	11	130	133	1	4	11	47	18	-1	1	12	39	4
1	3	10	88	101	0	6	10	72	80	-1	1	11	88	89	-8	5	11	53	41	-6	2	12	105	92
2	3	10	65	87	1	6	10	64	69	0	1	11	257	265	-7	5	11	73	82	-4	2	12	58	24
3	3	10	70	40	2	6	10	59	61	1	1	11	69	58	-4	5	11	90	92	-1	2	12	178	165
-9	4	10	67	38	-7	7	10	142	127	2	1	11	59	37	-1	5	11	98	91	-6	3	12	84	59
-7	4	10	90	72	-6	7	10	67	39	-7	2	11	57	37	0	5	11	81	65	-4	3	12	87	66
-4	4	10	54	24	-3	7	10	127	131	-6	2	11	74	67	1	5	11	55	19	-2	3	12	75	84
-2	4	10	153	135	-1	7	10	50	11	-5	2	11	67	45	-6	6	11	65	54	-1	3	12	121	109
-1	4	10	96	98	0	7	10	45	10	-4	2	11	54	49	-5	6	11	139	127	0	3	12	58	22
0	4	10	199	213	-6	8	10	52	30	-3	2	11	167	157	-3	6	11	70	56	-7	4	12	57	31
1	4	10	123	128	-5	8	10	56	12	0	2	11	56	40	-2	6	11	60	24	-6	4	12	87	65
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-3	6	10	195	181																				

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