The synthesis, analysis, and characterization of a group of platinum clusters
by Eric Spencer Peterson

A thesis submitted in partial fulfillment of the requirements for the degree of Doctor of Philosophy in Chemistry
Montana State University

Abstract:
There is a great deal of interest in the synthesis of materials which possess special physical and chemical properties. One such area of interest is concerned with the formation and chemistry of platinum-platinum bonds. The structures of platinum-platinum bonded species which exhibit the platinum(III) oxidation state have only recently been elucidated. The chemical pathways leading to the platinum(III) oxidation state are not well understood. Presented here is structural evidence for what is considered to be one of the initial steps in the pathway leading to platinum-platinum bonds. Two single crystal x-ray crystal structures exhibiting a bent nitrosyl ligand upon a monomeric platinum center are presented. To our knowledge, no other examples of bent nitrosyl ligands on platinum monomeric species exist in current literature. The single crystal x-ray crystallographic structures of three closely related complexes are also presented. ESCA studies, visible spectral and infrared spectral studies are also presented in support of the structural data. Additionally, the results of NMR and ESCA studies of a group of structurally related platinum(III) dimeric complexes are presented. The NMR data include complete sets of 195pt, 13C, and 1H spectral information. Generally, the solid state structure was found to remain intact in solution. Unusually large platinum-platinum coupling constants were observed during the course of the investigations. The ESCA studies of the same platinum-platinum bonded species lend support to the platinum(III) oxidation state. Finally, the synthesis, analysis, and chemical characterization of a group of tetrameric platinum-platinum bonded complexes is presented.

A newly developed synthetic scheme for the tetrameric complexes, along with an efficient method of chromatographic purification of the complexes is presented. Single crystal x-ray crystallographic information is presented about a new structural derivative of the octakisacetato platinum complex. The complex exhibits a pair of bridging carbonyl ligands on opposite sides of the tetrameric rectangle, and a pair of asymmetric bridging acetate ions trans to the carbonyl ligands. The short sides of the tetrameric rectangle are bridged by symmetric acetate ions. Infrared, visible, ESCA and elemental analytic studies are presented as evidence for the complexes. A novel application of NMR determining the total number of acetate ligands per cluster is also presented. Eighteen other derivatives of the octakisacetato tetrameric complex were made using different ligands. The reaction conditions under which the complexes were found to react appear unique for this set of complexes. Infrared, visible, ESCA and elemental analytic data are presented in support of the proposed structures for the complexes.

The possible oxidation states of each of the complexes is considered. It is hoped that this work will aid in future systematic synthetic efforts for exploratory studies of platinum-platinum bonded compounds.

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OF A GROUP OF PLATINUM CLUSTERS

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Eric Spencer Peterson

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of the requirements for the degree

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APPROVAL

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Eric Spencer Peterson

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

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Date 27 October, 1987

DEDICATION

To Mom and Dad.

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I would like to thank Dr. Edwin H. Abbott for his advice. I would also like to thank all of those people who have made my stay in graduate school quite pleasant.

TABLE OF CONTENTS

Page

LIST OF TABLES x

LIST OF FIGURES xiv

KEY ABBREVIATIONS xvii

ABSTRACT. xviii

INTRODUCTION. 1

Sulfate and Phosphate Bridged Species. 6
α-Oxopyridonate Bridged Platinum(III) Complexes. 11
Platinum Carboxylate Bridged Compounds 14

PURPOSE OF THE PRESENT INVESTIGATION. 20

EXPERIMENTAL. 22

Preparation of Compounds 22

Preparation of $K_2Pt(NO_2)_4 \cdot H_2O$ 22
Preparation of $K_2Pt(NO_2)_4(NO)(H_2O)$, 1 22
Method II for the Preparation of $K[Pt(NO_2)_4NO \cdot OH_2] \cdot OH_2$, 1, with $NOBF_4$ 23
Preparation of $K_2[Pt(Cl_3)(NO_2)_2NO]$, 2 23
Preparation of $K_2[Pt(NO_2)_2Cl_4]$, 3 23
Method II for Preparation of $K_2[Pt(NO_2)_2Cl_4]$, 3 . . . 25
Preparation of $K_2[Pt(NO_2)_4Br_2]$, 4 25
Preparation of $K_2[Pt(PO_3)_2Cl_2]$, 5 25
Preparation of $Pt_4(OAc)_8$ Blue from Platinum(IV) . . . 26
Synthesis of $Pt_4(OAc)_8$ from Platinum(II), 10. 27
Preparation of $[Pt_4(OAc)_6(CO)_2] \cdot 2HOAc$, 6. 28
Direct Preparation of $[Pt_4(OAc)_6(CO)_2] \cdot 2HOAc$, 6, from $Pt_4(OAc)_8$ Blue 28
Direct Method I for the Preparation of 6 Using Formic Acid. 28
Direct Method II for the Preparation of 6 Using Co Gas 30
Direct Preparation of $[Pt_4(OAc)_6(NO)_2] \cdot 2HOAc$, 12 30

TABLE OF CONTENTS (continued)

Page

Direct Method I for the Preparation of 12 Using Nitric Acid 31
Direct Method II for the Preparation of 12 Using NO Gas. 31
Preparation of [$Pt_2(POP)_4 \cdot H_2O$] from $Pt_4(OAc)_8$ Blue, 13 32
Preparation of $Pt_2(POP)_4 \cdot H_2O$ from $Pt_4(OAc)_8$ Blue with Ammonium Diphosphite, 13 32
Reaction of $Pt_4(OAc)_8$ with KOCN 33
Reaction of $Pt_4(OAc)_8$ Blue with 20 Equivalents KOCN, 14 33
Reaction of $Pt_4(OAc)_8$ Blue with 20 Equivalents KSCN, 15 33
Reaction of $Pt_4(OAc)_8$ Blue with Eight Equivalents KSCN, 16 34
Reaction of $Pt_4(OAc)_8$ with Four Equivalents KSCN, 17 35
Reaction of $Pt_4(OAc)_8$ Blue with Two Equivalents KSCN, 18 35
Reaction of $Pt_4(OAc)_8$ Blue with Acetylene Gas, 19. 36
Reaction of $Pt_4(OAc)_8$ Blue with Phenylacetylene, 20. 36
Reaction of $Pt_4(OAc)_8$ Blue with Diphenylacetylene, 21. 38
Reaction of $Pt_4(OAc)_8$ Blue with One Equivalent Triphenylphosphine, 22. 39
Reaction of $Pt_4(OAc)_8$ Blue with Two Equivalents Triphenylphosphine, 23 39
Reaction of $Pt_4(OAc)_8$ Blue with Four Equivalents Triphenylphosphine, 24 40
Reaction of $Pt_4(OAc)_8$ Blue with Excess HCN, 25 40
Reaction of $Pt_4(OAc)_8$ Blue with HCN Controlled Reaction, 26. 41
Reaction of $Pt_4(OAc)_8$ Blue with One and Two Equivalents of Cyanamide, 27 42
Reaction of $Pt_4(OAc)_8$ Blue with Eight Equivalents of Acetamide, 28 42
Reaction of $Pt_4(OAc)_8$ Blue with Trifluoroacetic Acid, 29 43
Reaction of $Pt_4(OAc)_8$ Blue with Sulfuric Acid, 30. 43
Reaction of $Pt_4(OAc)_8$ Blue with K_2SO_4, 31 44
Reaction of $Pt_4(OAc)_8$ Blue with Eight Equivalents Hydroxypyridine, 32. 44

TABLE OF CONTENTS (continued)

Page

Materials and Methods 45

Chromatographic Procedures 46

Preparation of Ag Salts 47

NMR Spectroscopy of Pt(III) Dimeric Species 47

X-Ray Crystallography 51

Structure Solution of $K[Pt(NO_2)_4(NO)(H_2O)\}$ $\cdot H_2O$, 1 52

Structure Solution for $K_2[Pt(NO_2)_2(NO)Cl_3]$, 2 55

Structure Solution for $K_2[Pt(NO_2)_4Br_2]$, 3 58

Structure Solution for $K_2[Pt(NO_2)_2Cl_4]$, 4 58

Structure Solution for $K_2[Pt(Cl)_2(PO_3)_2]$, 5 60

Structure Solution for $[Pt_4(OAc)_6(CO)_2]$ $\cdot 2HOAc$, 6 63

RESULTS 65

X-Ray Crystallographic Results 65

Structure of $K[Pt(NO_2)_4(NO)(OH_2)]$, 1 65

Structure of $K_32[Pt(NO_2)_2(NO)(Cl3]$, 2 69

Structure of $K_2[Pt(NO_2)_2Cl_4]$, 3 74

Structure of $K_2[Pt(NO_2)_4Br_2]$, 4 76

Structure of $K_2[Pt(Cl)_2(PO_3)_2]$, 5 79

Structure of $[Pt_4(OAc)_6(CO_2)]\cdot 2(HOAc)$, 6 82

Physical Measurements 88

Electron Spectroscopy for Chemical Analysis (ESCA) 88

NMR Spectra and Spectral Assignments for a Series of Pt(III) Complexes 91

Infrared Spectral Results 130

Total Ligands Per Metal Cluster Determination 143

Results of Elemental Analyses of Selected Compounds 143

TABLE OF CONTENTS (continued)

Page

DISCUSSION 150

Synthetic Procedures 162
Reactivity Studies 164
Structural Studies 165
NMR Studies 169
ESCA Studies 173
Infrared Spectral Studies 176
Elemental Analytical Studies 181
Proposed Structures 182

SUMMARY 188

REFERENCES CITED 191

APPENDIX. F_o F_c Tables for Compounds 1 - 6 197

LIST OF TABLES

Table		Page
1.	Crystallographic parameters for $K[Pt(NO_2)_4(NO)(H_2O)]\cdot H_2O$, 1.	53
2.	Crystallographic parameters for $K[Pt(NO_2)_2(NO)Cl_3]$, 2.	56
3.	Crystallographic parameters for $K_2Pt(NO_2)_4Br_2$, 3	59
4.	Crystallographic parameters for $K_2[Pt(NO_2)_2Cl_4]$, 4	61
5.	Crystallographic parameters for $K_2[PtCl_2(PO_3)_2]$, 5	62
6.	Crystallographic parameters for $[Pt_4(OOCCH_3)_6(CO)_2]$, 6	64
7.	Atomic coordinates ($\times 10^4$) and isotropic thermal parameters ($Å^2 \times 10^3$) for $K[Pt(NO_2)_4(NO)OH_2]\cdot(OH_2)$	66
8.	Bond lengths (Å) for $K[Pt(NO_2)_4(NO)OH_2]\cdot(OH_2)$.	67
9.	Bond angles (°) for $K[Pt(NO_2)_4(NO)OH_2]\cdot(OH_2)$	68
10.	Anisotropic thermal parameters ($Å\times 10^3$) for $K[Pt(NO_2)_4(NO)OH_2]\cdot(OH_2)$	69
11.	Atomic coordinates ($\times 10^4$) and isotropic thermal parameters ($Å\times 10^3$) for $K_2[Pt(NO_2)_2(NO)Cl_3]$	71
12.	Bond lengths (Å) for $K_2[Pt(NO_2)_2(NO)Cl_3]$	71
13.	Bond angles (°) for $K_2[Pt(NO_2)_2(NO)Cl_3]$.	72
14.	Anisotropic thermal parameters ($A^2 \times 10^3$) for $K_2[Pt(NO_2)_2(NO)Cl_3]$.	73
15.	Atomic coordinates ($\times 10^4$) and isotropic thermal parameters ($Å^2 \times 10^3$) for $K_2[Pt(NO_2)_2Cl_4]$.	75

LIST OF TABLES (continued)

Table		Page
16.	Bond lengths (Å) for $K_2[Pt(NO_2)_2Cl_4]$	75
17.	Bond angles (°) for $K_2[Pt(NO_2)_2Cl_4]$	75
18.	Anisotropic thermal parameters ($Å^2x10^3$) for $K_2[Pt(NO_2)_2Cl_4]$	76
19.	Atomic coordinates ($x10^4$) and isotropic thermal parameters ($Å^2x10^3$) for $K_2[Pt(NO_2)_2Cl_4]$	77
20.	Bond lengths (Å) for $K_2[Pt(NO_2)_2Cl_4]$	77
21.	Bond angles (°) for $K_2[Pt(NO_2)_2Cl_4]$	78
22.	Anisotropic thermal parameters ($Å^2x10^3$) for $K_2[Pt(NO_2)_4Br_2]$	78
23.	Atomic coordinates ($x10^4$) and isotropic thermal parameters ($Å^2x10^3$) for $K_2[Pt(PO_3)_2Cl_2]$	80
24.	Bond lengths (Å) for $K_2[Pt(PO_3)_2Cl_2]$	81
25.	Bond angles (°) for $K_2[Pt(PO_3)_2Cl_2]$	81
26.	Anisotropic thermal parameters ($Å^2x10^3$) for $K_2[Pt(PO_3)_2Cl_2]$	82
27.	Atomic coordinates ($x10^4$) and isotropic thermal parameters ($Å^2x10^3$) for $[Pt_4(OAc)_6(CO)_2 \cdot 2(HOAc)$	84
28.	Bond lengths (Å) for $[Pt_4(OAc)_6(CO)_2 \cdot 2(HOAc)$	85
29.	Bond angles (°) for $[Pt_4(OAc)_6(CO)_2 \cdot 2(HOAc)$	86
30.	Anisotropic thermal parameters ($Å^2x10^3$) for $[Pt_4(OAc)_6(CO)_2 \cdot 2(HOAc)$	88
31.	ESCA data for platinum complexes	90
32.	$Pt_2(mhp)_2(CH_3)_4(pyr)_1$ (head-to-head dimer)	93
33.	$Pt_2(CH_3)_4(hp)_2(Et_2S)_1$ (head-to-head dimer)	98
34.	$Pt_2(CH_3)_4(mhp)_2(Et_2S)_1$ (head-to-head dimer)	102
35.	$Pt_2(CH_3)_4(fhp)_2(pyr)_2$ (head-to-tail dimer)	106

LIST OF TABLES (continued)

Table | Page

36. $Pt_2(CH_3)_4(chp)_2(pyr)_1$ (head-to-head dimer) 110

37. $Pt_2(CH_3)_4(fhp)_2(Et_2S)_1$ (head-to-head dimer). 115

38. $Pt_2(CH_3)_4(fhp)_2(pyr)_1$ (head-to-head dimer) 119

39. $Pt_2(CH_3)_4(hp)_2(pyr)_2$ (head-to-tail dimer) and $Pt_2(CH_3)_4(hp)_2(pyr)_1$ (head-to-head dimer). 124

40. Infrared spectral results for $K[Pt(NO_2)_4(NO)(OH_2]\cdot OH_2$, 1 130

41. Infrared spectral results for $K[Pt(NO_2)_2Cl_3(NO)]$, 2. 130

42. Infrared spectral results for $Pt_4(OAc)_6(CO)_2$, purple fraction, 6 131

43. Infrared spectral results for $Pt_4(OAc)_8$, blue fraction, 7, 10 131

44. Infrared spectral results for $Pt_4(OAc)_8$, green fraction, 8. 132

45. Infrared spectral results for reaction of $Pt_4(OAc)$ blue and $NOBF_4$ or NO (gas) or HNO_3, two equivalents (purple solid), 12 132

46. Infrared spectral results for reaction of $Pt_4(OAc)_8$ blue and KOCN, 10 and 20 equivalents, 14. 133

47. Infrared spectral results for reaction of $Pt_4(OAc)_8$ blue and KSCN, 20 equivalents, 15. 133

48. Infrared spectral results for reaction of $Pt_4(OAc)_8$ blue and eight equivalents KSCN H_2O insoluble fraction, 16 134

49. Infrared spectral results for reaction of $Pt_4(OAc)_8$ blue and four equivalents KSCN H_2O soluble fraction, 17S. 134

50. Infrared spectral results for reaction of $Pt_4(OAc)$ blue and four equivalents KSCH H_2O insoluble fraction, 17I, 18I 135

LIST OF TABLES (continued)

Table		Page
51.	Infrared spectral results for reaction of $Pt_4(OAc)_8$ blue and KSCN (two equivalents), **18S**	135
52.	Infrared spectral results for reaction of $Pt_4(OAc)_8$ blue and HC≡CH (gas), **19**	136
53.	Infrared spectral results for $Pt_4(OAc)$ blue and phenylacetylene, **20**	136
54.	Infrared spectral results for reaction of $Pt_4(OAc)$ blue and PhC≡PCh, **21**	137
55.	Infrared spectral results for reaction of $Pt_4(OAc)_8$ and (PH_3P), two and four equivalents, **23**, **24**	137
56.	Infrared spectral results for reactions of $Pt_4(OAc)_8$ blue and HCN or KCN, two equivalents, **26**	138
57.	Infrared spectral results for $Pt_4(OAc)_8$ blue plus cyanamide, one and two equivalents, **27**	138
58.	Infrared spectral results for $Pt_4(OAc)_8$ blue with eight equivalents acetamide, **28**	139
59.	Infrared spectral results for $Pt_4(OAc)_8$ blue with trifluoroacetic acid, **29**	139
60.	Infrared spectral results for $Pt_4(OAc)_8$ blue with H_2SO_4, **30**	140
61.	Infrared spectral results for reaction of $Pt_4(OAc)_8$ blue and excess K_2SO_4, **31**	140
62.	Visible spectroscopic measurements	141
63.	Determination of total ligands per cluster by ^1H NMR	144
64.	Results of elemental analyses	147
65.	Proposed formulae, supporting data, and proposed structures for all of the platinum complexes presented	184

LIST OF TABLES (continued)

Table | Page

66. F_o F_c Tables for $F_K[Pt(NO_2)_4(NO)H_2O] \cdot H_2O$, 1. 197
67. F_o F_c Tables for $K_2[Pt(NO_2)_2(NO)Cl_3]$, 2. 240
68. F_o F_c Tables for $K_2[Pt(NO_2)_2(Br)_2]$, 3. 271
69. F_o F_c Tables for $K_2[Pt(NO_2)_2Cl_4]$, 4. 280
70. F_o F_c Tables for $K_2[Pt(Cl)_2(PO_3)_2]$, 5. 286
71. F_o F_c Tables for $[Pt_4(OAc)_6(CO)_2] \cdot 2HOAc$, 6 317

LIST OF FIGURES

Figure — Page

1. The reaction sequence leading to the dimeric platinum(III) phosphate and sulfate complexes. 8

2. Oxopyridonate ligands and their derivatives. 12

3. (a) Head-to-head configuration. (b) Head-to-tail configuration 12

4. The octakisacetatoplatinum(II) complex which is of interest in this investigation 15

5. The newer, somewhat safer synthesis of the oktakisacetatoplatinum(II) complex 18

6. The preparation of the octakisacetatoplatinum(II) complexes in this study. 19

7. Synthetic schemes for compounds 1-5. 24

8. Synthetic schemes for compounds 6-8. 29

9. Synthetic scheme for compounds 19-32 37

10. ORTEP view of $K[Pt(NO_2)_4(NO)(OH_2)]\cdot OH_2$, 1. 66

11. ORTEP view of $K_2[Pt(NO_2)_2(NO)(Cl)_3]$, 2 70

12. ORTEP view of $K_2[Pt(NO_2)_2Cl_4]$, 3 74

13. ORTEP view of $K_2[Pt(NO_2)_4Br_2]$, 4 76

14. ORTEP view of $K_2[Pt(Cl)_2(PO_3)_2]$, 5 80

15. ORTEP view of $[Pt_4(OAc)_6(CO)_2]\cdot 2(HOAc)$, 6. 83

16. The molecular numbering scheme used for this investigation: a) head-to-head platinum(III) dimer; b) head-to-tail platinum(III) dimer. 92

17. ^1H NMR spectrum of $[Pt_2(CH_3)_4(mhp)_2(pyr)]$. 94

LIST OF FIGURES (continued)

Figure | Page

18. $^{13}C(^{1}H)$ NMR spectrum of $[Pt_2(CH_3)_4(mhp)_2(pyr)]$ 95

19. Upfield region of ^{195}Pt NMR spectrum of $[Pt_2(CH_3)_4(mhp)_2(pyr)]$. 96

20. Downfield region of ^{195}Pt NMR spectrum of $[Pt_2(CH_3)_4(mhp)_2(pyr)]$. 97

21. Figure 21.^{1}H NMR spectrum of $[Pt_2(CH_3)_4(hp)_2(C_2H_5)_2S)]$. 99

22. $^{13}C(^{1}H)$ NMR spectrum of$[Pt_2(CH_3)_4(hp)_2((C_2H_5)_2S)]$. 100

23. ^{195}Pt NMR spectrum of $[Pt_2(CH_3)_4(hp)_2((C_2H_5)_2S)]$ 101

24. ^{1}H NMR spectrum of $[Pt_2(CH_3)_4(mhp)_2((C_2H_5)_2S)]$ 103

25. $^{13}C(^{1}H)$ NMR spectrum of $[Pt_2(CH_3)_4(mhp)_2((C_2H_5)_2S)]$. . . . 104

26. ^{195}Pt NMR spectrum of $[Pt_2(CH_3)_4(mhp)_2((C_2H_5)_2S)]$. 105

27. ^{1}H NMR spectrum of $[Pt_2(CH_3)_4(fhp)_2(pyr)_2]$ 107

28. $^{13}C(^{1}H)$ NMR spectrum of $[Pt_2(CH_3)_4(fhp)_2(pyr)_2]$. 108

29. ^{195}Pt NMR spectrum of $[Pt_2(CH_3)_4(fhp)_2(pyr)_2]$. 109

30. ^{1}H NMR spectrum of $[Pt_2(CH_3)_4(chp)_2(pyr)]$. 111

31. $^{13}C(^{1}H)$ NMR spectrum of $[Pt_2(CH_3)_4(chp)_2(pyr)]$ 112

32. Upfield region of ^{195}Pt NMR spectrum of $[Pt_2(CH_3)_4(chp)_2(pyr)]$. 113

33. Downfield region of ^{195}Pt NMR spectrum of $[Pt_2(CH_3)_4(chp)_2(pyr)]$. 114

34. ^{1}H NMR spectrum of $[Pt_2(CH_3)_4(fhp)_2((C_2H_5)_2S)]$ 116

35. $^{13}C(^{1}H)$ NMR spectrum of $[Pt_2(CH_3)_4(fhp)_2((C_2H_5)_2S)]$. . . . 117

36. ^{195}Pt NMR spectrum of $[Pt_2(CH_3)_4(fhp)_2((C_2H_5)_2S)]$. 118

37. ^{1}H NMR spectrum of $[Pt_2(CH_3)_4(fhp)_2(pyr)]$. 120

38. $^{13}C(^{1}H)$ NMR spectrum of $[Pt_2(CH_3)_4(fhp)_2(pyr)]$ 121

LIST OF FIGURES (continued)

Figure Page

39. Upfield region of ^{195}Pt spectrum of $[Pt_2(CH_3)_4(fhp)_2(pyr)]$. 122

40. Downfield region of ^{195}Pt NMR spectrum of $[Pt_2(CH_3)_4(fhp)_2(pyr)]$ 123

41. ^{1}H NMR spectrum of $[Pt_2(CH_3)_4(hp)_2(pyr)_2]$. 126

42. $^{13}C(^{1}H)$ NMR spectrum of $[Pt_2(CH_3)_4(hp)_2(pyr)_2]$ 127

43. Upfield region of ^{195}Pt NMR spectrum of $[Pt_2(CH_3)_4(hp)_2(pyr)_2]$. 128

44. Downfield region of ^{195}Pt NMR spectrum of $[Pt_2(CH_3)_4(hp)_2(pyr)_2]$. 129

45. Hypothetical mechanism for the generation of a nitrosyl complex. a) The protonation of the nitrito-group; b) displacement of the NO group; c) our proposed oxidative addition of the NO ligand to the platinum(II) species (33) 154

46. Head-to-tail dimeric platinum(III) arrangement showing the two types (I and II) of methyls on opposite platinum ions 159

47. Synthesis of the derivative species and their compound numbers as presented in this discussion 183

KEY ABBREVIATIONS

Å	=	Angstroms
chp	=	Chlorohydroxypyridine
DN	=	Downfield
ESCA	=	Electron Spectroscopy for Chemical Analysis (X. P. S.)
Et	=	Ethyl
Et_2S	=	Diethyl Sulfide $[(H_5C_2)_2S]$
E_b	=	Binding energy
eV	=	Electron volts
fhp	=	Fluorohydroxypyridine
H Form	=	Formic acid
$H_2NOC_2H_3$	=	Acetamide
HOAc	=	Acetic acid
hp	=	Hydroxypyridine
Hz	=	Hertz
Me	=	Methyl
mhp	=	Methylhydroxypyridine
MHz	=	Megahertz
nm	=	Nanometers
NCN^-	=	Cyanamide
NMR	=	Nuclear Magnetic Resonance
OAc^-	=	Acetate ion
OCN^-	=	Cyanate ion
ppm	=	Parts per million
Pt	=	Platinum
pyr	=	Pyridine
SCN^-	=	Thiocyanate ion
TPP	=	Triphenylphenylphosphine
UP	=	Upfield
ν	=	Frequency
X	=	Halogen, or <u>specified</u> functional group
Y	=	<u>Specified</u> functional group

ABSTRACT

There is a great deal of interest in the synthesis of materials which possess special physical and chemical properties. One such area of interest is concerned with the formation and chemistry of platinum-platinum bonds. The structures of platinum-platinum bonded species which exhibit the platinum(III) oxidation state have only recently been elucidated. The chemical pathways leading to the platinum(III) oxidation state are not well understood. Presented here is structural evidence for what is considered to be one of the initial steps in the pathway leading to platinum-platinum bonds. Two single crystal x-ray crystal structures exhibiting a bent nitrosyl ligand upon a monomeric platinum center are presented. To our knowledge, no other examples of bent nitrosyl ligands on platinum monomeric species exist in current literature. The single crystal x-ray crystallographic structures of three closely related complexes are also presented. ESCA studies, visible spectral and infrared spectral studies are also presented in support of the structural data. Additionally, the results of NMR and ESCA studies of a group of structurally related platinum(III) dimeric complexes are presented. The NMR data include complete sets of ^{195}Pt, ^{13}C, and ^{1}H spectral information. Generally, the solid state structure was found to remain intact in solution. Unusually large platinum-platinum coupling constants were observed during the course of the investigations. The ESCA studies of the same platinum-platinum bonded species lend support to the platinum(III) oxidation state. Finally, the synthesis, analysis, and chemical characterization of a group of tetrameric platinum-platinum bonded complexes is presented. A newly developed synthetic scheme for the tetrameric complexes, along with an efficient method of chromatographic purification of the complexes is presented. Single crystal x-ray crystallographic information is presented about a new structural derivative of the octakisacetato platinum complex. The complex exhibits a pair of bridging carbonyl ligands on opposite sides of the tetrameric rectangle, and a pair of asymmetric bridging acetate ions <u>trans</u> to the carbonyl ligands. The short sides of the tetrameric rectangle are bridged by symmetric acetate ions. Infrared, visible, ESCA and elemental analytic studies are presented as evidence for the complexes. A novel application of ^{1}H NMR determining the total number of acetate ligands per cluster is also presented. Eighteen other derivatives of the octakisacetato tetrameric complex were made using different ligands. The reaction conditions under which the complexes were found to react appear unique for this set of complexes. Infrared, visible, ESCA and elemental analytic data are presented in support of the proposed structures for the complexes. The possible oxidation states of each of the complexes is considered. It is hoped that this work will aid in future systematic synthetic efforts for exploratory studies of platinum-platinum bonded compounds.

INTRODUCTION

For 3000 years platinum has fascinated man (1). This interest stems from his recognition that platinum is a relatively rare element, occurring only in specific mineral deposits. These deposits are scattered in a mere handful of locations throughout our world, including the U.S.S.R., South Africa, South America, and Montana (2). A number of theories abound concerning the origins of the minerals which bear the platinum metals. One of the most highly publicized theories suggests these deposits originated with meteorite impacts on the earth's surface (3). Whatever the origins of such minerals, modern man has certainly been able to enjoy the resulting chemical characteristics which the platinum metals offer. The following discussion examines one of these characteristics of platinum chemistry: platinum-platinum bond formation.

Before proceeding with the discussion, a brief review of man's fascination with the platinum metals is in order. This fascination has existed for some 30 centuries; an Egyptian casket found at Thebes, dating from the seventh century B.C., contained an alloy of platinum, iridium and gold (4). There was, however, no evidence suggesting that the alloy of platinum was to the Egyptians anything more than a workable precious metal. Eight hundred years later, during the first century A.D., Pliny discussed platinum, known then as cassiteros or plumbum candidum. Pliny suggested the following:

> It is now known that cassiteros is a product of Lucitania, and Gallaecia. It is a sand found on the surface of the earth, and of a black color, can be detected only by its weight.... It is also found in the gold mines that are known as Alutice or Talutice, the stream of water which is passed through then detaches certain black pebbles, mottled with small white spots and of the same weight (density) as gold. Hence it is that they remain with gold in the baskets in which it is collected; and being separated in the furnace, are then melted, and become converted into album plumbum (5).

Other than this scanty knowledge, very little was really learned about the platinum family for centuries; however, there are a number of accounts of the mysterious "platina" metal found throughout some of the early literature (6). During the sixteenth century, J. C. Scaliger noted that there was a non-fusible metallic substance in the mines of Mexico and Darian (Panama) which did not melt in the Spanish gold smelting furnaces. Current thought is that the described substance was probably platinum, simply because platinum is known to occur in these very areas. During the middle of the eighteenth century, A. deUlloa accompanied the expedition sent from France to measure the arc of the meridian of the equator, and in his account of the voyage he mentioned that in the mines of El Chaco', Columbia, South America, there was an unworkable metallic stone which the Spanish called "platina" and which made gold ores useless if it were associated in large quantities (7). The Spanish considered the platina useless and commonly threw the platina into the rivers of South America.

The study of platinum began in earnest in 1741 when W. Brownigg received a specimen of native platina from C. Wood, a metallurgist in

Jamaica, who claimed that he had obtained the sample from Carthogina, New Grenada. A number of other platina samples began to find their way to Europe at about the same time and were examined by several different investigators (8). A number of theories sprouted, concerning both what the metal was and what its specific properties were. These were published in the metallurgical/ chemical literature of the period (9).

Some decades later, during April 1803, R. Chenevix received an anonymous circular to the effect that a new metal called palladium could be purchased at Forster's of Gerrard Street, Soho, London (10). The "new" metal had some very specific properties which were previously unknown for virtually any other element. Chenevix believed this to be a fraud; he bought up the entire stock and, after investigating the question, concluded that the substance was not a new element but rather a platinum amalgam of peculiar properties (11). Following Chenevix's publication at the Royal Society May 3, 1803, there appeared an advertisement offering a reward to anyone who could prepare a grain of the new substance, either by Chenevix's method or any other (12). Though no one succeeded in securing the reward, in 1804 W. H. Wallaston announced the discovery of a new element in platinum ore. Between 1804 and 1828 the other members of the platinum metal family were isolated and purified (1804--palladium, rhodium, iridium, osmium; 1828--ruthenium) (13).

The chemical exploration of the platinum metals began almost simultaneously and has, in the opinion of this author, proven to be quite a significant segment of the transition metal chemical literature. Much of the earliest literature concerning the chemical properties of the platinum metals resulted from simply questioning what would be the resultant compounds (and their chemical properties) upon combination with a plethora of metals and ligands. Descriptions of alloys of platinum with copper, mercury, uranium, iron, and other platinum metals began to appear in the literature as early as the 1840's (14). Additionally, reports of some of the earliest coordination/cluster complexes began to appear at roughly the same time. These early efforts were made using both simple ligands, such as Cl^-, Br^-, I^-, OH^-, SO_4^{2-}, PO_4^{2-}, and a number of much more complicated ligands (14). The only analytic method employed by many of the chemists was elemental analysis and generally a substantial amount of reaction chemistry. Of course, the chemist's eyes were also a very valuable analytic tool and provided a significant amount of the information which one observes in the literature, even to this day.

Studying the literature both old and relatively recent yields discovery of a number of complexes which reportedly contain polynuclear metal centers. These complexes are investigated for a number of reasons; a few of the major areas of interest follow:

1) biological activity of clusters;

2) electronic applications of clusters;

3) catalytic activity;

4) structure bonding relationships; and

5) systematic chemical properties;

Each of the above areas has a significant amount of literature associated with it; however, a review of such a broad spectrum of chemistry is inappropriate at this time. Nonetheless, the question of just what a platinum cluster is needs clarification. For the purposes of this dissertation, a platinum cluster will be defined as being two or more platinum atoms which are brought together either by the "bite" size of a ligand or by the formation of a platinum-platinum bond. Of course, the more interesting cases occur when a metal-metal bond is formed or broken due to the chemical interactions involved in such processes. Examples vary from relatively simple dimeric species which exhibit platinum-platinum bonds, through groups of trimeric, tetrameric, and one-dimensional polymeric species. Such examples only begin to touch upon the complexity with which the coordination chemist must attempt to cope.

Our interest in the platinum metal clusters has centered on developing the type of systematic chemistry that can be performed upon the clusters either in the formation or destruction of the platinum metal clusters themselves. To initiate this, we have set about investigating the chemistry of platinum-platinum bonded species. Our approach has been guided by several areas of specific interest which follow:

1) synthesis;

2) disproportionation reactions;

3) substitution reactions;

4) cluster redox chemistry; and

5) mechanistic considerations.

Reading the following pages will reveal that each of the five areas above will be addressed, either as a route to compounds, or as a method for the analysis of such complexes.

The initial portion of this work was undertaken to investigate the reaction chemistry of a group of binuclear platinum(III) complexes. Such binuclear d^7–d^7 metal complexes possess a net single bond between the metal atoms and exhibit an electronic configuration of $\sigma^2\pi^4\delta^2\delta^{*2}\pi^{*4}$ (15). Generally the systems have two or four ligands bridging the metal centers and possess axial positions which can be occupied by appropriate monodentate ligands. Such a style of bonding and electronic configuration is observed in Rh_2 +4 systems (16–18), for which several examples have been structurally characterized. By comparison, however, the Pt_2 +6 systems have only recently been studied in any detail, and few structural examples are known.

Sulfate and Phosphate Bridged Species

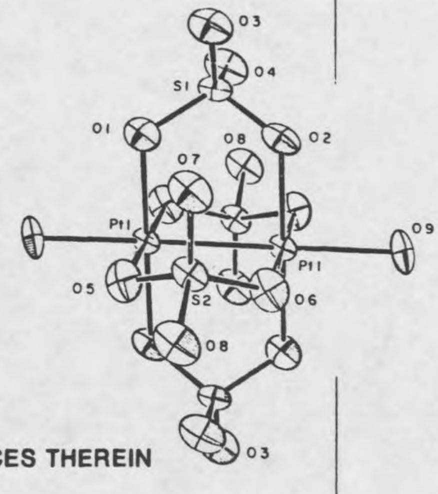
In 1905 Blondel prepared a complex which he suggested was a platinum(III) complex. This complex was the first example of such an oxidation state and still elicits questions about the electronic configuration of the metal atoms (19). In a complex reaction between platinum(IV) and an aqueous sulfuric acid solution which was reduced with oxalic acid, Blondel formed the binuclear platinum(III) complex $[H_2(Pt_2(SO_4)_4(H_2O)_2]\cdot 9.5H_2O$. Additionally, Blondel reported the sodium and potassium salts of the complex (20). Blondel's work was confirmed several years later by Wöhler and Frey (21), who also synthesized several closely related species. The potassium salt which Blondel reported proved to be significant in that it was the first structurally characterized platinum(III) complex (22) exhibiting platinum-platinum bonds (23-27).

The reaction conditions under which the complexes are prepared appear quite simple. Essentially all that is required is heating a given platinum(II) complex with an aqueous solution of either sulfuric or phosphoric acid. During the course of the reaction, at least four color changes are observed, as is exhibited in Figure 1. The reaction begins as a colorless solution, changing sequentially to blue, green, yellow; then the dimeric red-orange product precipitates from solution. Our efforts to perform nuclear magnetic resonance (NMR) spectroscopic studies upon the product proved exceptionally difficult due, as we found, to the low solubility of the product in all solvents. Additionally, a group of Australians were at the same time completing the nuclear magnetic resonance studies of the complexes (29). Since our interests were focused both upon the study of platinum-platinum bonds and upon the processes which must take place to form the bonds, we decided to investigate the events which precede platinum-platinum bond formation. Given the idea (in inorganic chemistry) that one color of a solution can indicate a single compound, there is in the above system the potential for

SYNTHESIS OF Pt(III):PO_4^- AND SO_4^{2-} DIMERS*

$$K_2PT(NO_2)_4 + H_2SO_4 \xrightarrow{110^\circ} \text{BLUE} \rightarrow \text{GREEN} \rightarrow \text{YELLOW} \rightarrow \text{RED}$$

$(Pt_2(SO_4)_4 \cdot 2H_2O)^{2-}$



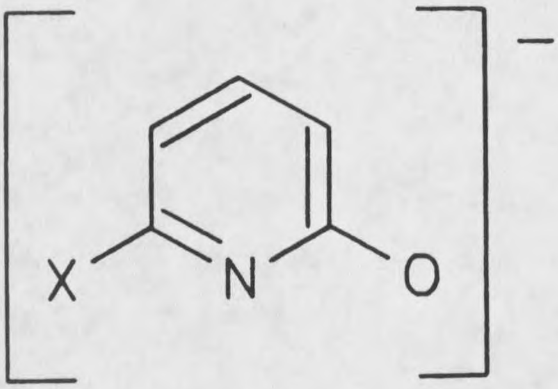
*COTTON et al. INORGANIC CHEMISTRY (1982) 21 1709, AND REFERENCES THEREIN

Figure 1. The reaction sequence leading to the dimeric platinum(III) phosphate and sulfate complexes.

describing at least two or three complexes. In theory, describing such a series of events could give a "snapshot" view of the sequence of events which lead to the formation of platinum-platinum bonds and perhaps present some insights into the mechanism of platinum-platinum bond formation. Therefore, this line of research was pursued and is described herein. We were able to obtain a group of blue crystals which were formed in the early part of the reaction sequence described previously. These crystals proved to be highly air and moisture sensitive. For platinum there seem to be three general classes of blue compounds. The best known class consists of linear tetrameric complexes of mixed valence (30). A second class, lesser known but well-characterized, is mononuclear, most probably with a charge transfer band in the long wavelength part of the visible spectrum (31-32). The third class has but a single well-characterized example—a mononuclear, blue, paramagnetic platinum species with rather bulky electron donating ligands which possibly function to prevent the dimerization of the platinum centers (33). A number of studies have been reported upon the blue solution which forms when platinum(II) nitrites react with phosphoric and/or sulfuric acids (23,28,34-36). The blue solutions owe their color to an absorption band near 630 nm. Some investigators have suggested that the blue compounds are nitrosyl complexes, but no structural information has been available due to the difficulties encountered with handling the complexes. The two complexes which are described in the following discussion (blue and green) each exhibit a bent nitrosyl ligand upon the platinum atom. Only one other example of a bent nitrosyl on a platinum center was previously structurally characterized (37). Both complexes were shown to be highly unstable to air, moisture, and elevated temperatures. Additionally, unless the crystals of each compound were kept in their mother liquor and stored at -20°C under airless conditions, the reaction was observed to proceed toward the red dimeric platinum(III) product. The blue species is believed to be one of two species present in solution during the initial steps of the platinum-platinum bond formation reaction sequence. The other species is probably a platinum(II) species which results from the well-characterized hydrolysis reaction of $K_2Pt(NO_2)_4 \cdot 2H_2O$ in aqueous acid solutions (38). Since these two complexes are the second and third structural examples of the bent nitrosyl ligand on a platinum center, they have given some interesting insight into the initial steps of platinum-platinum bond formation. The structural details of bent nitrosyls on platinum have also been of interest. During efforts to make analogues to the two new complexes, several closely related species were crystallized and their structures elucidated. Such compounds will also be discussed in light of their relationship to the formation of platinum-platinum bonds.

α-Oxopyridonate Bridged Platinum(III) Complexes

There have been a number of synthetic approaches for the preparation of complexes with the platinum ions in the formal +3 oxidation state; however, most approaches yield products which are insoluble, give poor chemical yields, or are not reproducible (as we observed in the formation of the binuclear sulfate and phosphate species). A synthetic approach for the preparation of binuclear platinum(III) complexes with properties including high yield, stability, and solubility has been suggested by Vrieze (39-40). Vrieze's method employs platinum(II) precursors which (by oxidative addition reactions) yield binuclear platinum(III) products. The method involves the use of silver(I) carboxylate salts, which have been shown to give the binuclear platinum(III) species. Such species possess many of the "desirable" properties described earlier. F. A. Cotton's research group has employed a variation of Vrieze's method to obtain a group of new and interesting platinum(III) complexes. The complexes contain hydroxypyridine (α-pyridone) derivatives which are known to give some interesting coordination geometries, especially as bridging ligands. The asymmetric ligands (Figure 2), typically stabilize metal-metal bonds by bridging the two metal centers (41-42). Examples of such ligands playing an important role in the chemistry of metal-metal bonds are found in a number of cases ranging from quadruple bonds (Cr, Mo, W) to single bonds (Rh, Pt) (15).



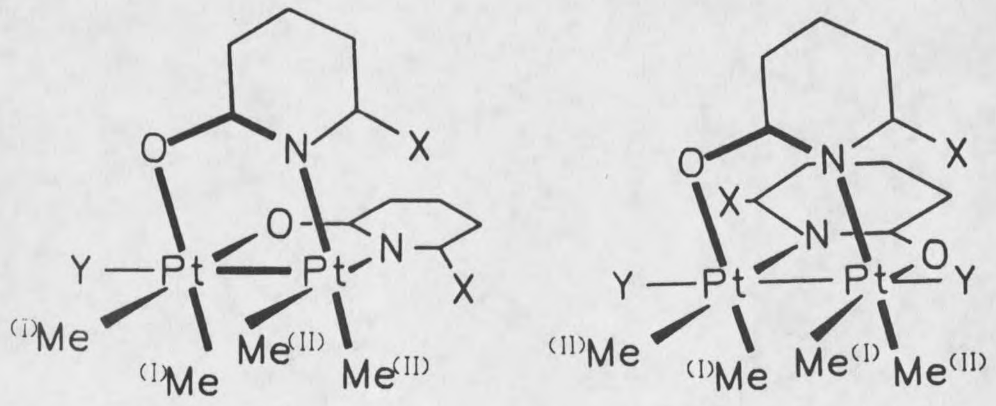
x = CH_3 mhp^-

x = Cl chp^-

x = F fhp^-

x = H hp^-

Figure 2. Oxopyridonate ligands and their derivatives.



a b

Figure 3. (a) Head-to-head configuration. (b) Head-to-tail configuration.

The resulting hydroxypyridinoate complexes have coordination geometries that are dependent upon the steric bulk of the substituted pyridine ring. If the substituent is large (e.g., Cl^- or CH_3), the complexes take the head-to-head bridging ligand arrangement, with one of the axial sites vacant due to the steric interference of the ring substituent (Figure 3). If, on the other hand, the substituent is relatively small (e.g., H or F), head-to-tail or head-to-head ligand arrangements can result. More interestingly, the complexes with the small substituents can inter-convert by the addition of an excess or the removal of the axial donor ligand (42). The preparation of the complexes follows the general scheme shown below:

$$[Pt_2(CH_3)_4(R_2S)_2] + 2Ag(xhp) \rightarrow [Pt_2(CH_3)_4(xhp)_2(R_2S)] + 2Ag^{\circ}$$

$$[Pt_2(CH_3)_4(xhp)_2(R_2S)] + xs\ pyridine \rightarrow [Pt_2(CH_3)_4(xhp)_2(py)_n] + nR_2S$$

where R = C_2H_5; x = H, F Cl, Br, or CH_3; and n = 1 or 2.

Using the above reaction sequences, Cotton's group has to date prepared ten new platinum(III) complexes, and they have structurally characterized the compounds by single crystal x-ray diffraction methods. Eight of the ten new complexes have been investigated by this author using nuclear magnetic resonance and x-ray photoelectron spectroscopic methods. In-solution structural details, NMR chemical shifts, and oxidation state information are reported here.

The platinum(III) complexes which were synthesized by Cotton's group are very stable in most organic solvents and can generally be isolated in high yield (70-90%). The NMR studies which appear here suggest that the head-to-head complexes are stable in solution for relatively long periods of time, while the head-to-tail complexes tend to revert to equilibrium mixtures of head-to-head and head-to-tail forms over the course of a few hours to days. Evidence for interconversion is found in the platinum-195 NMR spectral data. Nonetheless, there is no evidence for the dissociation of the complexes in either case. Additional studies of the reaction chemistry of these complexes continues both here at Montana State University and in Cotton's group at Texas A and M University.

Platinum Carboxylate Bridged Compounds

Vreize's and Cotton's success with the formation of platinum-platinum bonds through oxidative additions of various carboxylato species to metal centers led us to investigate a tetrameric carboxylato species which had been characterized as being platinum(II). The complex exhibits an interesting structure (Figure 4). The structure is composed of a nearly planar square of four platinum ions, with each platinum ion being 2.5 Å from each of its nearest neighbors. There are bridging acetate ions between each of the metal centers, such that each metal center exhibits pseudo-octahedral coordination. The acetate ligands are alternately axial and equatorial on each side of the square; the resulting symmetry of the complex gives it quite an aesthetic appeal. Besides the aesthetic aspects of the complex, one notes that the 2.5 Å distance between the metal centers suggests platinum-platinum bonds. Such an

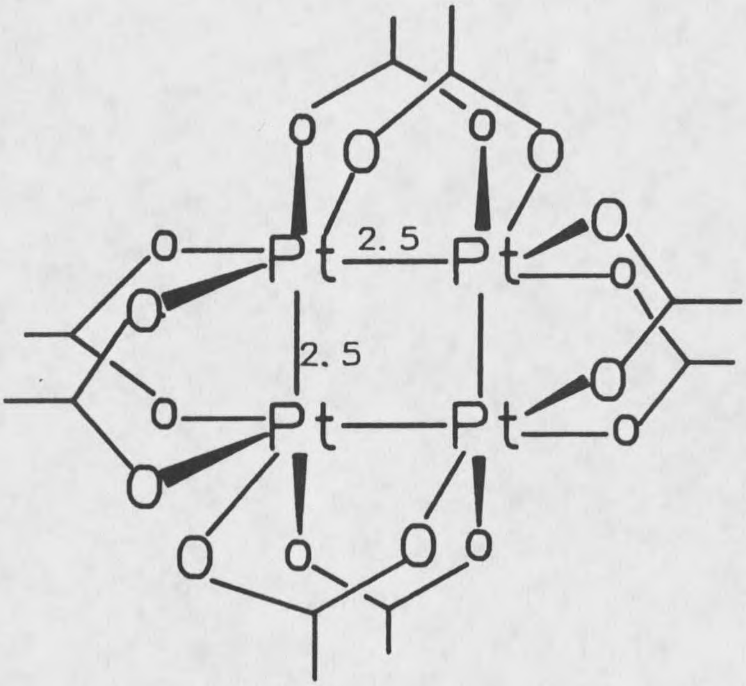


Figure 4. The octakisacetatoplatinum(II) complex which is of interest in this investigation.

arrangement potentially could yield a very sensitive measurement of platinum-platinum bonds. Coupling such information with systematic synthetic strategies could potentially elicit a variety of new chemical complexes. Such synthetic strategies could possibly lead to new (we hoped) syntheses of platinum(III) species. Therefore we began to investigate the synthesis of the square tetrameric species.

The preparation of the multinuclear platinum acetate species was first reported in 1965 (43). X-ray powder diffraction studies suggested that the complex was trimeric like diacetatopalladium(II) but not isomorphous (44). The first reported synthesis was an extremely complicated and somewhat convoluted approach to the complexes in question. The synthesis began with sodium hexahydroxyplatinate(IV) being dissolved in concentrated nitric acid and heated until a brown syrup containing crystals of sodium nitrate resulted. Glacial acetic acid was then added to the syrup and the mixture boiled until the nitrate crystals became white. After cooling, filtration, and washing, the solution was boiled over an open flame until a red orange syrup resulted. Most of the nitric acid was then thought to have been expelled. The addition of a 20% formic acid:80% acetic acid solution followed by heating gave a bright green solution. Further addition of formic acid along with boiling reportedly gave an aqua-marine blue solution, which became deep purple upon standing. Crystals of complex were then reported to precipitate along with a small amount of platinum metal. After washing with acetic acid and chloroform, the purple crystals were reportedly recrystallized from chloroform:acetic acid (1:1). A few years later the above synthesis was reported to give an explosion (45), and a safer synthetic approach appeared in the British patent literature (46). The color of the complex warranted a patent for I.C.I., Ltd., apparently due to the strong interest in the "platinum blues" which were thought to be very effective therapeutic agents in cancer patients (30), though another possibility stems from the way in which the complexes stack in the crystalline lattice, which could have prompted interest as a one-dimensional conducting polymer such as has been investigated recently (47).

The newer, safer synthesis employs tetrachloroplatinate(IV) with the addition of the appropriate carboxylato silver(I) salt. Reduction with a very slight excess of formic acid follows, and the resulting blue complex was claimed to be pure (Figure 5). Structural evidence for the blue tetrameric octakis-acetatotetraplatinate(II) complex was obtained (Figure 4) (48-50). One problem was noted in both syntheses--for both cases some platinum metal always resulted. Furthermore, yields were not at all consistent (they ranged from 0% to 75%). These two factors suggested to this author that the resulting blue solution even in the "new" synthesis contained at least one product and possibly more. In this investigation the blue solution was, in fact, found to contain several constituents which have been characterized. The major product, the blue fraction, was isolated and has been found to have only slight contamination from silver (Figure 6). The synthesis, isolation, purification, analysis, and characterization of each of the products has shown that there are at least two tetrameric species produced in the reaction. Some systematic reaction chemistry has also been performed upon the complex which has previously been characterized as "not being very reactive under normal conditions" (51). The systematic chemistry and some of the implications for this type of platinum clusters will be discussed in the third portion of the Discussion (Chapter 5).

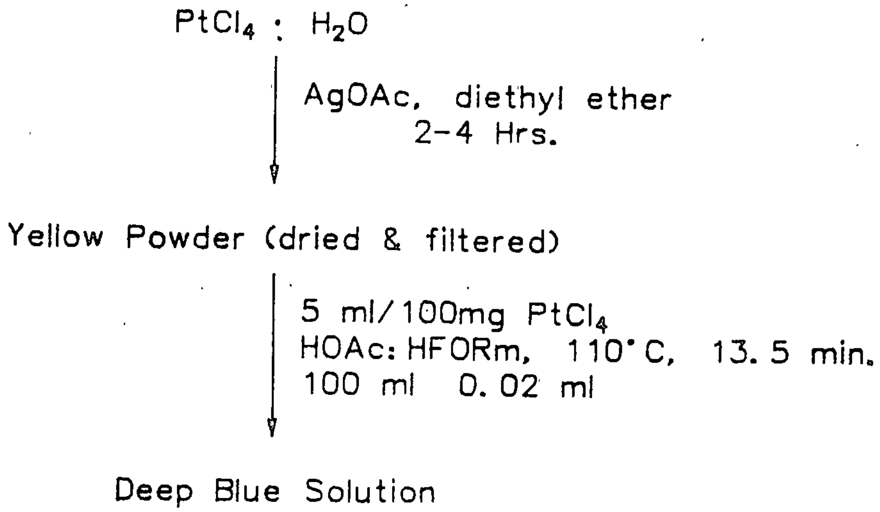


Figure 5. The newer, somewhat safer synthesis of the octakisacetatoplatinum(II) complex.

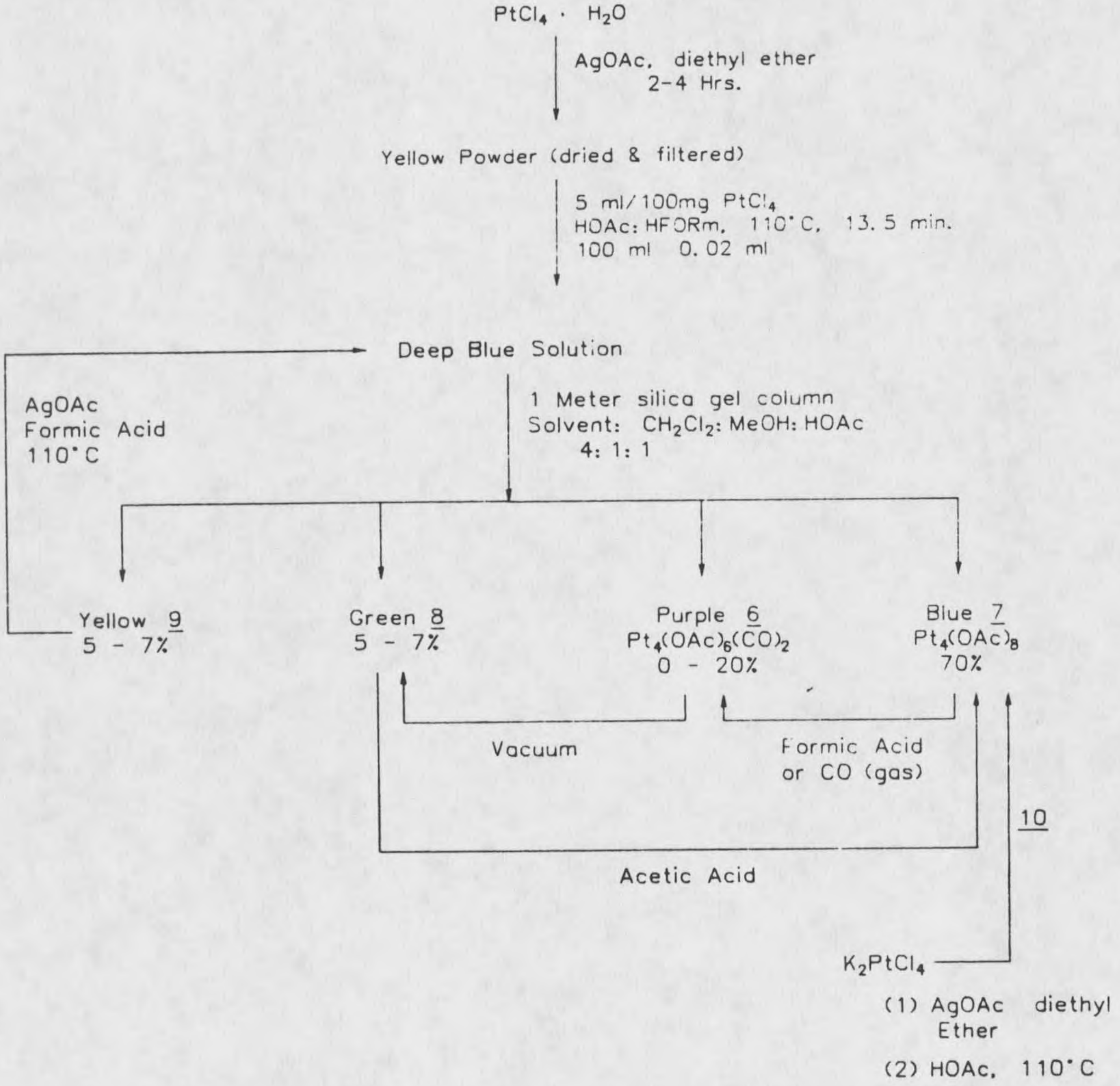


Figure 6. The preparation of the octakisacetatoplatinum(II) complexes in this study.

PURPOSE OF THE PRESENT INVESTIGATION

The general purpose of this investigation has been threefold. We have tried to 1) gain further insight into how platinum-platinum bonds are formed, 2) characterize the platinum-platinum bonds, and 3) understand some of the systematic chemistry which they will undergo. To achieve these goals several physical methods have been employed. These include: nuclear magnetic resonance spectroscopy, visible spectroscopy, electron spectroscopy for chemical analysis, single crystal x-ray crystallography, infrared spectroscopy, commercial elemental analyses, in-house heavy metal analyses, and chemical logic.

The thematic statement above, concerning the reason for interest in the complexes involved, is a rather broad statement. More specifically stated, there is a great deal of interest in making materials which possess certain physical and chemical properties. One such area concerns the formation and chemistry of platinum-platinum bonds. The work presented in this thesis addresses such chemistry.

This thesis is organized into six chapters. Chapter three examines the experimental methods used for the preparation and analysis of the complexes. Chapter four is divided into three parts and presents the results of each portion of this investigation. The three parts are each concerned with the following: complexes which are on the pathway to platinum-platinum bond formation, NMR and ESCA studies of eight complexes which are known to posses a platinum-platinum bond in the solid state, and, finally, the reactivity of a platinum-platinum bonded species in the third portion of chapter four. Chapter five discusses the results and their interpretations for this investigation. Any implications for structural details and platinum-platinum bonding are discussed in chapter five. Chapter six contains a summary of the work performed in this investigation and gives the significant advances achieved by this investigation.

EXPERIMENTAL

Preparation of Compounds

Preparation of $K_2Pt(NO_2)_4 \cdot H_2O$

$K_2Pt(NO_2)_4$ was prepared as described elsewhere (55). However for the purpose of this investigation it was found that recrystallizing the compound a minimum of three times, with a slight excess of KNO_2 present during each crystallization, was required to assure exclusion of all chloride ion. The resulting overall yield was approximately 50%.

Preparation of $K_2Pt(NO_2)_4(NO)(H_2O)$, 1

$K_2Pt(NO_2)_4$ was prepared as described above. A solution of phosphoric acid in water was prepared as a 3:1 mixture of 85% phosphoric acid and water by volume. The solution was degassed and stored under argon. To 1.5 ml of the solution was added 50 mg (1.08×10^{-4} moles) of $K_2Pt(NO_2)_4$. A very faint blue solution resulted. The solution was heated to 80°C for two to three minutes under argon during which time it became an intense dark blue. The solution was placed in a freezer at -20°C in the dark. Over a period of 53 days dark blue crystals suitable for x-ray diffraction where observed to form. Attempts to remove the mother liquor invariably resulted in color changes which indicated decomposition. The crystals retained their blue color only when handled under argon at reduced temperature and without the complete removal of the mother liquor (Figure 7).

Method II For the Preparation of $K[Pt(NO_2)_4NO{\cdot}OH_2]{\cdot}OH_2$, 1, with $NOBF_4$

$K_2Pt(NO_2)_4$ was prepared as described for 1. 0.050 g $K_2Pt(NO_2)_4$ (1.08×10^{-4} moles) were dissolved in a minimum amount of H_2O. To the solution were then added ten equivalents $NOBF_4$ (0.0125 g) under argon. Immediately the solution became a dark blue color. No crystals were obtained (Figure 7).

Preparation of $K_2[Pt(Cl_3)(NO_2)_2NO]$, 2

The deep blue solution containing 1 was prepared as described earlier. Three equivalents of KCl (0.023 g, 3.24×10^{-3} moles) were added to the solution and the resulting green solution refrigerated at -20°C. Dark green crystals of the potassium salt of 2 formed in three to five days. Approximately 0.010 g of product was obtained by filtration under argon. The mother liquor could not be completely removed without decomposition of the product, and so elemental analysis was not attempted (Figure 7).

Preparation of $K_2[Pt(NO_2)_2Cl_4]$, 3

0.050 g of $K_2Pt(NO_2)_4$ (1.08×10^{-4} moles) were dissolved in a minimal amount of distilled water, phosphoric acid (3:1) solution. The solution was heated at 80°C under argon until a bright yellow solution resulted. Four equivalents KCl were added from a stock solution in glass distilled H_2O. The solution was allowed to stand

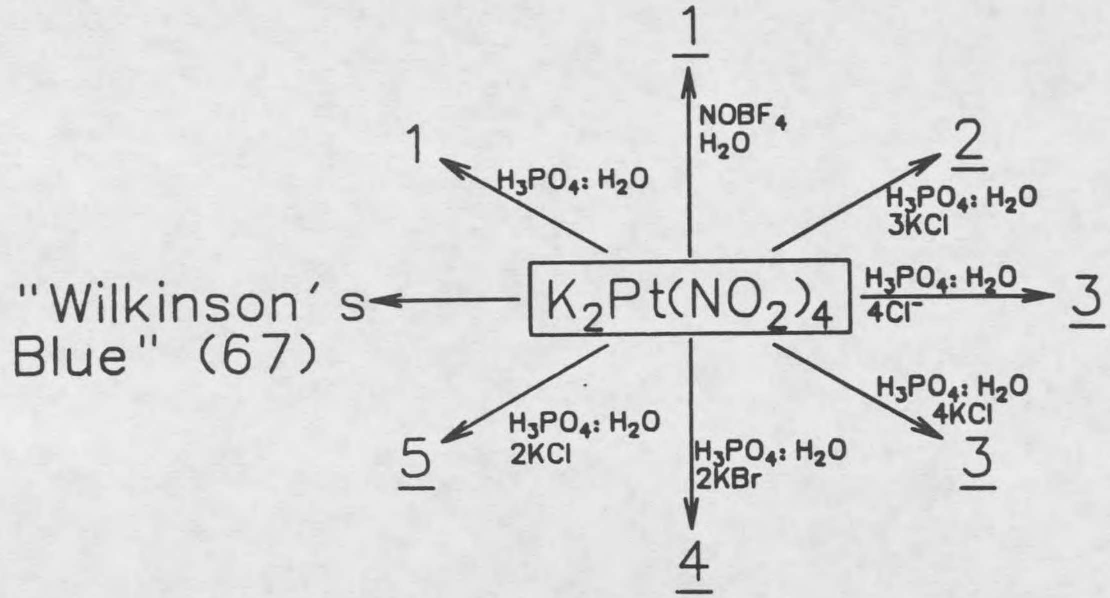


Figure 7. Synthetic schemes for compounds 1 - 5.

in a cold room at -20°C for 10-12 days when bright yellow air stable crystals suitable for x-ray crystallographic studies resulted (Figure 7).

Method II for Preparation of $K_2[Pt(NO_2)_2Cl_4]$, 3

The deep blue solution containing 1 was prepared as described above. Four equivalents of KCl (0.008 g, 3.12 x 10^{-4} moles) were added to the solution. The resulting yellow solution was refrigerated at -20°C. Bright yellow crystals of the potassium salt of 5 formed in eight to nine days. Approximately 0.015 g (61%) of product was obtained by filtration under argon (Figure 7). The crystals were found to be air stable and air dried.

Preparation of $K_2[Pt(NO_2)_4Br_2]$, 4

The deep blue solution containing 1 was prepared as described above. Two equivalents of KBr (1.27 x 10^{-2}g) were added to this solution and the resulting red solution refrigerated at -20°C. Dark red crystals of the potassium salt of 4 formed in five to seven days. Approximately 0.023 g (34%) of product was obtained by filtration under argon. The crystals were dried with 95% ethanol and diethyl ether, then found to be air-stable (Figure 7). Since this was a known compound no elemental analyses were attempted.

Preparation of $K_2[Pt(PO_3)_2Cl_2]$, 5

The deep blue solution containing 1 was prepared as described above. The solution was heated at 80°C under argon until a bright yellow solution resulted. Two equivalents of (1.56 x 10^{-4} moles) KCl were added. The solution was allowed to stand in a cold room at -20°C for four days when small, bright yellow, air stable crystals suitable for x-ray crystallographic studies resulted. No yields were measured (Figure 7).

Preparation of $Pt_4(OAc)_8$ Blue from Platinum(IV)

This preparation is a modified method of Davidson and Triggs (45). (See Figure 6.)

Silver(I) acetate was prepared as described earlier. To approximately 2.5 ml of diethyl ether was added 0.200 g (6×10^{-4} moles) $PtCl_4$ (platinic chloride). One or two drops of water then followed to give a bright red solution over a period of 15 to 30 minutes. 0.408 g (2.4×10^{-3} moles) of silver(I) acetate was added to the solution. The solution was stirred for two to three hours or until the solvent was colorless. The resulting yellow powder was dried under a stream of dry nitrogen gas and placed upon a vacuum line for one to three hours. The dry powder was suspended in 5 ml of acetic acid:formic acid which was freshly prepared. The concentration of formic acid in acetic acid was 2.52×10^{-5} moles/ml. The reduction reaction was then run at 110°C in an oil bath. Reaction times varied, but generally for a freshly-prepared sample 13.5 minutes were required to obtain a deep blue solution. The deep blue solution was then cooled with cold tap water, filtered twice through a medium or fine glass frit (to remove AgCl) and the solvent acetic acid-formic acid stripped away on a Buchi "R" rotary evaporator. The resulting blue solid was placed on a vacuum line at room temperature for 12 to 18 hours. The dried, micro-crystalline, deeply-colored solid, was chromotagraphed as described above. Four fractions resulted from the procedure, a blue fraction 7, a purple fraction 6, a green fraction 8, and a yellow fraction 9 Each of the fractions was stripped of solvent and dried over KOH under vacuum for 12 to 23 hours. Yield of the blue component was found to vary from 40% to 70% total yield.

Synthesis of $Pt_4(OAc)_8$ from Platinum(II), 10

0.250 g (6.05×10^{-4} moles) K_2PtCl_4 was suspended in diethyl ether. 0.480 g (2.9×10^{-3} moles) silver acetate, prepared as described above, was added to the platinous chloride-diethyl ether suspension. The pink slurry was stirred for about 24 hours. A salmon pink colored powder resulted. The salmon colored powder was dried under vacuum and then suspended in three to five ml of acetic acid. The resulting pink solution was then heated to 110°C for 8 to 15 minutes when a deep blue solution resulted. The solution was cooled with cold tap water, filtered twice through a medium or fine glass frit (to remove AgCl), and the acetic acid solvent stripped away on a Buchi "R" rotary evaporator. The resulting blue solid was then dried on a vacuum line at room temperature for 12 to 18 hours. The dried blue solid was then chromatographed as described above. Two fractions resulted from the procedure, a blue fraction 10, and a pink fraction 11. Each of the fractions was stripped of solvent and dried over KOH under vacuum for 12 to 14 hours; yield of the blue component was 38%.

Preparation of $[Pt_4(OAc)_6(CO)_2]\cdot 2HOAc$, 6

The purple fraction, which resulted from the chromatographic separation of the crude $Pt_4(OAc)_6$ complex, was observed to have the above formula. Yield of the purple complex was 0% to 20% by the chromatographic method (Figures 6 and 8).

Direct Preparation of $[Pt_4(OAc)_6(CO)_2]\cdot 2HOAc$, 6, from $Pt_4(OAc)_8$ Blue

Two methods for the direct preparation of the above complex were found. The first employs formic acid, while the second employs the direct addition of CO gas to the octakis-acetate complex (Figure 8).

Direct Method I for the Preparation of 6 Using Formic Acid

0.050 g $Pt_4(OAc)_8$ Blue (3.9×10^{-5} moles) was dissolved in 2.00 ml acetic acid. The solution was allowed to stir under argon until all of the powdered micro crystalline compound was dissolved. To the above solution was added 10 equivalents (3.9×10^{-4} moles) formic acid. The deep blue solution was then heated to 110°C. Within 10 minutes the solution was observed to become a dark purple color. The solution was cooled under tap water, and the solvent acetic acid stripped away on a Buchi "R" Rotary evaporator with a cool water bath. A deep purple micro-crystalline solid was obtained. Crystals were grown from acetic acid:chloroform (1:10) (Figure 8).

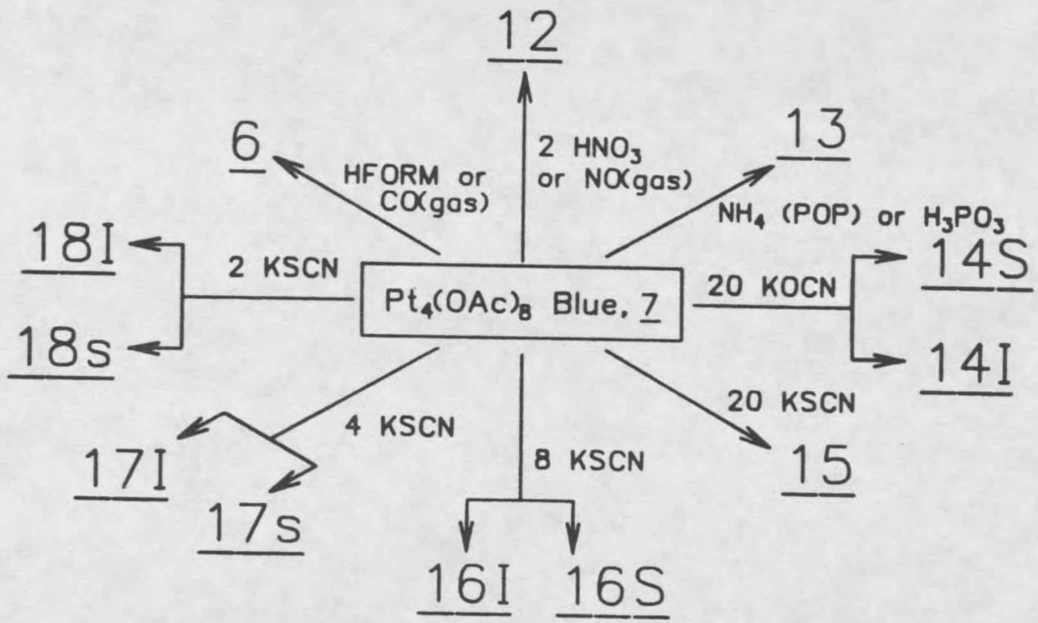


Figure 8. Synthetic scheme for compounds 6 - **18**.

Direct Method II for the Preparation of 6 Using CO Gas

0.050 g $Pt_4(OAc)_8$ (3.9×10^{-5} moles) Blue was dissolved in 2.0 ml Acetic acid. The solution was allowed to stir under argon until all of the powdered micro crystalline compound was dissolved. To the above solution was added a small portion of CO gas; then the reaction vessel was resealed. Stirring was continued at room temperature. Over the course of several minutes the solution gradually became a deep purple color. The color had to be watched most closely; if one allowed the reaction to go too long, the complex would be destroyed and platinum(0) metal would precipitate. The resulting purple solution was purged with dry nitrogen or dry argon and the solvent acetic acid removed with a Buchi "R" rotary evaporator in a cool water bath, Figures 6 and 8. Crystals were grown from acetic acid: chloroform 1:10 yield was 20%.

Direct Preparations of $[Pt_4(OAc)_6(NO)_2]\cdot 2HOAc$, 12

Two direct preparation methods were found for the preparation of the above complex. The first employs the addition of a stoichiometric amount of nitric acid, while the second employs the addition of a limited amount of nitric oxide gas, Figure 8. Both methods yield purple solids which give appropriate elemental analyses.

Direct Method I for the Preparation of 12 Using Nitric Acid

0.050 g $Pt_4(OAc)_8$ Blue (3.9×10^{-5} moles) was dissolved in 2.0 ml acetic acid. The solution was allowed to stir under argon until all of the powdered, micro-crystalline octakis-acetatoplatinate(II) complex was dissolved. To the above solution was added two equivalents (7.8×10^{-5} moles) nitric acid. The deep blue solution was allowed to stir for several hours. Invariably, the solution color darkened to a nearly black color, then gradually became a very dark red/purple. The solution was allowed to stir for 12 to 24 hours. Work up of the reaction consisted of a filtration to remove any precipitated platinum metal, then removal of solvent acetic acid by rotary evaporation. A dark purple micro-crystalline solid resulted, Figure 8. Crystals were grown from acetic acid:D_2O (1:20).

Direct Method II for the Preparation of 12 Using NO Gas

0.050 g (3.9×10^{-5} moles) $Pt_4(OAc)_8$ Blue was dissolved in 2.0 ml acetic acid. The solution was allowed to stir under argon until all of the powdered micro-crystalline compound was dissolved. To the above solution was added a small amount of NO gas; then the reaction vessel was reclosed. Stirring was continued at room temperature. Over the course of several minutes the solution gradually became a deep purple color. The color had to be watched most closely; if one allowed the reaction to go too long the complex was destroyed, and platinum(0) metal would precipitate. The purple solution was purged with dry argon or dry nitrogen, and the solvent acetic acid removed with a Buchi "R" rotary evaporator in a cool water bath. The resulting micro-crystalline purple solid exhibited all of the same physical characteristics as the compound in direct method I, Figure 8. However, no crystals were obtained.

Preparation of [$Pt_2(POP)_4 \cdot H_2O$] from $Pt_4(OAc)_8$ Blue, 13

The green luminescent dimeric species $Pt_2(POP)_4 \cdot 2H_2O$ was initially reported by Roundhill et. al., (56). 0.050 g $Pt_4(OAc)_8$ Blue (3.9×10^{-5} moles) was dissolved in 2.0 ml acetic acid. The solution was placed in a small glass petri dish cover. To the above solution was added 0.100 g of crystalline phosphorous acid which dissolved immediately. The solution was then heated to dryness at 110°C. Upon reaching dryness a green residue remained. The green residue was shown to be luminescent with U.V. irradiation at 254 nm Figure 8.

Preparation of $Pt_2(POP)_4 \cdot H_2O$ from $Pt_4(OAc)_8$ Blue with Ammonium Diphosphite, 13

0.050 g $Pt_4(OAc)_8$ Blue (3.9×10^{-5} moles) was dissolved in 2.0 ml acetic acid. To the solution was added 0.100 g $NH_4(POP)$. The solution was allowed to stir at 110°C. Over a period of two hours, the solution color changed from dark blue to a very deep green color. Upon cooling, the solution was shown to contain the complex 13 by monitoring its fluorescence upon irradiation at 254 nm (Figure 8).

Reaction of $Pt_4(OAc)_8$ with KOCN

Several reactions between KOCN and $Pt_4(OAc)_8$ Blue were carried out. Using varying concentrations of KOCN, varying results were observed. Due to their extreme physical hardness and chemical inertness very few solution data were available for evaluation; what was obtained will be described.

Reaction of $Pt_4(OAc)_8$ Blue with 20 Equivalents KOCN, 14

0.050 g (3.9×10^{-5} moles) $Pt_4(OAc)_8$ Blue was dissolved in acetic acid. To the deeply colored blue solution was added 6.4×10^{-3} g KOCN (7.8×10^{-4} moles). The solution immediately darkened to a nearly black color. Over a time of two minutes the color became a red/brown. From the above solution a dark brown solid was deposited upon the removal of the solvent acetic acid. The dark brown solid was then washed with water. No brown color was transferred to the water; however upon lyophilization of the water, a small amount of light tan colored solid resulted (five to eight percent); each fraction was appropriately designated water soluble or water insoluble, Figure 8.

Reaction of $Pt_4(OAc)_8$ Blue with 20 Equivalents KSCN, 15

0.0250 g $Pt_4(OAc)_8$ Blue (1.8×10^{-5} moles) was dissolved fully in 1.5 ml acetic acid. 0.0380 g (3.7×10^{-4} moles) of solid KSCN was added to the solution. Over the course of thirty to forty minutes the solution gradually became an orange-red color. The solution was filtered (to remove excess KSCN). The solvent was then stripped away from the product on a Buchi "R" rotary evaporator. The product was placed under vacuum for 24 hours and finally washed with ethyl alcohol, Figure 8. Bright red crystals of the complex were grown from ethyl alcohol and recrystallized twice. Yield was 35%.

Reaction of $Pt_4(OAc)_8$ Blue with Eight Equivalents KSCN, **16**

0.050 g (3.9×10^{-5} moles) $Pt_4(OAc)_8$ Blue was dissolved in acetic acid. To the deep blue solution was added eight equivalents of solid KSCN (0.030 g KSCN). The solution gradually became a dark red color, and finally a brown solid precipitated. The mother liquor remained a bright yellow to nearly tan color. The solvent acetic acid was removed using the Buchi "R" rotary evaporator. The solid was then placed under vacuum for 48 hours. To the dried solid was added approximately 2.0 ml of deionized glass distilled water. An orange or tan solution resulted, with an insoluble brown solid remaining. Four more successive 2-ml water washes followed, with the liquid being decanted each time. The final water wash was colorless. All five washings were combined, shell-frozen, and lyophilized. An extremely hydroscopic, red solid resulted, **16S**. The water insoluble fraction, **16I**, was also shell frozen and lyophilized. A light brown to tan solid resulted, Figure 8. Yields water insoluble fraction: 0.028 g (56%); water soluble fraction: 0.013 g (26%).

Reaction of $Pt_4(OAc)_8$ with
Four Equivalents KSCN, **17**

0.050 g (3.9×10^{-5} moles) $Pt_4(OAc)_8$ Blue was dissolved in 2.0 ml acetic acid. To the deep blue solution was added four equivalents of solid KSCN (0.0152 g KSCN). The solution gradually darkened to a deep green color over several hours. The reaction was allowed to stir an additional 12 hours with no further color changes observed. The acetic acid solvent was removed using the Buchi "R" rotary evaporator. The solid was then placed under vacuum for 48 hours. To the dried solid approximately 2 ml of deionized glass distilled water was added. Water-soluble and water-insoluble fractions resulted. The insoluble fraction was washed as previously described with all washings combined. The water soluble fraction, **17S**, was a moderately colored green solution, while the water insoluble fraction, **17I**, was a dark green powdery solid, Figure 8. Both fractions were shell frozen and lyophilized. Yields water soluble: 0.004 g (13%); water insoluble: 0.026 g (87%).

Reaction of $Pt_4(OAc)_8$ Blue with
Two Equivalents KSCN, **18**

0.050 g (3.9×10^{-5} moles) $Pt_4(OAc)_8$ Blue was dissolved in 2.0 ml acetic acid. To the deep blue solution was added two equivalents of solid KSCN (0.0076 g KSCN). The solution gradually became a blue green color, and was stirred for 24 hours. The acetic acid solvent was removed using the Buchi "R" rotary evaporator. The blue-green solid was then placed under vacuum for 48 hours. To the dried solid 2.0 ml of glass distilled water was added. Water soluble, **18S**, and water insoluble, 18I, fractions resulted, Figure 8. The washings were combined previously described. Yields were not measured but were approximately equal in mass.

Reaction of $Pt_4(OAc)_8$ Blue with Acetylene Gas, 19

0.050 g (3.9 x 10^{-5} g) $Pt_4(OAc)_8$ Blue was dissolved in approximately 2 ml of acetic acid. The solution was vacuum filtered and placed in a glass desiccator which contained three other containers. The containers each contained 25 ml of water, 5.06 g. potassium hydroxide, and approximately 2 g of calcium carbide. The cover of the desiccator was replaced and the solution color observed. Within two hours the solution color was observed to become green. If one allowed the solution to sit in the presence of the acetylene gas for more than two hours, platinum metal was invariably precipitated. The green solution was then removed from the acetylene gas-containing environment and placed in a fresh, clean, dry desiccator. The cover of the new desiccator was removed once each twelve hours in an attempt to grow crystals of the complex, Figure 10. No crystals suitable for single crystal x-ray diffraction resulted. Yield of the purple micro-crystalline solid was approximately 70%.

Reaction of $Pt_4(OAc)_8$ Blue with Phenylacetylene, 20

0.050 g $Pt_4(OAc)_8$ Blue (3.9 x 10^{-5} moles) was dissolved in 2.0 ml acetic acid. The solution was filtered through a fine glass frit, no solid was noted to be present. To the solution, 1.0 μl (9.95 x 10^{-4} g) phenylacetylene was added. The solution was vigorously

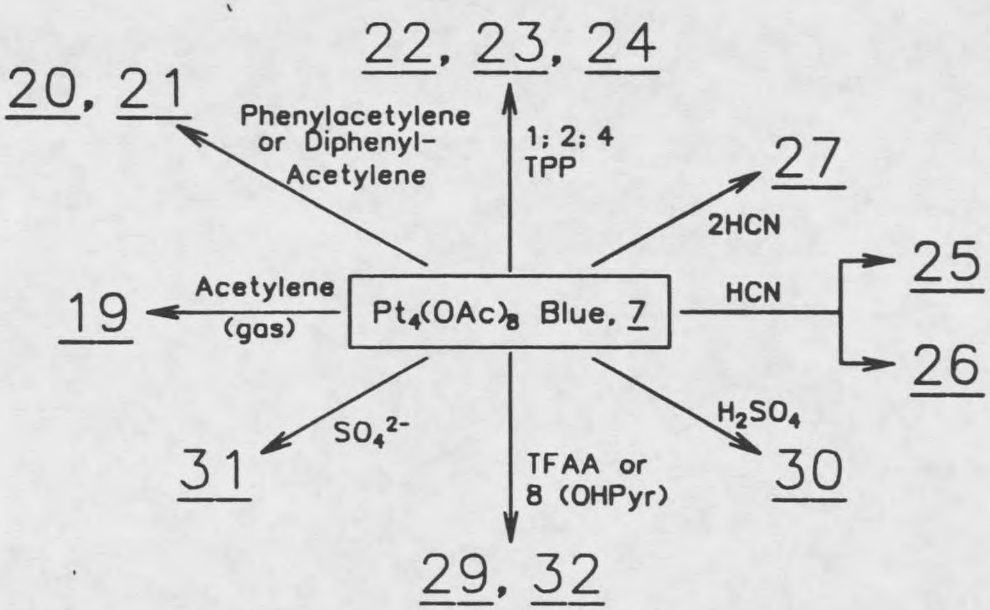


Figure 9. Synthetic scheme for compounds 19 - 32.

stirred and the color changes observed quite carefully. Initially the color of the solution became green (15 minutes). After 30 minutes, a green solid precipitated. The green solid redissolved over the next hour, and the solution color faded to a brownish color. Visible spectra were taken, and the solution was then allowed to stir for 24 hours to assure complete reaction. Neither the color changed nor did the visible spectrum, so the reaction was considered complete. The solvent acetic acid was removed on the Buchi "R" rotary evaporator. The yellow-green solid was then dissolved in acetic anhydride, and crystal growth was attempted, Figure 9. The solution precipitated a green solid. No crystals were obtained.

Reaction of $Pt_4(OAc)_8$ Blue with Diphenylacetylene, 21

0.0050 g $Pt_4(OAc)_8$ Blue (3.9×10^{-6} moles) was dissolved in 2.0 ml acetic acid. The solution was filtered through a fine glass frit, and no solid was noted to be present. To the solution was added 1.75 mg of diphenylacetylene. The solution remained a very deep blue color and was allowed to stir over 24 hours. The color was still blue at the end of 24 hours. The solvent acetic acid was removed using the Buchi "R" rotary evaporator. The blue solid was placed under vacuum for 25 hours. The blue solid was found to be freely soluble in acetic anhydride only, Figure 9. The acetic anhydride solution was placed in a cold room (4°C) in the dark. A dark blue solid was precipitated from the solution, and the supernatant color became brown. No crystals were obtained, and no yields were measured.

Reaction of $Pt_4(OAc)_8$ Blue with One Equivalent Triphenylphosphine, 22

0.050 g (3.9×10^{-5} moles) $Pt_4(OAc)_8$ Blue was dissolved in 5.0 ml acetic acid. The deep blue solution was filtered with no solid being removed. To the deep blue solution was added 10.2 mg (one equivalent) from a stock solution of triphenylphosphine in acetic acid which had been previously prepared (concentration of triphenylphosphine was 51.0 mg/ml). The solution was allowed to stir while color changes were observed. Initially the solution darkened (30 minutes), and within two hours an evenly-green-colored solution had resulted. After 24 hours of stirring, the solution remained green. The solvent acetic acid was removed using a Buchi "R" rotary evaporator. The resulting green solid was put under vacuum for 24 hours. The green solid was found to be soluble in dichloromethane. Crystal growth was attempted; however, a black solid was found to precipitate leaving a very faintly yellow solution, Figure 9.

Reaction of $Pt_4(OAc)_8$ Blue with Two Equivalents Triphenylphosphine, 23

0.050 g (3.9×10^{-5} moles) $Pt_4(OAc)_8$ Blue was dissolved in 5.0 ml acetic acid. The deep blue solution was filtered with no solid being removed. To the deep blue solution was added 20.4 mg triphenylphosphine (two equivalents) from the stock solution described above. The solution was allowed to stir while the color changes were observed. Initially the solution darkened (30 minutes), and within two hours and evenly red colored solution had resulted. The solution remained red after 24 hours of stirring. The solvent acetic acid was removed using a Buchi "R" rotary evaporator. The resulting dark red solid was found to be soluble in dichloromethane and chloroform, Figure 9. Crystal growth was attempted; however, a black solid was found to precipitate, leaving a very faintly yellow solution.

Reaction of $Pt_4(OAc)_8$ Blue with Four Equivalents Triphenylphosphine, 24

0.050 g (3.9×10^{-5} moles) $Pt_4(OAc)_8$ Blue was dissolved in 5.0 ml acetic acid. The deep blue solution was filtered with no solid being removed. To the deep blue solution was added 40.4 mg (four equivalents) of solid triphenylphosphine. The solution was allowed to stir while color changes were observed. Initially the solution darkened (15 minutes), and within 15 minutes an evenly yellow colored solution had resulted. After 24 hours of stirring, the solution remained bright yellow. The solvent acetic acid was removed using a Buchi "R" rotary evaporator. The resulting bright yellow solid was found to be soluble in dichloromethane and chloroform, Figure 9. Crystal growth was attempted; however, no crystals resulted.

Reaction of $Pt_4(OAc)_8$ Blue with Excess HCN, 25

0.050 g (3.9×10^{-5} moles) $Pt_4(OAc)_8$ Blue was dissolved in 5.0 ml acetic acid. The deep blue solution was placed in half of a small petri dish. The container was placed into a closed desiccator with solid KCN (5.08 g) in a small petri dish, and the base well area of the desiccator was filled with approximately 50 ml of acetic acid.

Thus HCN was generated. The blue solution was observed to become a purple-red color within 15 minutes, and within 30 minutes the solution had become faintly yellow or nearly colorless. No solids were present in the solution. The solution was allowed to air dry. A very light yellow solid resulted. A yield of 0.011 g (22%) was obtained after pumping on the solid for 24 hours. The yellow solid was washed with hexane and chloroform to remove excess acetic acid, Figure 9. Final yield was 0.0105 g (17.5%).

Reaction of $Pt_4(OAc)_8$ Blue
with HCN Controlled Reaction, 26

0.050 g (3.9×10^{-5} moles) $Pt_4(OAc)_8$ Blue was dissolved and prepared as described above. The solution was exposed to HCN as described above. The solution was removed from the desiccator within 15 minutes when the color changed to purple-red. The solvent acetic acid was removed using a Buchi "R" rotary evaporator. The purple-red solution commonly reverted to a blue color at this point in the reaction sequence; thus it was extremely difficult to isolate the purple-red solid. Generally, reduction of the volume of the purple-red solution on the rotary evaporater with a cool water bath gave a dark purple solid. The dark purple solid could then be dried but only with great care because, again, the color commonly reverted to blue. Therefore, it was not possible to expose the solid to reduced pressure (as on a vacuum line), Figure 9. Yields were not measured, and because of the difficulties in handling the compounds further reactions were not pursued.

Reaction of $Pt(OAc)_8$ Blue with One and Two Equivalents of Cyanamide, 27

0.0050 g (3.9×10^{-6} moles) $Pt_4(OAc)_8$ Blue was dissolved in 2.0 ml of acetic acid. The deep blue solution was stirred until all solid was observed to have dissolved. To the blue solution was added one or two equivalents (1.6×10^{-5} g or 3.2×10^{-5}g) of cyanamide. The solution was stirred and observed for 24 hours; no significant color changes were apparant. The solvent acetic acid was removed using a Buchi "R" rotary evaporator. A reddish-brown solid resulted, Figure 9. The solid was found to be insoluble in most common solvents from polar water to nonpolar ethers. Due to the extreme "hardness" of the solid and its insolubility, this series of compounds was not further pursued.

Reaction of $Pt_4(OAc)_8$ Blue with Eight Equivalents of Acetamide, 28

0.010 g $Pt_4(OAc)_8$ Blue (7.8×10^{-6} moles) was dissolved in 2.0 ml acetic acid. The solution was filtered through a fine glass frit, and no solid resulted. To the deep blue solution was added two equivalents of acetamide (9.3×10^{-4} g). The solution was stirred for 24 hours. No obvious color changes were observed; however a dark blue, nearly black precipitate was observed to form after 48 hours without any further stirring. Deep blue crystals were obtained, Figure 9. Yield of blue solid plus crystals was 0.0053 g (53%). The blue mother liquor was allowed to stand several days longer; however observation revealed no further crystal formation.

Reaction of $Pt_4(OAc)_8$ Blue with Trifluoroacetic Acid, 29

0.050 g $Pt_4(OAc)_8$ Blue (3.9×10^{-5} moles) was dissolved in 2.5 ml of trifluoroacetic acid. The solution was originally prepared for nuclear magnetic resonance studies. Nonetheless, following the nuclear magnetic resonance experiments, the solution was observed to have taken on an unusual purple color. The color continued to deepen over the next few days at which time the excess solvent trifluoroacetic acid was removed by blowing dry nitrogen over the solution, Figure 9. The dark blue, nearly-black solid was exposed to vacuum for 48 hours. Yield of the solid was 0.040 g (80%).

Reaction of $Pt_4(OAc)_8$ Blue with Sulfuric Acid, 30

0.015 g $Pt_4(OAc)_8$ Blue (1.17×10^{-5} moles) was dissolved in 15.0 molar concentrated sulfuric acid under argon. The solution was initially dark blue. However, over a period of three days at room temperature the solution gradually became a dark red color. Heating the solution to 110°C did not appreciably decrease the time needed for reaction. A small amount of yellow, powdery precipitate formed and was isolated by decanting the red mother liquor. The yellow powder was washed with 2 to 3.0 ml portions of water and dried with 3 to 5.0 ml portions of ethyl alcohol and diethyl ether, Figure 9. Yield of the bright yellow, insoluble powder was 0.004 g (26%).

Reaction of $Pt_4(OAc)_8$ Blue with K_2SO_4, 31

0.0200 g $Pt_4(OAc)_8$ Blue (1.54×10^{-5} moles) was dissolved in 5 to 7 ml of acetic acid. The solution was filtered through a fine glass frit; no residual solid was observed. To the dark blue solution 50 equivalents (0.126 g) K_2SO_4 were added. The solution was then heated to 110°C for 12 hours. The color of the solution gradually changed from dark blue through a dark green color, to an extremely deep red or brown. The solution was once again filtered through a fine glass frit, and a dark gray solid resulted. The solvent acetic acid was removed from the dark red filtrate using a Buchi "R" rotary evaporator. The red solid was then put under vacuum for 48 hours, Figure 9. Yield of the red, powdery solid was 0.0150 g (26%).

Reaction of $Pt_4(OAc)_8$ Blue with Eight Equivalents Hydroxypyridine, 32

0.025 g (1.95×10^{-5} moles) $Pt_4(OAc)_8$ Blue was dissolved in acetic acid. The deep blue solution was filtered through a fine or medium glass frit. To the deep blue solution was added eight equivalents (0.0152 g) of hydroxypyridine (α-pyridone). The solution was heated to 110°C until a dark purple solution was obtained (2-2.5 hours). The solution was filtered through a fine glass frit with no solid resulting. The solvent acetic acid was removed using a Buchi "R" rotary evaporator. Thin layer chromatography gave a single spot which moved with pure acetic acid ($R_f = 0.4$). Column chromatography on a 2 cm column gave one purple band. The solvent acetic acid was removed using the Buchi "R" rotary evaporator. The complex was found to be soluble in most common organic solvents, Figure 9. Efforts to grow crystals failed.

Materials and Methods

The ^{1}H, ^{13}C, ^{195}Pt NMR spectra were obtained on a Bruker WM-250 NMR spectrometer. Infrared spectra for compounds 1 and 2 were obtained upon a Nicolet Mx-1 spectrometer in I.R. tran cells. All other spectra were obtained on a Nicolet 5 DX B spectrometer.

Visible spectra were obtained upon a Cary 14A spectrophotometer. Electron Spectra for Chemical Analysis (ESCA) were obtained upon a L-H EAII (Leybold-Heraeus) spectrometer. Single crystal x-ray crystallographic data were obtained at both room temperature and at liquid nitrogen-cooled temperature on a Nicolet R3m/E diffractometer. Structure solution and refinement was performed as described for each compound.

Elemental analyses for C-H, N, S, and Ag were performed by Galbraith Labs, Knoxville, Tennessee. Platinum analyses were performed in-house using the method of Browning (52).

The platinum used in all compounds was loaned by Johnson Matthey, Inc. All reagents were analytical grade and not further purified.

Magnetic moments for compounds 1 and 2 were measured by the Evans method (53) using tris(ethylenediamine)chromium(III) chloride as a calibrant. The ratios of the number of ligands per cluster were determined using ^{1}H NMR spectroscopy. Destruction of the platinum complexes was effected by hydrolysis in D_2O, or by the addition of 5.8 M $DCl:D_2O$ solutions purchased from Aldrich. The peak intensities were measured by integration, and the concentrations of H^+ and OAc^- were determined using methyl alcohol as an internal standard.

Chromatographic Procedures

The acetate complexes were normally purified using the following procedure. Chromatography columns were prepared by suspending silica gel (Baker 50-200 mesh) first in methyl alcohol, acetic acid (3:1), and drying the silica at 110°C for 24 hours. The silica was then suspended in a methylene chloride, methyl alcohol, acetic acid (4:4:1) mixture. Wet packed columns of about one meter height were prepared by pouring the slurry into a 1.25 meter glass column; a small ball of glass of wool and a stopcock were used to control the flow rate. Approximately 1 cm of glass wool was also placed at the top of the silica gel bed to inhibit disruption of the silica upon introduction of the sample. The silica gel bed was normally washed with three to five bed volumes of solvent prior to application of samples. Samples were dissolved in a slight excess of the methylene chloride, methanol, acetic acid (4:4:1) and introduced to the column by careful layering onto the layer of glass wool. Upon introduction of the sample to the column bed, elution was made using the same methylene chloride, methanol, acetic acid (4:4:1) solvent. The eluents were then collected and treated as described in the preparative procedures.

Preparation of Ag Salts

Silver acetate and silver benzoate were prepared as described by Fales and Kenny (54). Silver trifluoroacetate was purchased from Aldrich Chemical Company. All of the silver salts were generally an off white color and somewhat light sensitive.

NMR Spectroscopy of Pt(III) Dimeric Species

Platinum-195, carbon-13, and proton NMR spectra were recorded in $CDCl_3$ solutions. The spectra were measured on a Bruker WM 250 MHz multinuclear spectrometer. The platinum-195 spectra were recorded at 53.518 MHz and were referenced to H_2PtCl_6 (1.0 M) (59). The carbon-13 spectra were recorded at 62.898 MHz and referenced to external tetramethylsilane; broad band proton decoupling was employed in recording all carbon-13 spectra. Proton NMR spectra were referenced to internal tetramethylsilane. For all spectral observations, shifts to greater shielding were taken as positive.

The referencing of platinum-195 chemical shifts has been a controversial problem (57-58). We have followed the convention of Sadler, et. al., (59), in which 1.0 molar H_2PtCl_6 was used as an external reference, and the chemical shifts for the platinum resonances were then calculated from the absolute frequency at which they occured. The major reason for their method being employed stems from the size of the platinum-195 NMR chemical shift range (up to 1.5 MHz). The absolute frequency of H_2PtCl_6 was calculated as follows (Equation 1 is taken from the Bruker WM-250 Operating Manual):

$$SY = \frac{250.132 + [01] - x}{2} \qquad \text{Eq. 1}$$

where x is the absolute resonance frequency of the spectrum, 01 is the observation window of the NMR spectrometer, and 250.132 MHz is the base synthesizer frequency for the WM 250 NMR spectrometer at Montana State University. All multinuclear frequencies are generated by beating an appropriate frequency against the 250.132 synthesizer frequency to obtain the desired frequency.

SY is the frequency at which the synthesizer is set. Rearranging to obtain the absolute frequency which one is observing:

$$X = 250.132 + [01] - 2SY \qquad \text{Eq. 2}$$

Since the result shown in equation 2 is an algebraic expression in one variable, calculation of absolute frequencies for any resonance are possible. To further simplify matters even more, the spectrometer reference (SR command) can be set equal to the observation window (01), and all frequencies are then given in terms of Hertz from the base frequency of the instument within the observation window relative to the detector setting. For example, the case of H_2PtCl_6 would follow as below:

01 = 898.44 Hz
SR = 01
SY = 98.180 MHz
SF = 250.1320 MHz
Cursor on Screen Value = −217.75 Hz

X = 250.132 + 01 − 2SY (equation 2)

Substituting:

$$\nu H_2PtCl_6 = 250{,}132{,}000 \text{ Hz} + 898.44 \text{ Hz} = (-217.75 \text{ Hz}) \cdot 2(98{,}180{,}000)$$
$$= 53{,}772{,}680 \text{ Hz} \qquad \text{Eq. 3}$$

One can vary SY (synthesizer position) or 01 and, provided that the spectrum is not "folded-over" (both observation and synthesizer frequencies are correct), can determine the absolute frequency for H_2PtCl_6 or any other platinum species.

Once the absolute frequencies for each of the observed platinum-195 species have been determined, the value is simply substracted from the value for H_2PtCl_6, and the chemical shift for the resonance in question is obtained (in Hz). Conversion to the more standard parts-per-million chemical shift scale requires division by 53.518 MHz (the frequency at which the spectra were taken). Therefore, one more example should be given here and is shown below in equations 2.4 through 2.9. For this example the species $Pt_2(MHP)(CH_3)_4(Pyr)_1$ has been selected. Two sets of triplets were observed at substantially different SY values, indicating a significant amount of difference in the chemical environment for each of the platinum atoms. Remembering:

$$\nu_{PT} = 250.132 \text{ MHz} = 01 - 2SY$$

where 01 = SR,

Downfield Pt-195 Spectra	Upfield Pt-195 Spectra
01 = -6825 Hz	01 = 4149.9 Hz
SY = 98.220 MHz	SY = 98.260 MHz
Cursor = -49.73 Hz	Cursor = 170.66 Hz

$$\nu DN = [250{,}132000 \text{ Hz} + (-6825 \text{ Hz} + (-49.7 \text{ Hz}))-2(98220 \text{ Hz})]$$

$$\nu DN = 53795125 \text{ Hz} \qquad \text{(Eq. 4)}$$

Chemical Shift for Pt-195 Down Field shift relative to H_2PtCl_6:

$$53772680 - 53685125 = 87555 \qquad \text{(Eq. 5)}$$

$$\frac{87{,}555}{535{,}188{,}000} = -1635.9 \text{ ppm} \qquad \text{(Eq. 6)}$$

$$\nu UP = 250132000 \text{ Hz} + (4115 + 170) - 2(98.260 \text{ Hz})$$

$$\nu UP = 53616285 \text{ Hz} \qquad \text{(Eq. 7)}$$

Chemical shifts for Pt-195 Up Field Shift relative to H_2PtCl_6:

$$53772680 \text{ Hz} - 53616285 \text{ Hz} = 156395 \text{ Hz} \qquad \text{(Eq. 8)}$$

$$\frac{156395 \text{ Hz}}{53518000} = -2922.2 \text{ ppm} \qquad \text{(Eq. 9)}$$

From the above method the chemical shift of any platinum-195 species in solution can be determined. The spin-spin coupling constants are then measured in hertz.

X-Ray Crystallography

Crystals of the platinum compounds which were suitable for X-ray diffraction studies were prepared for such studies in a variety of ways. For room temperature data collection many of the crystals were either coated with a thin film of epoxy cement, or Paratone "N" (60) after being mounted on glass fibers. Some crystals were mounted in Lindemann glass capillaries under argon. The "mounting" of such crystals consisted of wedging the crystal into the capillary. The Lindemen capillaries were then flame sealed, taking care not to heat the crystals. For extremely air-sensitive, moisture-sensitive, or solvent-losing crystals, low temperature data collection methods were employed. In most cases the crystals for low-temperature data collection were immersed in Paratone "N" which had been diluted (3:1) with mineral oil. The crystals were transferred under dry argon. Once the crystals were in the Paratone "N", they were examined under a microscope and the best choices mounted onto a glass fiber. The glass fiber with a crystal encased in a small droplet of Paratone "N" was then placed in the liquid nitrogen-cooled stream of nitrogen gas where it was immediately frozen in place. X-ray intensity data were collected on a Nicolet R3m/E four circle diffractometer equipped with graphite monochromated Mo Kα radiation (λ = 0.71073 Å). Further details of structure solution and refinements follow for each complex.

Structure Solution for $K[Pt(NO_2)_4(NO)(H_2O)]\cdot H_2O$, 1:

A blue crystal fragment with approximate dimensions of 0.2 x 0.5 x 0.8 mm was sealed in a Lindemann glass capillary surrounded by mother liquor to prevent decomposition or reaction with air. Unit cell dimensions were obtained by least squares refinement using 25 centered refections for which $26° < 2\Theta < 34°$. Three check reflections, monitored every 100 reflections, showed no significant loss in intensity over the course of data collection. Crystal data, further information on data collection, and structure refinement are given in Table 1.

Data reduction, including corrections for Lorentz and polarization effects, gave 4069 independent reflections in the range $3° < 2\Theta < 65°$ of which 3148 with $I > 3\sigma(I)$ were used for structure refinement. The volume of the triclinic unit cell was appropriate for two formula units, so the centrosymmetric space group was assumed, and later confirmed, by successful structure solution and refinement. A Patterson synthesis gave the platinum position and the remaining non-hydrogen atoms were located by difference syntheses. These positions were refined with anisotropic thermal parameters by blocked cascade least squares, minimizing $\Sigma W\Delta 2$ with 101 parameters refined in each full matrix block. Absorption corrections were calculated by Gaussian integration using indexed planes to

Table 1. Crystallographic parameters for $K[Pt(NO_2)_4(NO)(H_2O)]\cdot H_2O$, 1

Formula wt	474.09
Crystalline System	Triclinic
Space Group	$P\bar{1}$
a, Å	6.695
b, Å	8.712
c, Å	9.829
α. degrees	91.04
β. degrees	100.36
γ degrees	92.11
V, Å	562.6
z	2
α cal g/cm3	2.85
d measured.	2.85
Crystal Size	0.15 x 0.25 x 0.35 mm
μ Mo Kα, cm-1	135.0
Radiation (Monochromated in incident Beam	Mo Kα (g = 0.71073 Å)
Orientation Reflections, Number, range (2Θ)	25, 19°-32
Temperature, °C	24
Scan Method	Omega
Data Collection Range	3.0-65.0
No. Unique data, total $W/f_o^2 \geq 3\sigma(f_o^2)$	4069, 3148
Number of parameters Refined	167
R^a	0.065
Rw^b	0.068
G.O.O.F.[c]	1.03
Largest Shift/esd, final cycle	1.08
Largest Peak, e/Å^3	

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

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

c. $$G.O.O.F. = \frac{\Sigma(||F_o|-|F_c||)w^{\frac{1}{2}}}{(m-n)^{\frac{1}{4}}}$$

$$w = (\sigma F^2 = gF^2)^{-1}$$

approximate the crystal shape with measured crystal dimensions. Atomic scattering factors, including terms for analomous dispersion, were taken from Cromer and Waber (61). The weighting scheme used was $W = K[2(F_o) + 0.0045 f_o2]-1$. There was no evidence of significant secondary extinction. Structure refinement led to an unreasonably short (0.91 Å) NO distance for the nitrosyl ligand suggestive of rotational disorder of the oxygen position, a relatively common feature in structures with bent NO groups (62). The equivalent isotropic thermal parameter for the nitrosyl oxygen was very large (μ = 0.16 cm^{-2}), and difference electron density maps showed a broad peak with three areas of greater electron density spread across an area of about 90°. The model was refined with the N-O distance constrained to 1.19 Å, the nitrosyl bond length in the structure of 2. The site occupancy parameters for the three oxygen disorder positions were allowed to vary. Refinement of the disordered model gave a reasonable nitrosyl oxygen thermal parameter (μ = 0.08 cm^2), and the refined occupancy parameters for the disordered oxygen positions summed to 0.96, indicating that the model accounts for most of the electron density for the nitrosyl oxygen. The final difference map was featureless except for the usual "ripple" near the platinum atom. Hydrogen atom positions could not be identified with any certainty, and as such were not included in the structure refinement.

Structure Solution for $K_2[Pt(NO_2)_2(NO)Cl_3]$, 2

A green plate-shaped crystal with approximate dimensions of 0.04 x 0.12 x 0.12 mm was transferred under argon to a 3:1 mixture of Paratone-N and mineral oil. It was then removed from the Paratone-N:Mineral oil on the end of a glass fiber and immediately placed into a stream of nitrogen gas at approximately -120°C. Thus isolated from air, the crystal remained stable as long as the low temperature environment was maintained. All crystallographic procedures were conducted at -120°C. Unit cell dimensions were obtained from 24 reflections $19° < 2\Theta < 32°$. Crystal data, intensity measurement, and structure refinement parameters are given in Table 2. Procedures were otherwise as described above.

After all atoms had been refined anisotropically and absorption corrections had been applied, a difference map showed a relatively large peak (2.9 e cm^{-3}) at 1.3 Å from one of the chlorine positions, indicating possible disorder. The equivalent isotropic thermal parameter for the proximate chlorine (Cl(2)) was twice as large as for the other two chlorines in the complex. This suggested that for a relatively small fraction of sites (the R value at this point was 0.052), there was an alternative orientation of the complex where the position of the nitrosyl and Cl(2) ligands were exchanged. In the minor orientation the nitrite ligands would also be exchanged, and Cl(1) and Cl(3) would replace each other. To model the apparent disorder, additional positions were introduced for Cl(2) and the nitrosyl ligand, using the peak from the difference map for the

Table 2. Crystallographic Parameters for $K[Pt(NO_2)_2(NO)(Cl)_3]$, 2

Formula Wt	395.14
Crystalline System	MonoClinic
Space Group	$P2_1/c$
a, Å	6.227
b, Å	11.690
c, Å	14.525
α degrees	90.000
β degrees	99.13
γ degrees	90.000
c, Å	1043.4
z	4
d calc g/cm^3	3.19
Crystal Size	0.04 x 0.12 x 0.12 mm
Mo Kα, cm^{-1}	159.9
Radiation (Monochromated in incident beam	Mo Kα (g = 0.71073 Å)
Orientation Reflections	
Number, range (2Θ)	24, 19°-32°
Temperature, °C	-120
Scan Method	1
Data Collection Range	3°-65°
No. Unique data, total $W/f_o^2 \geq 3\sigma\ (gf_o^2)$	3032,1783
Number of parameters refined	148
R[a]	0.051
Rw[b]	0.050
G.O.O.F.[c]	1.01
Largest Shift/esd, final cycle	0.051
Largest Peak, $e/Å^3$	0.63

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

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

c. $$\text{G.O.O.F.} = \frac{\Sigma(||F_o|-|F_c||)w^{1/2}}{(m-n)^{1/4}}$$

$$w = (\sigma F^2 = gF^2)^{-1}$$

nitrosyl oxygen. Because of a significant difference in bond distance (Results), additional positions for Cl(1) and Cl(3) were also included in the disorder model. The nitrites were oriented such that their alternate positions were nearly superimposed; thus additional nitrite ligands were not needed.

The disorder model was refined with some constraints imposed on parameters for the minor orientation. Bond distances were constrained to corresponding values from the major orientation, as was the nitrosyl bond angle. Isotropic thermal parameters were assigned in like manner except for (Cl 2′), which was refined with anisotropic thermal parameters. Refinement of the disordered model led to smaller thermal parameters for Cl (2), a slightly shorter nitrosyl Pt–N distance (2.06 Å vs. 2.12 Å), and a longer N–O distance (1.19 Å vs. 1.09 Å) compared to values obtained without disorder. These differences were in agreement with the assumed disorder, and the nitrosyl distance was closer to expected values when the disorder model was included in the refinement. Other bond distances and angles were not significantly affected by including disorder in the model, nor were the refinement statistics. The site occupancy ratio for the two orientations refines to approximately 84% to 16% and was fixed in the final least squares cycles to facilitate convergence. The final difference map was featureless, except for the "ripple" near the platinum and chlorine positions. Corrections for extinction were not made.

Structure Solution for $K_2[Pt(NO_2)_4Br_2]$, 3

A crystal with dimensions of 0.16 x 0.14 x 0.18 mm was mounted on top of a glass fiber. The crystal was coated with Paratone N, mineral oil, 3:1 to avoid contact with the air. A Nicolet R3m/E diffractometer was used to collect 3478 unique reflections, of which 1449 had $I>3\sigma(I)$. Lorentz and polarization and absorption corrections were applied: six sets of faces were identified and indexed. Relevant crystal parameters and data are given in Table 3.

Preliminary examination of the crystal showed it to be of monoclinic symmetry. The space group was determined to be P21/c from the systematic abscences and the structure was refined in this space group. The platinum position was obtained from the Patterson function; the remaining non-hydrogen atoms were revealed by alternating difference Fourier maps and least-squares cycles. Blocked cascade least squares refinement converged to final residuals of R = 0.0610, (Rw = 0.0631). All atoms were refined with anisotropicthermal parameters. The largest peak in the final difference map was 0.95 e/Å^3 and was located near the platinum.

Structure Solution for $K_2[Pt(NO_2)_2Cl_4]$, 4

A crystal with dimensions of 0.21 x 0.08 x 0.05 mm was immersed in Paratone N. The crystal was removed from the Paratone N on the top of a glass fiber and frozen into position at -120°C on the Nicolet R3m/E diffractometer, which was equipped with a low temperature device. A total of 2816 reflections were collected, of which 1449 had $I>3\sigma(I)$. Lorentz and polarization and absorption

Table 3. Crystallographic Parameters for $K_2Pt(NO_2)_4Br_2$, 3

Formula	$K_2Pt(NO_2)_4Br_2$
Formula Wt	617.15
Crystalline System	Monoclinic
Space Group	$P\ 2_1/C$
a, Å	7.303
b, Å	9.413
c, Å	8.810
α. degrees	90.000
β degrees	108.230
γ degrees	90.000
c, Å	575.23
z	2
d cal c g/cm	2.97
Crystal Size	0.10 x 0.14 x 0.18 mm
μ Mo Kα, cm^{-1}	204.21
Radiation (Monochromated in incident Beam	Mo Kα (g = 0.71073 Å)
Orientation Reflection,	24
Number range (2Θ)	21°-41°
Temperature, °C	24
Scan Method	1
Data Collection Range, 2Θ,deg.3.0-75.0	
No. Unique data, total	3166
$W/f_o^2 > 3\ \sigma\ (F_o^2)$	1766
Number of parameters refined	79
R[a]	0.0610
Rw[b]	0.0631
G.O.O.F.[c]	1.68
Largest Shift/esd, final cycle	.001
Largest Peak, e/Å^3	2.5

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

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

c. $$G.O.O.F. = \frac{\Sigma(||F_o|-|F_c||)w^{\frac{1}{2}}}{(m-n)^{\frac{1}{4}}}$$

$$w = (\sigma F^2 = gF^2)^{-1}$$

corrections were applied. Six pairs of faces were identified and indexed. Relevant crystal parameters and data are given in Table 4.

Preliminary examination of the crystal showed it to be of orthorhombic symmetry. The space group was determined to be Fdddfrom systematic absences and some trial and error. The structure was refined in this space group. The platinum position was obtained from the Patterson function. The remaining non-hydrogen atoms were revealed by alternating difference Fourier maps and least squares cycles. Blocked cascade refinement converged to final residuals of R = 0.0352, (Rw = 0.0385). All atoms were refined with anisotropic thermal parameters. The largest peak in the final difference map was 0.80 e/$Å^3$ and was located 1.9 Å from the platinum atom.

Structure Solution for $K_2[Pt(Cl)_2(PO_3)_2]$, 5

A crystal with dimensions of 0.029 x 0.06 x 0.43 mm was immersed in Paratone N. The crystal was removed from the Paratone N on the tip of a glass fiber and frozen into position at -141°C (±5°C) on the Nicolet R3m/E diffractometer, which was equipped with a low-temperature device. A total of 3401 unique reflections were collected, of which 2290 had $I>3\sigma(I)$. Lorentz, polarization, and absorption corrections were applied. Six pairs of faces were identified and indexed. Relevant crystal parameters and data are given in Table 5.

Preliminary examination of the crystal showed it to be of triclinic symmetry, and the space group was determined to be P1. The structure was refined in this space group. The platinum position

Table 4. Crystallographic Paramenters for $K_2[Pt(NO_2)_2Cl_4]$, 4

Formula	$K_2Pt(NO_2)_2Cl_4$
Formula Wt	507.05
Crystalline System	Orthorhombic
Space Group	F ddd
a, Å	7.365
b, Å	15.373
c, Å	18.385
a. degrees	90.000
β. degrees	90.000
γ degrees	90.000
V, $Å^{-3}$	2081.70
z	8
α cal c g/cm^3	3.24 g/cm^{-3}
d measured	3.22 g/cm^3
Crystal Size	0.21 x 0.08 x 0.05 mm
μ Mo Kα, cm^{-1}	159.70
Radiation (Monochromated in incident Beam	Mo Kα (g = 0.71073 Å)
Orientation Reflection, Number range (2Θ)	24, 20.47-29.11
Temperature, °C	-120° 0°C
Scan Method	Wykoff ω and ω
Data Collection Range	3.0-60.0
No. Unique data, total $W/f_o^2 > 3\sigma(F_o^2)$	3605, 2510
Number of parameters refined	32
R[a]	0.0352
Rw[b]	0.0385
G.O.O.F.[c]	0.949
Largest Shift/esd, final cycle	.002
Largest Peak, $e/Å^3$	0.97

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

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

c. $$\text{G.O.O.F.} = \frac{\Sigma(||F_o|-|F_c||)w^{1/2}}{(m-n)^{1/4}}$$

$$w = (\sigma F^2 = gF^2)^{-1}$$

Table 5. Crystallographic Parameters for $K_2[PtCl_2(PO_3)_2]$, 5

Formula	$K_2[Pt(Cl)_2(PO_3)_2$
Formula Wt	502.07
Crystalline System	Triclinic
Space Group	P1
a, Å	8.612
b, Å	13.538
c, Å	9.367
α. degrees	90.000
β. degrees	105.674
γ degrees	90.000
V, $Å^{-3}$	1051.53
z	4
α cal c g/cm^3	----
d measured	----
Crystal Size	0.29 x 0.06 x 0.43 mm
μ Mo Kα, cm^{-1}	
Radiation (Monochromated in incident Beam	Mo Kα (g = 0.71073 Å)
Orientation Reflections, Number, range (2Θ)	24, 8.31-27.12
Temperature, °C	-141 ± 5
Scan Method	1
Data Collection Range	3.0-60.0
No. Unique data, total W/fo^2> 3 σ (Fo)	3401, 2290
Number of parameters refined	97
R[a]	0.0657
Rw[b]	0.0694
G.O.O.F.[c]	1.515
Largest Shift/esd, final cycle	.003
Largest Peak, e/$Å^3$	2.61

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

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

c. $$\text{G.O.O.F.} = \frac{\Sigma(||F_o|-|F_c||)w^{\frac{1}{2}}}{(m-n)^{\frac{1}{4}}}$$

$$w = (\sigma F^2 = gF^2)^{-1}$$

structure was refined in this space group. The platinum position was obtained from the Patterson function. The remaining non-hydrogen atoms were revealed by alternating difference Fourier maps and least squares cycles. Blocked cascade least squares refinement converged to final residuals of R = 0.0657 (Rw = 0.0694). All atoms were refined with anisotropic thermal parameters. The largest peak in the final difference map was located 1.8 Å from the platinum and 0.74 Å from the heavy ligands and was 2.61 e/$Å^3$ in size.

Structure Solution for $[Pt_4(OAc)_6(CO)_2]$ $\cdot 2(HOAc)$, 6

A crystal with dimensions of 0.037 x 0.17 x 0.10 mm was mounted on top of a glass fiber with epoxy cement. A Nichalet R3m/E diffractometer was used to collect 4210 unique reflections of which 1495 had $I>3\sigma(I)$. Lorentz and polarization and absorption corrections were applied. Faces were not indexed; an empirical absorption correction was applied. Relevant crystal parameters and data are found in Table 6.

Preliminary examination of the crystal showed it to be of monoclinic C symmetry. The space group was found to be C 2/c from the systematic absences, and the structure was refined in this space group. The platinum positions were obtained from the Patterson function. The remaining non-hydrogen atoms were revealed by alternating difference Fourier maps and least squares cycles. Full matrix least squares refinement converged to final residuals of R = 0.00473, (Rw = 0.0426). All atoms were refined with anisotropic

Table 6. Crystallographic Parameters for $[Pt_4(OOCCH_3)_6(CO)_2] \cdot 2(HOOCCH_4)$, 6

Formula $[Pt_4(OOCCH_3)_6(CO)_2] \cdot 2(HOOCCH_3)$	
Formula Wt	1254.36
Crystalline System	Monoclinic
Space Group	C 2/c
a, Å	23.710
b, Å	8.682
c, Å	14.206
α. degrees	90.000
β. degrees	92.940
γ degrees	90.000
V, $Å^{-3}$	2916.34
z	4
α cal c g/cm^3	2.87
d measured	2.867
Crystal Size	0.037 x 0.17 x 0.10 mm
μ Mo Kα, cm^{-1}	201.56
Radiation (Monochromated in incident Beam	Mo Kα (g = 0.71069 Å)
Orientation Reflection, Number range (2Θ)	25, 22.03–29.94
Temperature, °C	25
Scan Method	1
Data Collection Range	3.0–60.0
No. Unique data, total $W/fo^2 > 3\ \sigma\ (Fo^2)$	4210, 1495
Number of parameters refined	182
R^a	0.0473
Rw^b	0.0426
G.O.O.F.[c]	1.002
Largest Shift/esd, final cycle	0.008
Largest Peak, $e/Å^3$	1.39

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

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

c. $$G.O.O.F. = \frac{\Sigma(||F_o|-|F_c||)w^{\frac{1}{2}}}{(m-n)^{\frac{1}{4}}}$$

$$w = (\sigma F^2 = gF^2)^{-1}$$

RESULTS

X-Ray Crystallographic Results

The structural results of the various complexes for which crystals of sufficient quality were obtained are described in the following section; supporting results follow the x-ray crystallographic structures.

Structure of $K[Pt(NO_2)_4(NO)(OH_2)]$, 1

An ORTEP view of the mononuclear, blue, bent nitrosyl complex is shown in Figure 10. Tables 7-10 contain the final positional, equivalent isothermal temperature parameters, bond distances, and angles. Values for F_o and f_c are found in Table 66 (Appendix).

The structure consists of a mononuclear platinum(IV) molecule exhibiting a bent nitrosyl ligand. The platinum atom exhibits octahedral coordination with a water molecule *trans* to the bent nitrosyl ligand. The reliability of the bond angle and distance for light atoms in the structures can be gauged by the ranges in their values for the nitrite ions in the complexes. The nitrite N-O distances range from 1.17 to 1.26 Å (average= 1.21 Å), while the angles around the nitrite nitrogen atoms range from 118° to 124°. For the structure, the accuracy determining factor is probably the absorption correction.

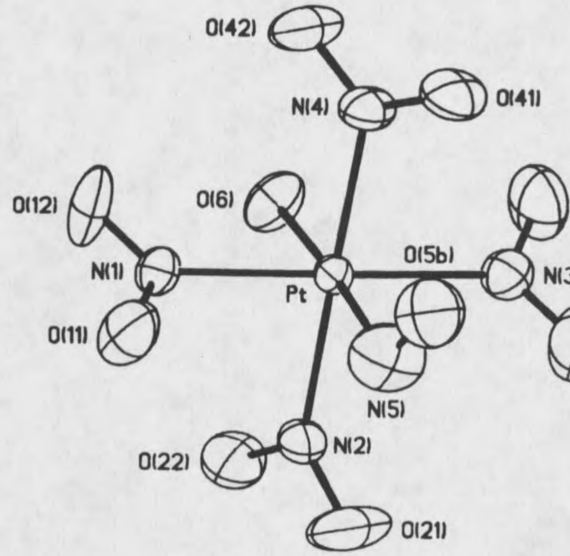


Figure 10. ORTEP view of $K[Pt(NO_2)_4(NO)(OH_2)]\cdot OH_2$, 1

Table 7. Atomic coordinates ($x10^4$) and isotropic thermal parameters ($Å^2x10^3$) for $K[Pt(NO_2)_4(NO)OH_2]\cdot(OH_2)$.

	x	y	z	
Pt	755(1)	2572(1)	2664(1)	28(1)*
K	4129(4)	8425(4)	2563(3)	43(1)*
N(1)	2865(17)	2318(12)	4438(11)	40(2)*
O(11)	2726(24)	3098(16)	5447(14)	79(2)*
O(12)	4146(19)	1363(17)	4414(14)	74(2)*
N(2)	2156(18)	4654(12)	2466(13)	46(2)*
O(21)	1224(22)	5852(13)	2653(20)	88(2)*
O(22)	3846(18)	4779(15)	2306(18)	75(2)*
N(3)	−1292(19)	2778(13)	869(13)	48(2)*
O(31)	−2556(26)	3760(19)	783(20)	105(2)*
O(32)	−1302(23)	1851(19)	−58(16)	83(2)*
N(4)	−658(17)	469(12)	2867(15)	46(2)*
O(41)	−2486(16)	423(13)	2800(17)	71(2)*
O(42)	345(17)	−656(11)	2960(18)	71(2)*
N(5)	−1164(21)	3760(19)	3745(18)	78(2)*
O(5A)	−1762(35)	3182(30)	4695(22)	80(4)
O(5B)	−2624(29)	3278(33)	4165(30)	80(4)
O(5C)	−2961(21)	3549(40)	3610(40)	80(4)
O(6)	3048(18)	1481(13)	1374(12)	55(2)*
O(7)	2947(20)	2835(15)	−1148(13)	65(2)*

Table 8. Bond lengths (Å) for $K[Pt(NO_2)_4(NO)OH_2]\cdot(OH_2)$.

Pt-N(1)	2.057(10)
Pt-N(2)	2.039(11)
Pt-N(3)	2.044(12)
Pt-N(4)	2.059(11)
Pt-N(5)	2.095(17)
Pt-O(6)	2.372(13)
N(1)-O(11)	1.211(18)
N(1)-O(12)	1.219(18)
N(2)-O(21)	1.262(18)
N(2)-O(22)	1.170(19)
N(3)-O(31)	1.218(21)
N(3)-O(32)	1.205(20)
N(4)-O(41)	1.211(16)
N(4)-O(42)	1.204(15)
N(5)-O(5A)	1.192(30)
N(5)-O(5B)	1.192(29)
N(5)-O(5C)	1.192(20)

Table 9. Bond angles (°) for $K[Pt(NO_2)_4(NO)OH_2]\cdot(OH_2)$.

N(1)-Pt-N(2)	87.4(4)
N(1)-Pt-N(3)	178.2(5)
N(2)-Pt-N(3)	93.0(5)
N(1)-Pt-N(4)	92.5(5)
N(2)-Pt-N(4)	180.0(6)
N(3)-Pt-N(4)	87.1(5)
N(1)-Pt-N(5)	91.9(5)
N(2)-Pt-N(5)	86.5(6)
N(3)-Pt-N(5)	89.9(6)
N(4)-Pt-N(5)	93.5(6)
N(1)-Pt-O(6)	89.0(4)
N(2)-Pt-O(6)	87.7(5)
N(3)-Pt-O(6)	89.3(5)
N(4)-Pt-O(6)	92.3(5)
N(5)-Pt-O(6)	174.1(5)
Pt-N(1)-O(11)	118.1(10)
Pt-N(1)-O(12)	117.7(9)
O(11)-N(1)-O(12)	124.2(12)
Pt-N(2)-O(21)	118.4(11)
Pt-N(2)-O(22)	122.4(10)
O(21)-N(2)-O(22)	118.9(13)
Pt-N(3)-O(31)	120.0(12)
Pt-N(3)-O(32)	118.7(11)
O(31)-N(3)-O(32)	121.2(15)
Pt-N(4)-O(41)	117.8(9)
Pt-N(4)-O(42)	118.7(10)
O(41)-N(4)-O(42)	123.4(12)
Pt-N(5)-O(5A)	120.3(16)
Pt-N(5)-O(5B)	128.5(18)
Pt-N(5)-O(5C)	125.6(21)

Table 10. Anisotropic thermal parameters ($Å^2x10^3$) for $K[Pt(NO_2)_4(NO)OH_2]\cdot(OH_2)$.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Pt	27(1)	27(1)	28(1)	1(1)	3(1)	-2(1)
K	36(1)	49(1)	43(1)	10(1)	1(1)	-1(1)
N(1)	47(3)	39(3)	30(3)	7(3)	-1(3)	2(3)
O(11)	118(4)	65(4)	43(4)	-13(3)	-18(4)	32(4)
O(12)	61(4)	106(4)	49(4)	12(4)	-11(3)	37(4)
N(2)	49(3)	36(3)	49(4)	12(3)	-3(3)	-11(3
O(21)	94(4)	31(3)	146(4)	8(4)	40(4)	5(3)
O(22)	53(4)	57(4)	114(4)	20(4)	14(4)	-14(3
N(3)	54(4)	43(3)	43(3)	3(3)	5(3)	-0(3)
O(31)	106(4)	95(4)	98(4)	-21(4)	-29(4)	39(4)
O(32)	84(4)	99(4)	58(4)	-21(4)	-10(4)	11(4)
N(4)	43(3)	34(3)	64(4)	5(3)	16(3)	-7(3)
O(41)	42(3)	47(3)	124(4)	0(4)	21(4)	-12(3
O(42)	54(3)	32(3)	136(4)	9(3)	36(4)	4(3)
N(5)	79(4)	75(4)	87(4)	-16(4)	39(4)	9(4)
O(6)	61(4)	58(3)	52(3)	12(3)	21(3)	19(3)
O(7)	78(4)	71(4)	50(3)	13(3)	20(3)	12(4)

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

Structure of $K_2[Pt(NO_2)_2(NO)(Cl)_3]$, 2

An ORTEP view of the mononuclear, green, bent nitrosyl complex is shown in Figure 11. Tables 11-14 contain the final positional, equivalent isothermal temperature parameters, bond distances, and angles. Values for F_o and f_c values are found in Table 67 (Appendix).

The structure consists of a mononuclear platinum(IV) molecule exhibiting a bent nitrosyl ligand. The platinum atom exhibits octahedral coordination with a chloride ion trans to the bent nitrosyl ligand. The reliability of the bond angles and distances

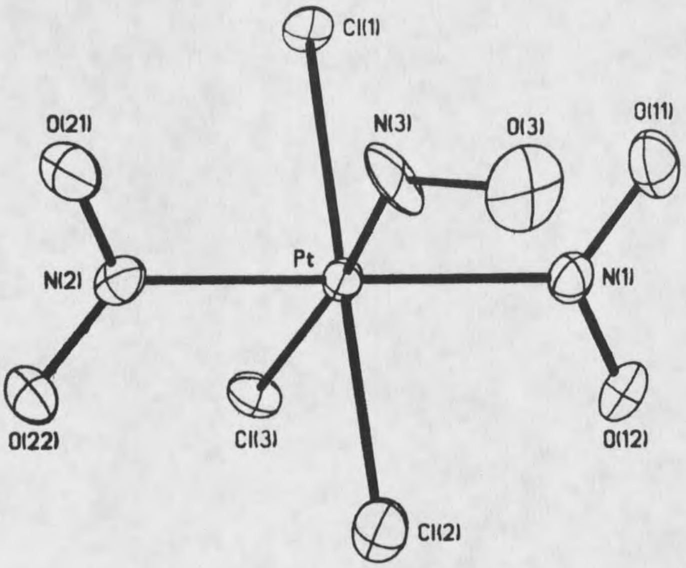


Figure 11. ORTEP view of $K_2[Pt(NO_2)_2(NO)(Cl)_3]$, 2

Table 11. Atomic coordinates ($x10^4$) and isotropic thermal parameters ($Å^2x10^3$) for $K_2[Pt(NO_2)_2(NO)Cl_3]$.

	x	y	z	U
Pt	1145(1)	2704(1)	1261(1)	14(1)*
K(1)	4432(7)	8946(3)	6538(3)	32(1)*
K(2)	-1778(7)	9512(3)	969(3)	31(1)*
Cl(1)	3928(9)	3389(5)	2361(4)	18(1)*
Cl(2)	-1722(8)	2089(4)	149(3)	28(1)*
Cl(3)	2972(10)	740(4)	1259(4)	19(1)*
N(1)	-564(19)	2192(11)	2289(8)	21(3)*
O(11)	-741(18)	2843(10)	2940(8)	29(3)*
O(12)	-1375(18)	1207(10)	2260(8)	28(3)*
N(2)	2733(20)	3279(10)	231(8)	19(3)*
O(21)	3487(23)	4236(10)	260(8)	40(3)*
O(22)	2924(19)	2664(10)	-457(7)	28(3)*
N(3)	-88(37)	4340(19)	1227(17)	40(4)*
O(3)	-1757(24)	4510(14)	1507(12)	44(4)*
Cl(1')	2915(53)	968(15)	1367(28)	18
Cl(2')	-451(54)	4488(15)	1333(29)	46(5)*
Cl(3')	4308(41)	3317(33)	2519(20)	19
N(3')	-1243(71)	2402(36)	133(29)	40
O(3')	-2337(59)	3184(47)	-205(26)	44

Table 12. Bond lengths (Å) for $K_2[Pt(NO_2)_2(NO)Cl_3]$.

Pt-Cl(1)	2.303(5)
Pt-Cl(2)	2.320(5)
Pt-Cl(3)	2.562(5)
Pt-N(1)	2.058(13)
Pt-N(2)	2.037(13)
Pt-N(3)	2.058(22)
N(1)-O(11)	1.232(17)
N(1)-O(12)	1.255(17)
N(2)-O(21)	1.211(17)
N(2)-O(22)	1.252(17)
N(3)-O(3)	1.192(30)

Table 13. Bond angles (°) for $K_2[Pt(NO_2)_2(NO)Cl_3]$.

Cl(1)-Pt-Cl(2)	177.6(2)
Cl(1)-Pt-Cl(3)	91.6(2)
Cl(2)-Pt-Cl(3)	90.8(2)
Cl(1)-Pt-N(1)	91.0(3)
Cl(2)-Pt-N(1)	89.2(3)
Cl(3)-Pt-N(1)	91.3(4)
Cl(1)-Pt-N(2)	89.7(3)
Cl(2)-Pt-N(2)	90.0(3)
Cl(3)-Pt-N(2)	91.5(4)
N(1)-Pt-N(2)	177.1(5)
Cl(1)-Pt-N(3)	86.0(6)
Cl(2)-Pt-N(3)	91.7(6)
Cl(3)-Pt-N(3)	175.1(7)
N(1)-Pt-N(3)	93.1(8)
N(2)-Pt-N(3)	84.2(8)
Pt-N(1)-O(11)	119.8(10)
Pt-N(1)-O(12)	119.6(10)
O(11)-N(1)-O(12)	120.5(13)
Pt-N(2)-O(21)	120.7(10)
Pt-N(2)-O(22)	121.1(9)
O(21)-N(2)-O(22)	118.2(13)
Pt-N(3)-O(3)	119.3(17)

Table 14. Anisotropic thermal parameters ($Å^2x10^3$) for $K_2[Pt(NO_2)_2(NO)Cl_3]$.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Pt	13(1)	18(1)	12(1)	1(1)	1(1)	-1(1)
K(1)	36(2)	30(2)	33(2)	8(1)	18(2)	10(2)
K(2)	43(2)	24(2)	23(2)	0(1)	3(2)	-9(2)
Cl(1)	12(2)	26(2)	12(2)	2(2)	-5(1)	-0(2)
Cl(2)	23(2)	44(3)	17(2)	7(2)	-1(2)	-3(2)
Cl(3)	22(2)	15(2)	19(2)	-5(2)	2(2)	3(2)
N(1)	14(5)	33(6)	17(5)	-1(5)	2(4)	-3(5)
O(11)	23(5)	42(6)	24(5)	-1(4)	8(4)	6(4)
O(12)	21(5)	33(5)	33(5)	-2(4)	11(4)	-11(4)
N(2)	19(5)	20(5)	17(5)	4(4)	0(4)	-4(4)
O(21)	74(6)	28(5)	25(5)	-5(4)	26(5)	-29(5)
O(22)	30(5)	37(5)	19(4)	-5(4)	7(4)	-2(5)
N(3)	50(7)	39(7)	37(7)	-21(6)	25(6)	10(6)
O(3)	17(6)	50(6)	64(7)	2(6)	1(6)	21(5)
Cl(2')	44(8)	47(8)	37(8)	6(8)	-23(8)	16(8)

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

can be gauged by the range in their values for the nitrite ions in the complex. The nitrite N-O distances range from 1.21 Å to 1.26 Å (average = 1.24 Å), and the bond angles range from 118° to 121°. As for the structure of 1, the accuracy of the absorption correction is probably the limiting factor determining the quality of the crystallographic data. For both 1 and 2 the positional coordinates and their derived values were probably affected to some degree by the models chosen to treat the disorder effects; however, both models exhibited well-behaved structure refinements under the limited constraints described previously.

Structure of $K_2[Pt(NO_2)_2Cl_4]$, 3

An ORTEP view of the mononuclear, yellow complex is shown in Figure 12. Tables 15-18 contain the final positional, equivalent isothermal temperature parameters, bond distances, and angles. Values for F_o and f_c are found in Table 68 (Appendix).

The structure consists of a mononuclear platinum(IV) molecule exhibiting four chloride ions and two nitrite ions. The platinum atom exhibits octahedral coordination. The nitrite N-O distances are 1.22 Å and their bond angle is 127.6°. As with the structure of 1 and 2, the accuracy of the absorption correction is probably the limiting factor determining the quality of the crystallographic data. No disorder was noted in the solution of the structure.

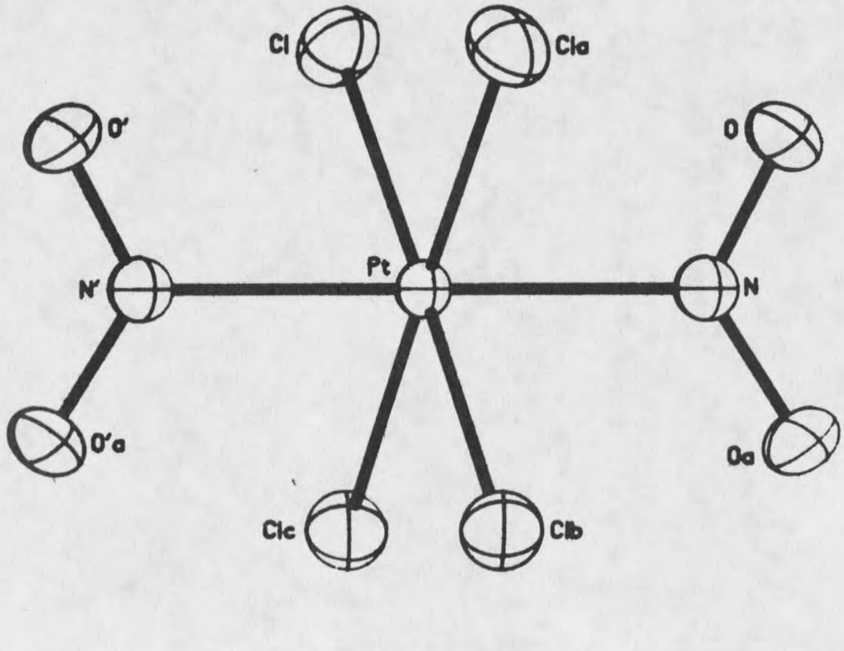


Figure 12. ORTEP view of $K_2[Pt(NO_2)_2Cl_4]$, 3

Table 15. Atomic coordinates ($x10^4$) and isotropic thermal parameters ($Å^2x10^3$) for $K_2[Pt(NO_2)_2Cl_4]$.

	x	y	z	U
Pt	1250	1250	6250	18(1)*
K	6250	2696(2)	6250	40(1)*
Cl	-1011(4)	1233(2)	5369(1)	33(1)*
N	1250	2587(7)	6250	26(4)*
O	-174(10)	2994(5)	6162(6)	36(3)*

Table 16. Bond lengths (Å) for $K_2[Pt(NO_2)_2Cl_4]$.

Pt-Cl	2.323(3)
Pt-N	2.056(11)
Pt-Cl(A)	2.323(3)
Pt-Cl(B)	2.323(3)
Pt-Cl(C)	2.323(3)
Pt-N'	2.056(11)
N-O	1.232(9)
N-O(A)	1.232(9)

Table 17. Bond angles (°) for $K_2[Pt(NO_2)_2Cl_4]$.

Cl-Pt-N	90.7(1)
Cl-Pt-Cl(A)	88.4(1)
N-Pt-Cl(A)	89.4(1)
Cl-Pt-Cl(B)	178.7(2)
N-Pt-Cl(B)	90.7(1)
Cl(A)-Pt-Cl(B)	91.6(1)
Cl-Pt-Cl(C)	91.6(1)
N-Pt-Cl(C)	89.4(1)
Cl(A)-Pt-Cl(C)	178.7(2)
Cl(B)-Pt-Cl(C)	88.4(1)
Cl-Pt-N'	89.3(1)
N-Pt-N'	180.0(1)
Cl(A)-Pt-N'	90.6(1)
Cl(B)-Pt-N'	89.3(1)
Cl(C)-Pt-N'	90.7(1)
Pt-N-O	120.5(6)
Pt-N-O(A)	120.5(6)
O-N-O(A)	119.0(11)

Table 18. Anisotropic thermal parameters ($Å^2x10^3$) for $K_2[Pt(NO_2)_2Cl_4]$.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Pt	17(1)	14(1)	23(1)	0	0	0
K	24(2)	29(2)	66(2)	0	8(3)	0
Cl	31(1)	33(1)	34(1)	1(1)	-10(1)	3(2)
N	21(6)	19(5)	38(7)	0	0(10)	0
O	23(4)	25(4)	60(6)	0(4)	-0(4)	7(3)

The anisotropic temperature factor exponent takes the form:

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

Structure of $K_2[Pt(NO_2)_4Br_2]$, 4

An ORTEP view of the mononuclear, red complex is shown in Figure 13. Tables 19-22 contain the final positional, equivalent isothermal temperature parameters, bond distances, and angles. Values for F_o and f_c are found in Table 69 (Appendix).

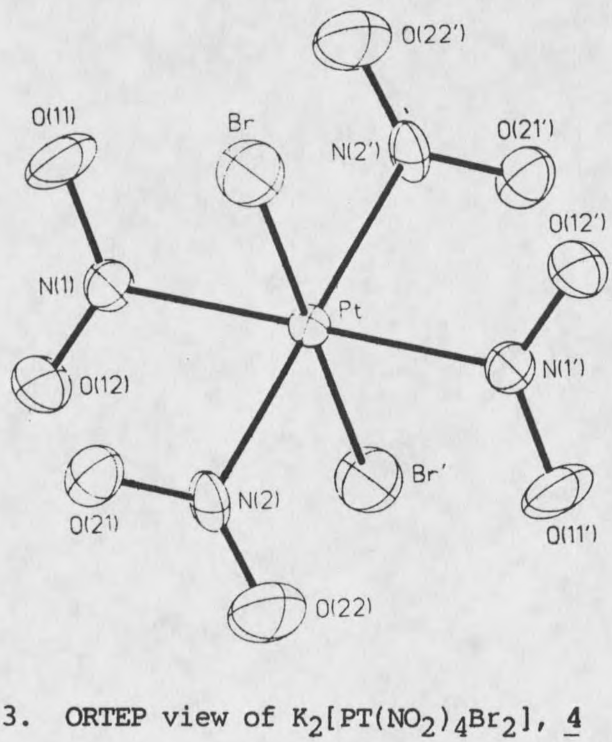


Figure 13. ORTEP view of $K_2[PT(NO_2)_4Br_2]$, 4

Table 19. Atomic coordinates ($\times 10^4$) and isotropic thermal parameters ($Å^2 \times 10^3$) for $K_2[Pt(NO_2)_4Br_2]$.

	x	y	z	U
K	1712(5)	4620(4)	8491(4)	32(1)*
Pt	5000	5000	5000	17(1)*
Br	2053(3)	6260(2)	5056(2)	41(1)*
N(1)	6323(19)	5335(13)	7447(14)	24(4)*
O(11)	5357(19)	5155(16)	8372(14)	48(5)*
O(12)	7959(16)	5736(14)	7920(13)	33(4)*
N(2)	6204(19)	6966(12)	4641(13)	25(4)*
O(21)	6020(19)	7921(12)	5494(13)	35(4)*
O(22)	7002(25)	7054(17)	3674(18)	61(7)*

Table 20. Bond lengths (Å) for $K_2[Pt(NO_2)_4Br_2]$.

Pt-Br	2.471(2)
Pt-N(1)	2.092(11)
Pt-N(2)	2.115(12)
Pt-Br′	2.471(2)
Pt-N(1′)	2.092(11)
Pt-N(2′)	2.115(12)
N(1)-O(11)	1.245(21)
N(1)-O(12)	1.198(17)
N(2)-O(21)	1.205(17)
N(2)-O(22)	1.176(24)

Table 21. Bond angles (°) for $K_2[Pt(NO_2)_4Br_2]$.

Br–Pt–N(1)	91.8(4)
Br–Pt–N(2)	89.3(4)
N(1)–Pt–N(2)	86.7(5)
Br–Pt–Br′	180.0(1)
N(1)–Pt–Br′	88.2(4)
N(2)–Pt–Br′	90.7(4)
Br–Pt–N(1′)	88.2(4)
N(1)–Pt–N(1′)	180.0(1)
N(2)–Pt–N(1′)	93.3(5)
Br′–Pt–N(1′)	91.8(4)
Br–Pt–N(2′)	90.7(4)
N(1)–Pt–N(2′)	93.3(5)
N(2)–Pt–N(2′)	180.0(1)
Br′–Pt–N(2′)	89.3(4)
N(1′)–Pt–N(2′)	86.7(5)
Pt–N(1)–O(11)	118.7(9)
Pt–N(1)–O(12)	119.7(11)
O(11)–N(1)–O(12)	121.5(12)
Pt–N(2)–O(21)	115.2(11)
Pt–N(2)–O(22)	119.5(11)
O(21)–N(2)–O(22)	125.2(15)

Table 22. Anisotropic thermal parameters ($Å^2 x10^3$) for $K_2[Pt(NO_2)_4Br_2]$.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
K	32(2)	35(2)	32(2)	1(1)	13(1)	1(1)
Pt	19(1)	17(1)	17(1)	−0(1)	6(1)	−1(1)
Br	40(1)	40(1)	45(1)	−2(1)	15(1)	2(1)
N(1)	27(6)	26(6)	18(5)	3(4)	5(5)	−2(5)
O(11)	37(6)	90(12)	21(5)	2(6)	15(5)	−6(7)
O(12)	23(5)	45(7)	30(5)	−1(5)	4(4)	−6(5)
N(2)	38(7)	14(5)	20(5)	−2(4)	3(5)	−5(5)
O(21)	50(8)	26(6)	34(6)	−0(5)	20(6)	1(5)
O(22)	87(12)	52(9)	62(9)	−5(8)	50(9)	−23(9)

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

The structure consists of a mononuclear platinum(IV) molecule exhibiting four nitrite ions in a square plane about the platinum and two bromide ions trans to each other. The platinum atom therefore exhibits octahedral coordination. The nitrite N–O distances range from 1.176 Å to 1.234 Å (average = 1.189 Å), and their bond angles range from 121.4° to 125.2P (average = 123.25°). As with the previous structures, the limiting factor for determining the quality of the crystallographic data was most likely the absorption correction. No evidence for disorder in the system was noted. Despite this being a known compound, the quality of the data and structure solution has shown a significant improvement over the original structure solution (78), which therefore warrants the inclusion of this structure in this investigation.

Structure of $K_2[Pt(Cl)_2(PO_3)_2]$, 5

An ORTEP view of the mononuclear, yellow complex is shown in Figure 14. Tables 23–26 contain the final positional, equivalent isothermal temperature parameters, bond distances, and angles. F_o and f_c values are found in Table 70 (Appendix).

The structure consists of a mononuclear square planar platinum(II) molecule with two chloride ions cis to each other and one PO_3 group trans to each chloride. The P–O distances range from 1.47 Å to 1.459 Å for double-bonded oxygens (average = 1.465 Å). Single-bonded P–O distances range from 1.752 Å to 1.778 Å (average = 1.766 Å). Bond angles for the PO_3 groups are approximately 109°, which are normal for tetrahedral coordination about the phosphorus. No evidence for disorder in the system was noted.

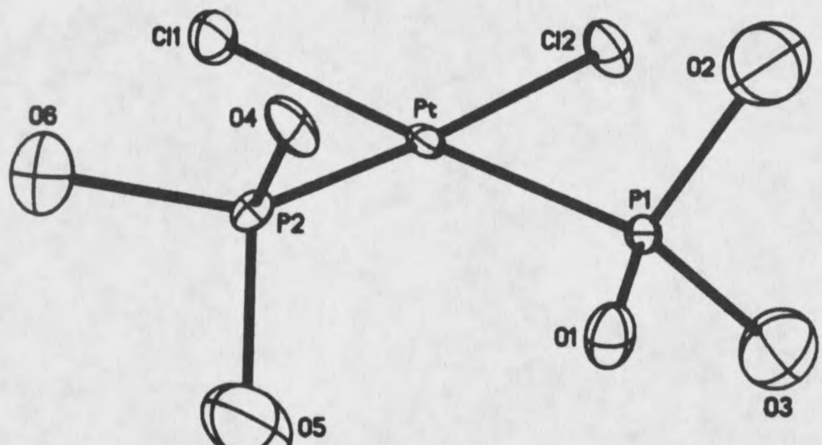


Figure 14. ORTEP view of $K_2[Pt(Cl)_2(PO_3)_2]$, 5

Table 23. Atomic coordinates ($x10^4$) and isotropic thermal parameters ($Å^2x10^3$) for $K_2[Pt(PO_3)_2Cl_2]$.

	x	y	z	U
Pt	267(1)	5160(1)	7857(1)	11(1)*
Cl(1)	21(4)	3548(2)	8603(4)	20(1)*
Cl(2)	3040(4)	4943(3)	8621(4)	19(1)*
P(1)	678(4)	6695(2)	7166(4)	12(1)*
P(2)	-2425(4)	5328(2)	6912(4)	10(1)*
O(1)	-732(13)	7349(7)	6704(12)	22(3)*
O(2)	1659(23)	6606(12)	5726(19)	63(4)*
O(3)	2096(19)	7332(12)	8556(16)	51(4)*
O(4)	-2868(13)	5526(8)	5322(11)	21(3)*
O(5)	-3255(21)	6248(11)	7812(19)	59(4)*
O(6)	-3489(18)	4275(10)	7257(17)	47(4)*

Table 24. Bond lengths (Å) for $K_2[Pt(PO_3)_2Cl_2]$.

Pt-Cl(1)	2.318(3)
Pt-Cl(2)	2.319(4)
Pt-P(1)	2.234(3)
Pt-P(2)	2.259(3)
P(1)-O(1)	1.470(11)
P(1)-O(2)	1.778(21)
P(1)-O(3)	1.752(14)
P(2)-O(4)	1.459(10)
P(2)-O(5)	1.761(18)
P(2)-O(6)	1.772(16)

Table 25. Bond angles (°) for $K_2[Pt(PO_3)_2Cl_2]$.

Cl(1)-Pt-Cl(2)	87.6(1)
Cl(1)-Pt-P(1)	176.2(1)
Cl(2)-Pt-P(1)	88.7(1)
Cl(1)-Pt-P(2)	92.6(1)
Cl(2)-Pt-P(2)	175.0(1)
P(1)-Pt-P(2)	91.1(1)
Pt-P(1)-O(1)	117.5(5)
Pt-P(1)-O(2)	107.6(5)
O(1)-P(1)-O(2)	110.0(7)
Pt-P(1)-O(3)	112.1(5)
O(1)-P(1)-O(3)	106.1(7)
O(2)-P(1)-O(3)	102.6(8)
Pt-P(2)-O(4)	112.1(5)
Pt-P(2)-O(5)	112.9(5)
O(4)-P(2)-O(5)	109.3(7)
Pt-P(2)-O(6)	112.0(5)
O(4)-P(2)-O(6)	109.2(7)
O(5)-P(2)-O(6)	100.7(8)

Table 26. Anisotropic thermal parameters ($Å^2x10^3$) for $K_2[Pt(PO_3)_2Cl_2]$.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Pt	14(1)	9(1)	14(1)	0(1)	9(1)	1(1)
Cl(1)	22(2)	14(1)	26(2)	4(1)	11(1)	1(1)
Cl(2)	14(1)	22(2)	25(2)	4(1)	9(1)	2(1)
P(1)	17(2)	8(1)	14(1)	1(1)	10(1)	-2(1)
P(2)	12(1)	8(1)	10(1)	0	0	0
O(1)	21(4)	16(4)	29(5)	6(4)	6(4)	-1(4)
O(2)	101(7)	49(6)	53(6)	-7(5)	43(6)	-20(6)
O(3)	50(6)	58(6)	45(6)	-18(5)	14(5)	-19(5)
O(4)	25(4)	27(4)	18(4)	10(4)	14(4)	2(4)
O(5)	77(7)	39(6)	78(7)	11(5)	53(6)	13(6)
O(6)	51(6)	38(6)	57(6)	-3(5)	26(5)	-15(5)

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

Structure of $[Pt_4(OAc)_6(CO_2)]\cdot 2(HOAc)$, 6

An ORTEP view of the rectangular, tetrameric, purple complex is shown in Figure 15. Tables 27-30 contain the final positional, equivalent isothermal temperature parameters, bond distances, and angles. F_o and f_e values are found in Table 71 (Appendix).

The structure consists of a nearly planar, rectangular tetramer of four platinum ions in which each of the platinum ions is located at a corner of the rectangle. The short ends of the rectangle are bridged by a pair of symmetric acetate ions, and the long sides of the rectangle are bridged by a single asymmetric acetate ion and a single symmetric carbonyl ligand. The C-O distances in the symmetric acetate ligands are 1.23(3) Å. In the asymmetric ligands the C-O distances are 1.26(3) Å and 1.48(3) Å. In the carbonyl ligands the Pt-C distances are 1.88(2) Å and 1.92(2) Å. The Pt-O-C angles for the asymmetric acetate ligands are 126.1(1.3)° and 134.6(1.2)°, while the symmetric ligands exhibit Pt–O–C angles of 125.2(1.8)°. The structure is interesting for a number of reasons which will be discussed later. No evidence for disorder was found during the solution and refinement of the structure.

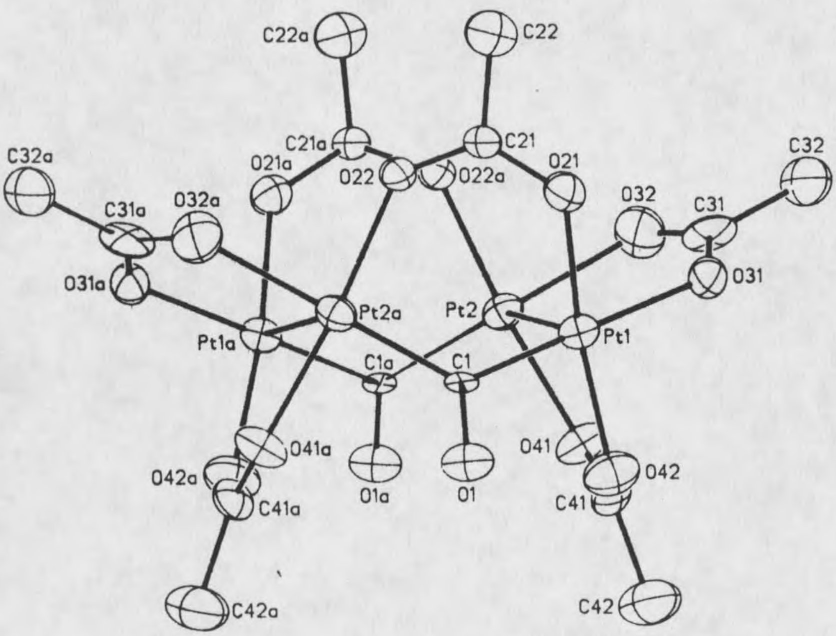


Figure 15. ORTEP view of $[Pt_4(OAc)_6(CO)_2]\cdot 2(HOAc)$, <u>6</u>

Table 27. Atomic coordinates ($x10^4$) and isotropic thermal parameters ($Å^2x10^3$) for $[Pt_4(OAc)_6(CO)_2]\cdot 2(HOAc)$.

	x	y	z	U
Pt(1)	963(1)	936(1)	2412(1)	33(1)*
Pt(2)	200(1)	617(1)	3966(1)	33(1)*
C(1)	467(8)	1690(18)	1407(12)	16(6)*
O(1)	576(7)	2906(16)	1020(10)	47(6)*
O(21)	998(7)	-1208(16)	1883(10)	43(6)*
O(22)	-125(6)	-1513(15)	3689(9)	34(5)*
C(21)	584(10)	-1987(22)	1553(13)	29(7)*
C(22)	654(11)	-3665(24)	1491(17)	51(10)*
O(31)	1525(6)	134(17)	3458(10)	44(6)*
O(32)	911(8)	-572(18)	4498(11)	63(7)*
C(31)	1389(11)	-541(23)	197(16)	49(9)*
C(32)	1850(11)	-1320(27)	4770(16)	60(10)*
O(41)	584(7)	2640(16)	4315(10)	46(6)*
O(42)	1030(7)	3104(18)	2976(11)	54(7)*
C(41)	861(10)	3432(24)	3785(17)	39(8)*
C(42)	1016(13)	5082(28)	4122(19)	74(12)*
C(51)	2434(17)	7336(43)	1342(23)	98(17)*
C(52)	2404(15)	7322(44)	2340(26)	119(19)*
O(51)	2703(9)	8440(24)	992(14)	94(10)*
O(52)	2152(10)	6429(27)	792(18)	97(10)*
H(22A)	1031	-3938	1707	105(31)
H(22B)	589	-3988	848	105(31)
H(22C)	389	-4165	1877	105(31)
H(32A)	2199	-1220	4461	105(31)
H(32B)	1760	-2392	4835	105(31)
H(32C)	1887	-851	5382	105(31)
H(42A)	1230	5584	3656	105(31)
H(42B)	1237	5032	4707	105(31)
H(42C)	676	5654	4211	105(31)
H(52A)	2181	6462	2524	105(31)
H(52B)	2234	8261	2540	105(31)
H(52C)	2778	7236	2629	105(31)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized $_{ij}$ tensor

Table 28. Bond lengths (Å) for $[Pt_4(OAc)_6(CO)_2].2(HOAc)$.

Pt(1)-Pt(2)	2.940(1)
Pt(1)-C(1)	1.919(17)
Pt(1)-O(1)	2.738(14)
Pt(1)-O(21)	2.011(14)
Pt(1)-O(31)	2.063(14)
Pt(1)-O(42)	2.049(15)
Pt(1)-Pt(2B)	3.312(1)
Pt(2)-O(22)	2.033(13)
Pt(2)-O(32)	2.086(17)
Pt(2)-O(41)	2.029(14)
Pt(2)-Pt(1A)	3.312(1)
Pt(2)-Pt(2A)	3.309(2)
Pt(2)-C(1A)	1.887(18)
Pt(2)-O(1A)	2.709(15)
C(1)-O(1)	1.224(22)
C(1)-Pt(2B)	1.887(18)
O(1)-Pt(2B)	2.709(15)
O(21)-C(21)	1.264(26)
O(22)-C(21A)	1.198(27)
C(21)-C(22)	1.469(28)
C(21)-O(22A)	1.198(27)
O(31)-C(31)	1.259(27)
O(32)-C(31)	1.232(33)
C(31)-C(32)	1.491(35)
O(41)-C(41)	1.233(27)
O(42)-C(41)	1.269(29)
C(41)-C(42)	1.548(33)
C(51)-C(52)	1.423(50)
C(51)-O(51)	1.267(44)
C(51)-O(52)	1.275(43)

Table 29. Bond angles (°) for $[Pt_4(OAc)_6(CO)_2].2(HOAc)$.

Pt(2)-Pt(1)-C(1)	102.3(6)
Pt(2)-Pt(1)-O(1)	113.9(3)
C(1)-Pt(1)-O(1)	22.9(6)
Pt(2)-Pt(1)-O(21)	103.4(4)
C(1)-Pt(1)-O(21)	94.2(6)
O(1)-Pt(1)-O(21)	109.1(5)
Pt(2)-Pt(1)-O(31)	80.1(4)
C(1)-Pt(1)-O(31)	177.6(7)
O(1)-Pt(1)-O(31)	155.6(5)
O(21)-Pt(1)-O(31)	85.4(6)
Pt(2)-Pt(1)-O(42)	80.3(5)
C(1)-Pt(1)-O(42)	90.6(7)
O(1)-Pt(1)-O(42)	74.0(5)
O(21)-Pt(1)-O(42)	173.2(6)
O(31)-Pt(1)-O(42)	89.7(6)
Pt(2)-Pt(1)-Pt(2B)	84.8(1)
C(1)-Pt(1)-Pt(2B)	29.3(5)
O(1)-Pt(1)-Pt(2B)	52.2(3)
O(21)-Pt(1)-Pt(2B)	75.6(4)
O(31)-Pt(1)-Pt(2B)	152.2(4)
O(42)-Pt(1)-Pt(2B)	110.7(5)
Pt(1)-Pt(2)-O(22)	100.4(4)
Pt(1)-Pt(2)-O(32)	78.5(5)
O(22)-Pt(2)-O(32)	84.9(6)
Pt(1)-Pt(2)-O(41)	79.3(4)
O(22)-Pt(2)-O(41)	174.5(6)
O(32)-Pt(2)-O(41)	89.7(6)
Pt(1)-Pt(2)-Pt(1A)	94.3(1)
O(22)-Pt(2)-Pt(1A)	70.5(4)
O(32)-Pt(2)-Pt(1A)	152.8(4)
O(41)-Pt(2)-Pt(1A)	115.0(4)
Pt(1)-Pt(2)-Pt(2A)	155.8(1)
O(22)-Pt(2)-Pt(2A)	75.8(4)
O(32)-Pt(2)-Pt(2A)	77.4(5)
O(41)-Pt(2)-Pt(2A)	102.1(4)
Pt(1A)-Pt(2)-Pt(2A)	106.5(1)
Pt(1)-Pt(2)-C(1A)	106.4(5)
O(22)-Pt(2)-C(1A)	95.3(7)
O(32)-Pt(2)-C(1A)	175.0(7)
O(41)-Pt(2)-C(1A)	90.1(7)
Pt(1A)-Pt(2)-C(1A)	29.8(5)
Pt(2A)-Pt(2)-C(1A)	97.8(5)
Pt(1)-Pt(2)-O(1A)	112.4(3)
O(22)-Pt(2)-O(1A)	114.7(5)
O(32)-Pt(2)-O(1A)	153.8(5)
O(41)-Pt(2)-O(1A)	70.1(6)

Table 29. (continued)

Pt(1A)-Pt(2)-O(1A)	53.0(3)
Pt(2A)-Pt(2)-O(1A)	90.3(3)
C(1A)-Pt(2)-O(1A)	23.1(6)
Pt(1)-C(1)-O(1)	119.5(14)
Pt(1)-C(1)-Pt(2B)	120.9(9)
O(1)-C(1)-Pt(2B)	119.5(14)
Pt(1)-O(1)-C(1)	37.6(10)
Pt(1)-O(1)-Pt(2B)	74.9(4)
C(1)-O(1)-Pt(2B)	37.3(10)
Pt(1)-O(21)-C(21)	126.0(14)
Pt(2)-O(22)-C(21A)	134.2(13)
O(21)-C(21)-C(22)	117.6(20)
O(21)-C(21)-O(22A)	127.0(18)
C(22)-C(21)-O(22A)	115.4(19)
Pt(1)-O(31)-C(31)	125.1(15)
Pt(2)-O(32)-C(31)	127.2(15)
O(31)-C(31)-O(32)	125.4(22)
O(31)-C(31)-C(32)	117.1(23)
O(32)-C(31)-C(32)	117.5(20)
Pt(2)-O(41)-C(41)	125.5(14)
Pt(1)-O(42)-C(41)	122.6(14)
O(41)-C(41)-O(42)	129.0(20)
O(41)-C(41)-C(42)	116.9(21)
O(42)-C(41)-C(42)	114.0(20)
C(52)-C(51)-O(51)	116.7(32)
C(52)-C(51)-O(52)	123.6(34)
O(51)-C(51)-O(52)	119.0(30)

Table 30. Anisotropic thermal parameters ($Å^2 x10^3$) for $[Pt_4(OAc)_6(CO)_2]\cdot 2(HOAc)$.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Pt(1)	38(1)	28(1)	33(1)	-2(1)	3(1)	-3(1)
Pt(2)	39(1)	30(1)	29(1)	0(1)	2(1)	-6(1)
C(1)	20(12)	9(8)	19(9)	-8(7)	13(9)	3(8)
O(1)	63(12)	33(9)	44(9)	-0(7)	7(9)	-3(8)
O(21)	43(11)	38(9)	49(9)	-6(7)	-5(8)	7(8)
O(22)	38(11)	25(7)	37(9)	5(6)	-9(8)	-2(7)
C(21)	45(16)	24(11)	15(10)	1(8)	-13(10)	1(11)
C(22)	48(18)	50(15)	59(17)	7(13)	26(14)	2(13)
O(31)	37(10)	41(9)	54(10)	-12(8)	-5(8)	3(8)
O(32)	65(13)	63(11)	61(11)	28(9)	-7(10)	-5(10)
C(31)	71(19)	30(12)	47(14)	22(11)	5(13)	-21(12)
C(32)	76(22)	56(16)	47(15)	-1(13)	-19(15)	-4(15)
O(41)	57(11)	39(9)	43(9)	-8(7)	10(8)	-18(8)
O(42)	65(13)	46(10)	53(11)	-2(8)	18(10)	-11(9)
C(41)	28(15)	39(13)	51(15)	-2(11)	13(12)	-9(11)
C(42)	105(28)	47(16)	69(19)	5(15)	-11(19)	-14(18)
C(51)	118(35)	107(28)	66(22)	-3(22)	-33(22)	50(27)
C(52)	77(29)	134(33)	152(38)	-25(30)	63(28)	7(25)
O(51)	96(19)	90(15)	93(16)	13(13)	-16(14)	5(14)
O(52)	62(15)	110(18)	119(19)	-19(16)	-4(14)	7(14)

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

Physical Measurements

Electron Spectroscopy for Chemical Analysis (ESCA)

ESCA has been developed as a very powerful method for chemical bond studies because it addresses the electons involved in bond formation, along with the atomic-like non-bonding electrons, which act as local probes of the molecular and solid state structures. In this investigation we analyzed the electronic properties of $Pt\text{-}X^+$ transition metal ions (X = 0, 1.5, 2, 3, 4) under the influence of various chemical environments. From these studies it was quite evident that the ligands have a significant effect upon the chemical shift (E_b eV) of the electrons on platinum. Surface charging effects in the solid sample are a significant problem in the applications of ESCA to chemical systems. Such a problem may be compensated by monitoring the chemical shift of the C(1s) binding energy. Should a significant change in chemical shift be detected, charging effects can be empirically corrected for by normalizing to a constant figure as was suggested by Riggs in his original work on complexes of platinum (76). The normalization probably is not completely correct.

In this investigation, the samples were mounted by physically rolling individual "pies" from bulk Indium metal. The samples were then adhered to the metallic surface by simply rolling them into the soft metal "pie". Excess loose powders were removed by a series of gentle bursts of dry nitrogen gas applied to the pie. The samples were then secured on the sample rod and introduced to the vacuum chamber immediately.

To correct for surface charging effects, the Indium (3d 3/2, 5/2) and aliphatic C(1s) signals were monitored, with the aliphatic C(1s) being corrected to a chemical shift of 285.0 eV. Data from this investigation are presented in Table 31.

Table 31. ESCA data for platinum complexes.

Complex	Formal Ox. State	E_b Pt(4f 7/2)	E_b C(1s)	E_b Other Elements
K_2PtCl_6	4+	75.9		199.4 Cl(2p)
$K_2Pt(CN)_4$	2+	74.0	285.0	
$K_2Pt(Cl)_4$	2+	73.4		199.4 Cl(2p)
$PtCl_2$	2+	75.9		199.6 Cl(2p)
$KPt(NO_2)_4 \cdot H_2O$	4+	75.2	285.0	(Major Species)
$KPt(NO_2)_3 \cdot H_2O$	2+	72.9	285.0	(Minor Species)
Pt(metal)	0	70.1	284.6	
$Pt_2(HP)_2(Et_2S)_1$	+3	74.7	285.0	
$Pt_2(FHP)_2(ET_2S)_1$	+3	74.6	285.0	
$Pt_2(MHP)_2(Et_2S)$	+3	74.7	285.0	
$Pt_2(FPH)_2(Pyr)_1$	+3	74.5	285.0	
$Pt_2(MHP)(Pyr)_1$	+3	74.2	285.0	
$Pt_2(CHP)_2(Pyr)_1$	+3	74.5	285.0	
$Pt_2(HP)_2(Pyr)_2$	+3	74.3	285.0	
$Pt_2(FHP)_2(Pyr)_2$	+3	74.2	285.0	
$Pt_2(MHP)_2(Pyr)_2$	+3	73.8	285.0	
$Pt_2(PO_3)_4 \cdot 2H_2O$	+3	75.2	285.0	
$Pt_2(POP)Cl_2$	+3	75.1	285.0	
$Pt_4(OAc)_8$ Blue	+2	74.3	285.0	
$Pt_4(OAc)_8$Green	+2	74.7	285.0	
$Pt_4(OAc)_6(CO)_2 \cdot 2HoAc$	1.5	74.4	285.0	
$Pt_4(OOCCF_3)_8$ Blue	+2		285.0	
$Pt_4(POP)_y$ Red Lumin. Complex	+2	72.6		131.6(P)
Pt(en)(ox)	+2	74.3	285.0	
$Pt_4(OAc)_8$ Blue + Excess Trifluoro- Acetic Acid	+4	75.3	285.0	562.4(F)
"German Yellow Complex"	+4	75.8	285.5	
"German Red Complex", "Vzez's Salt"	+4	75.3	285.0	

NMR Spectra and Spectral Assignments for a Series of Pt(III) Complexes

The compounds which are described below were synthesized by Dr. D. P. Bancroft while working with Professor F. A. Cotton at Texas A & M University, College Station, Texas. The molecular structures were elucidated by Dr. Bancroft using single crystal x-ray crystallographic methods. The proton, carbon-13, and platinum-195 NMR spectra and chemical shift assignments were performed at Montana State University as part of a collaborative effort to explore the chemistry of the complexes. Studies of the complexes' reaction chemistry continue both here and at Texas A & M University. The structures of the complexes are shown in Figure 3. There are two structures known for the complexes. One is described as a head-to-head or polar form, and the other is the head-to-tail or nonpolar form. Some of the complexes have been shown by Cotton's group to undergo conversion from one form to the other under specific conditions. For each of the following compounds the chemical shifts and their assignments are shown. The molecular numbering scheme which will be employed for this purpose is shown in Figure 16. The NMR spectral data and assignments are shown in Tables 32 to 39. The ^{1}H, ^{13}C, and ^{195}Pt NMR spectra are shown in Figures 18 to 45. The methods used to make the assignments are described in the Discussion.

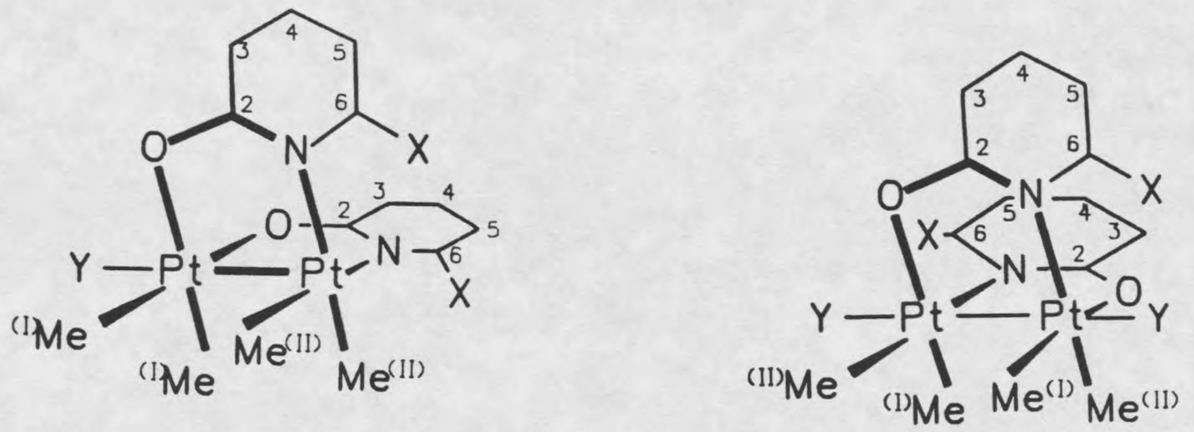


Figure 16. The molecular numbering scheme used for this investigation: a) head-to-head platinum(III) dimer; b) head-to-tail platinum(III) dimer.

Table 32. $Pt_2(mhp)_2(CH_3)_4pyr_1$ (head-to-head dimer).

Resonance	(Mult.)	Assignment	Coupling Constants
Proton Assignments			
1.03		MeI	$^2J_{CH_3-Pt}$ 69.84Hz
1.50		MeII	$^2J_{CH_3-Pt}$ 79.34Hz
2.36		Me(X)(Ring Substituent)	
6.23 6.25	(d)	5H	
6.48 6.52	(d)	3H	
7.15(t)		4H	
7.24		$CDCl_3$	
7.39		β-Pyridine	
7.91		γ-Pyridine	
8.49		α-Pyridine	
Carbon-13 Assignments			
-8.95(t)		MeI	$^1J_{CH_3-Pt}$ 705.72 Hz $^2J_{CH_3}$ 37.3 Hz
-1.39(t)		MeII	$^2J_{CH_3-Pt}$ 705.7Hz $^2J_{CH_3-Pt}$ 37.3Hz
26.27		Me(Ring Substituent)	
111.21		C_5	
113.5		C_3	
125.3		β-Pyridine	
137.14		C_4	
138.6		γ-Pyridine	
150.04		α-Pyridine	
153.5		C_2	
Platinum-195 Spectra			
-2922.2		Pt_1	12,060.5Hz
-1635.9		Pt_2	

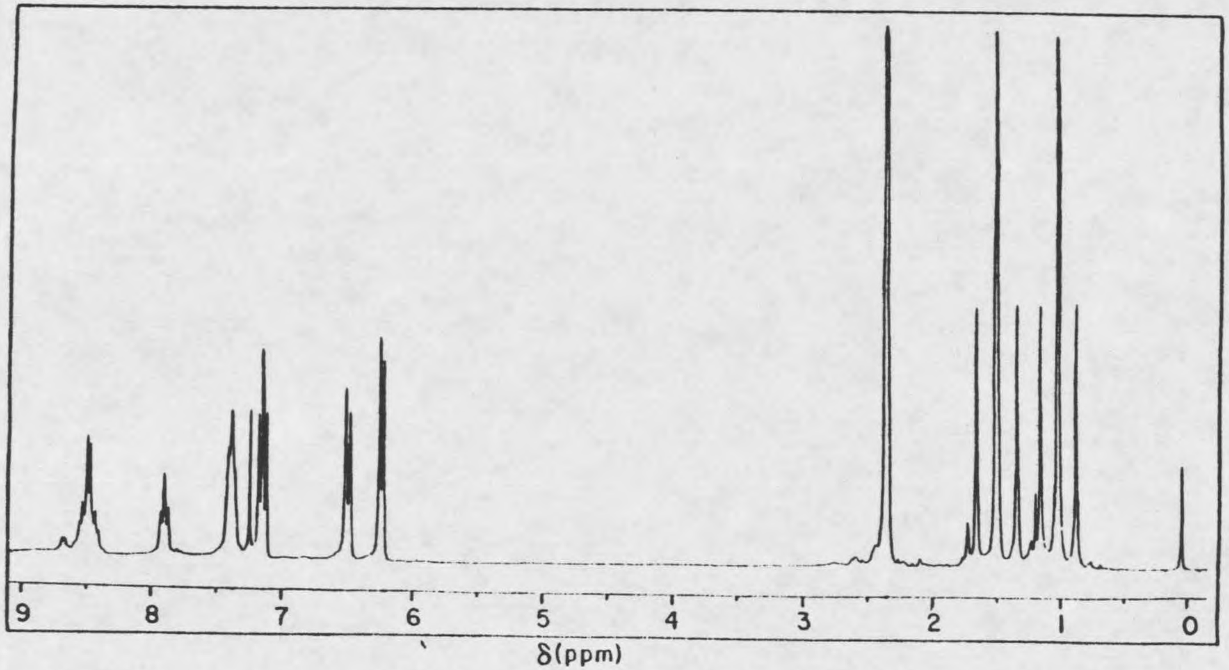


Figure 17. ^{1}H NMR spectrum of $[Pt_2(CH_3)_4(mhp)_2(pyr)]$.

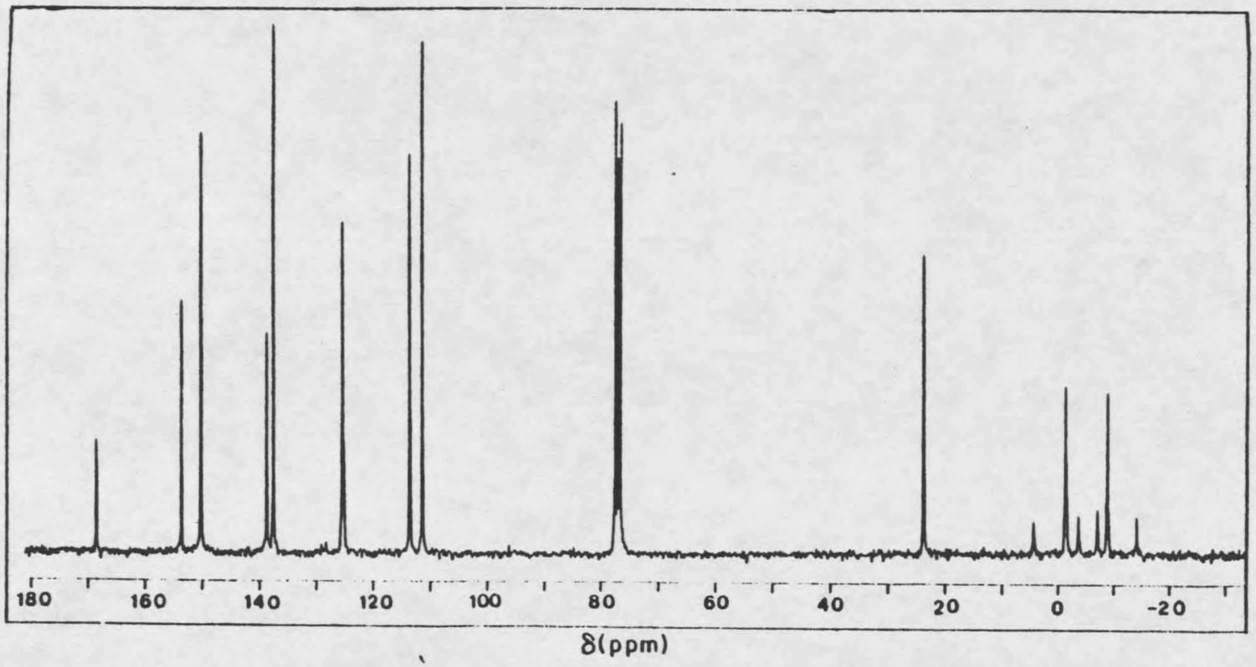


Figure 18. $^{13}C(^{1}H)$ NMR spectrum of $[Pt_2(CH_3)_4(mhp)_2(pyr)]$.

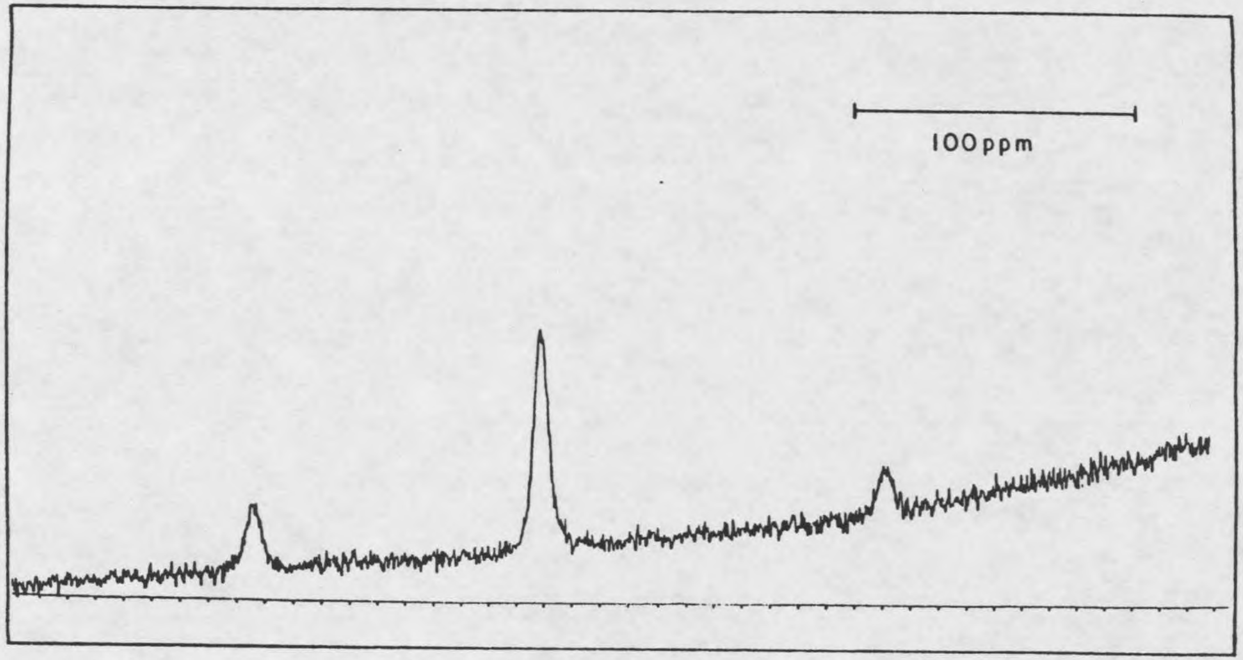


Figure 19. Upfield region of ^{195}Pt NMR spectrum of $[Pt_2(CH_3)_4(mhp)_2(pyr)]$.

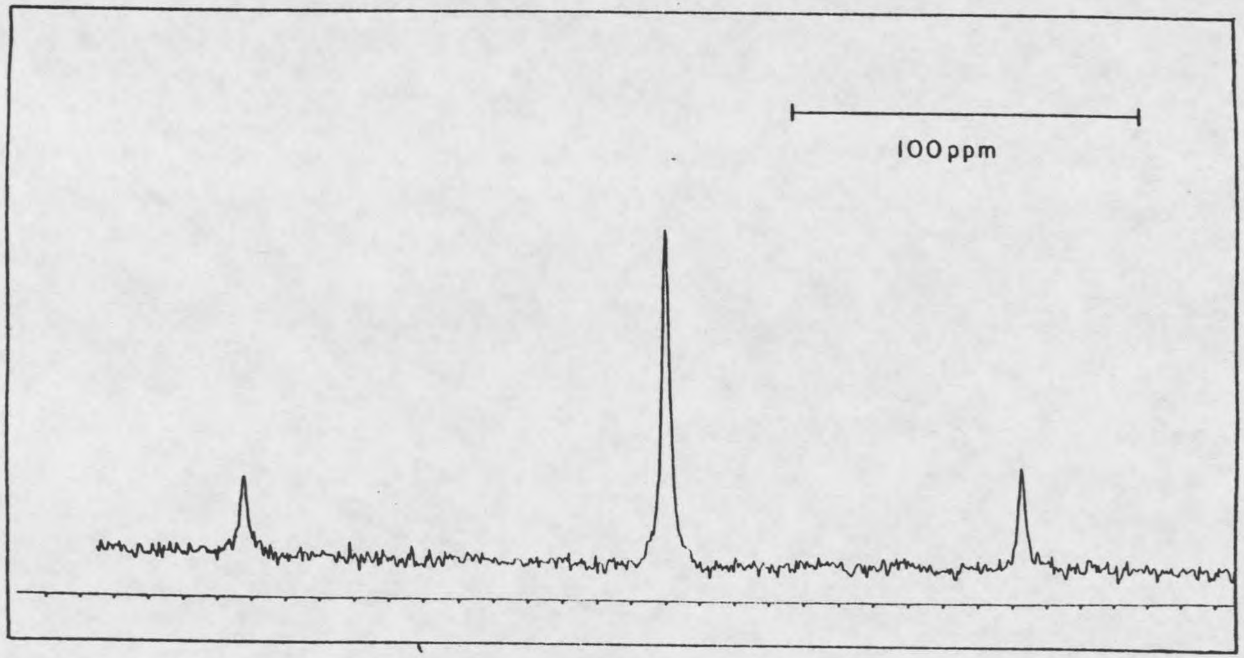


Figure 20. Downfield region of ^{195}Pt NMR spectrum of $[Pt_2(CH_3)_4(mhp)_2(pyr)]$.

Table 33. $Pt_2(CH_3)_4(hp)_2(Et_2S)_1$ (head-to-head dimer).

Resonance	(Mult.)	Assignment	Coupling Constants
Proton Assignments			
1.03		MeI	$^2J_{CH_3-Pt}$ 5.85Hz
1.21		MeII	$^2J_{CH_3-Pt}$ 10.23Hz
1.35		$S-CH_3$	
2.72(Broad Meth)		$S-CH_2$	
6.26	(t)	5H	
6.42	(d)	3H	
7.24	(Mult)	4H	
7.69	(d)	6H	
Carbon-13 Assignments			
-12.8	(t)	MeI	$^2J_{CH_3-Pt}$ 31.5Hz
-2.51	(t)	MeII	$^2J_{CH_3-Pt}$ 23.63Hz
11.40		$S-CH_3$	
28.54		$S-CH_2$	
110.74		C_5	
116.16		C_3	
138.07		C_4	
144.18		C_5	
168.00		C_2	
Platinum-195 Spectra			
-2607		Pt_1	10,599.8Hz
-2436		Pt_2	

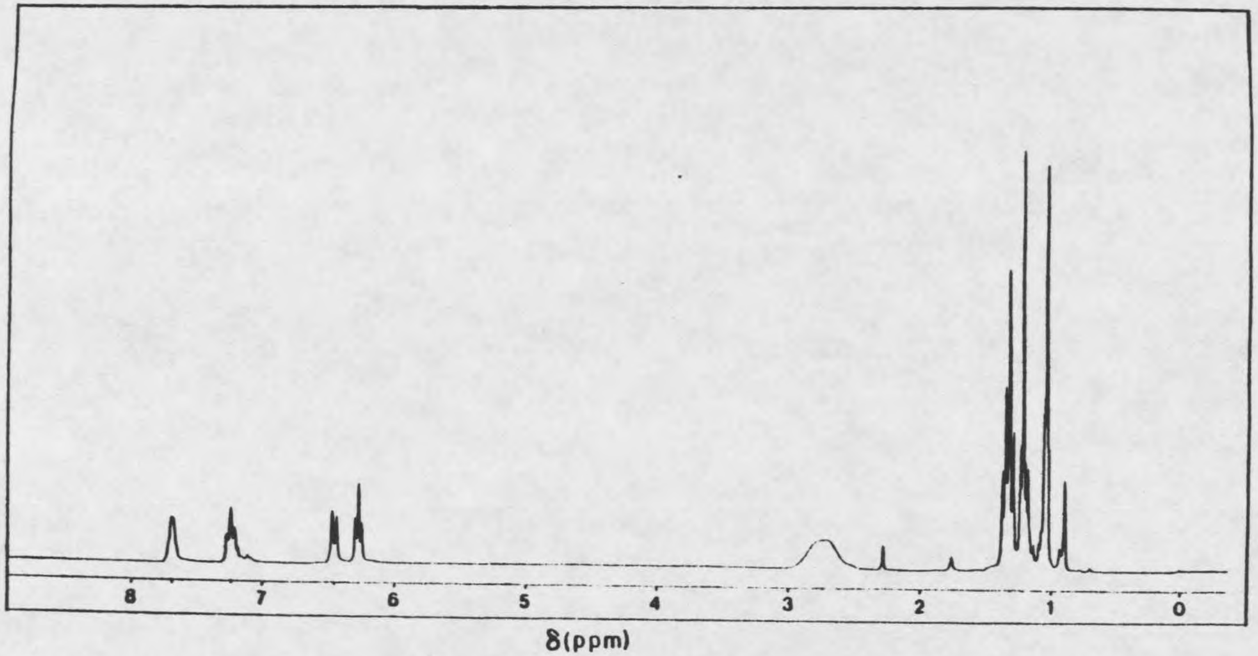


Figure 21. ^1H NMR spectrum of $[Pt_2(CH_3)_4(hp)_2(C_2H_5)_2S)]$.

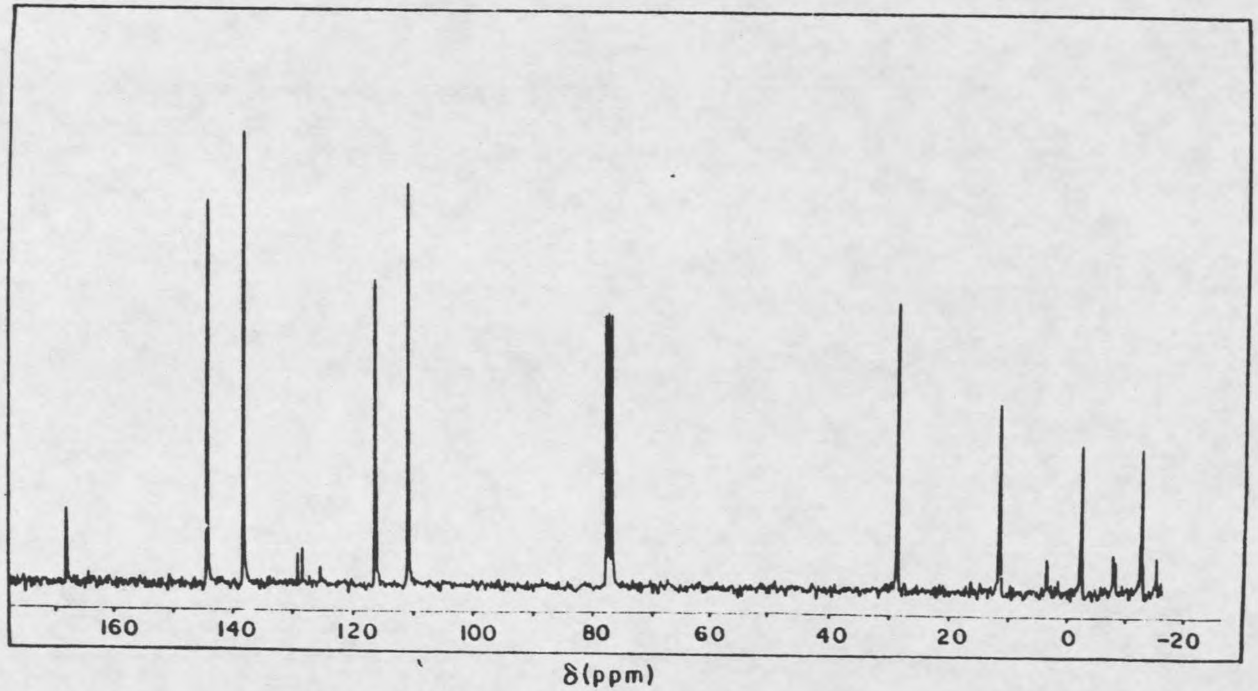


Figure 22. $^{13}C(^{1}H)$ NMR spectrum of$[Pt_2(CH_3)_4(hp)_2((C_2H_5)_2S)]$.

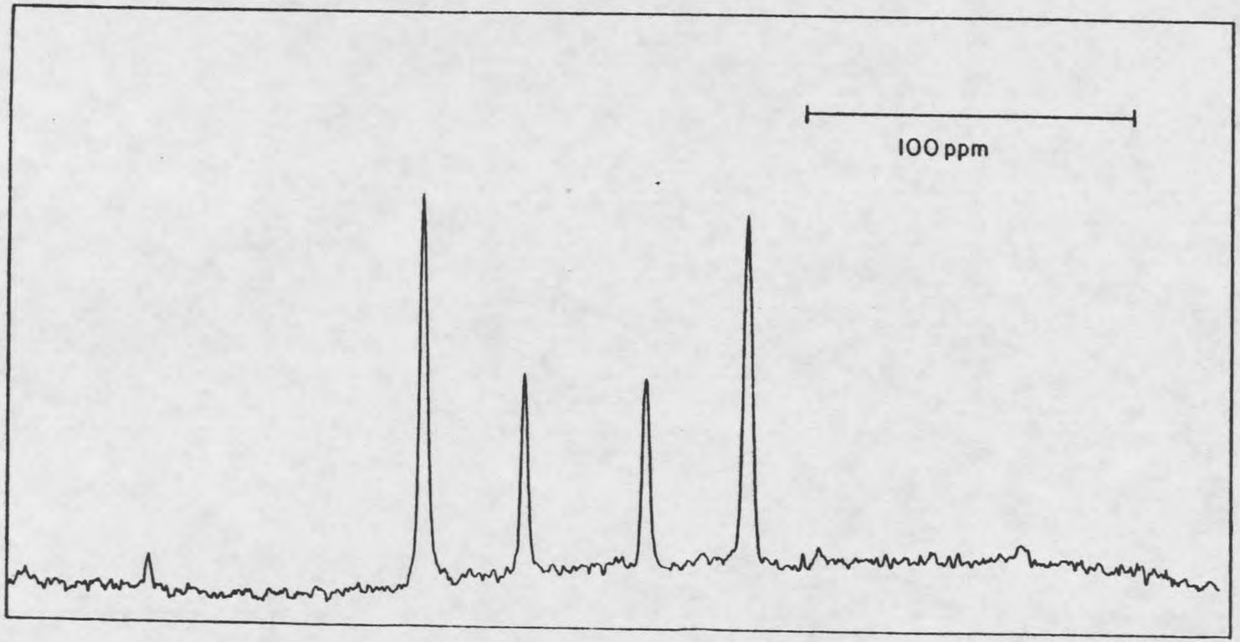


Figure 23. ^{195}Pt NMR spectrum of $[Pt_2(CH_3)_4(hp)_2((C_2H_5)_2S)]$.

Table 34. $Pt_2(CH_3)_4(mhp)_2(Et_2S)_1$ (head-to-head dimer).

Resonance	(Mult.)	Assignment	Coupling Constants
Proton Assignments			
1.03	(t)	MeI	$^2J_{CH_3-Pt}$ 10.83Hz
1.15	(t)	MeII	$^2J_{CH_3-Pt}$ 14.85Hz
1.38	(t)	$S-CH_3$	
2.10	(t)		
2.32		Me(X)(Ring Subst.)	
2.75		$S-CH_2$	
6.21	(d)	5H	
6.24			
6.40	(d)	3H	
6.44			
7.14	(t)	4H	
Carbon-13 Assignments			
-12.34	(t)	MeI	$^1J_{CH_3-Pt}$ 618.23Hz $^2J_{CH_3-Pt}$ 25.60Hz
-2.40	(t)	MeII	$^1J_{CH_3-Pt}$ 730.45Hz $^2J_{CH_3-Pt}$ 23.63Hz
11.39		$S-CH_3$	
24.00		$S-CH_2$	
28.30		Me-(Ring Subst.)	
111.08		C_5	
113.32		C_3	
137		C_4	
153		C^6	
168		C_2	
Platinum-195 Spectra			
-2672		Pt_1	11,311.0Hz
-2367		Pt_2	

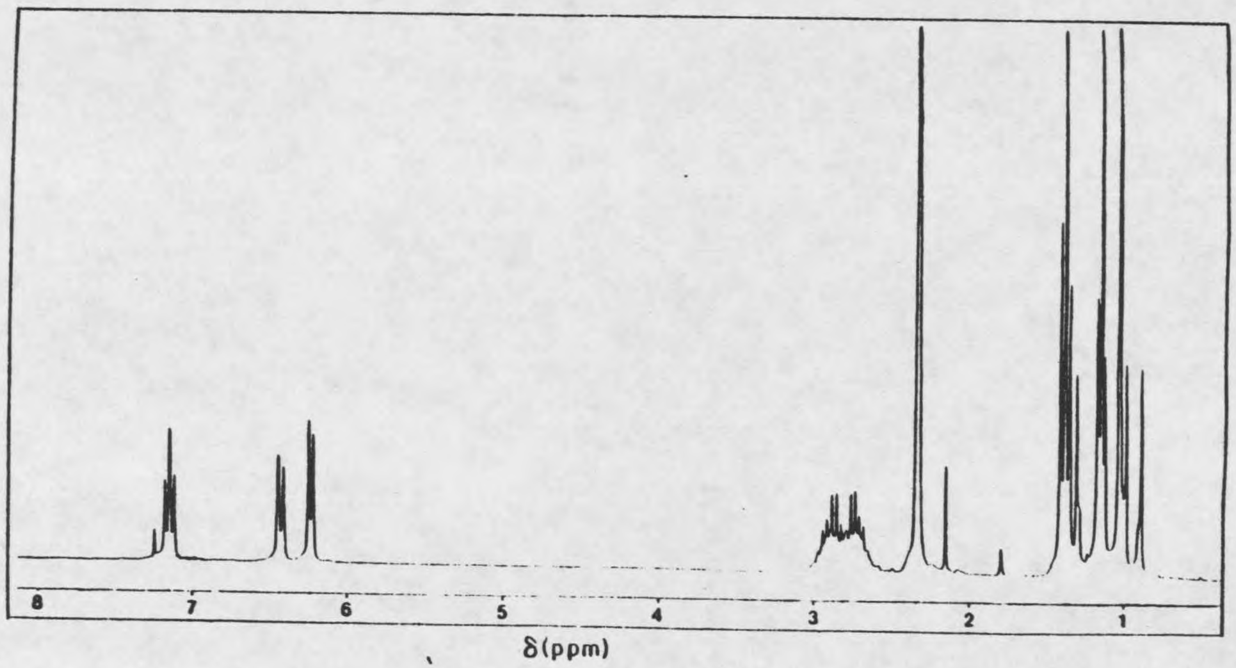


Figure 24. ^{1}H NMR spectrum of $[Pt_2(CH_3)_4(mhp)_2((C_2H_5)_2S)]$.

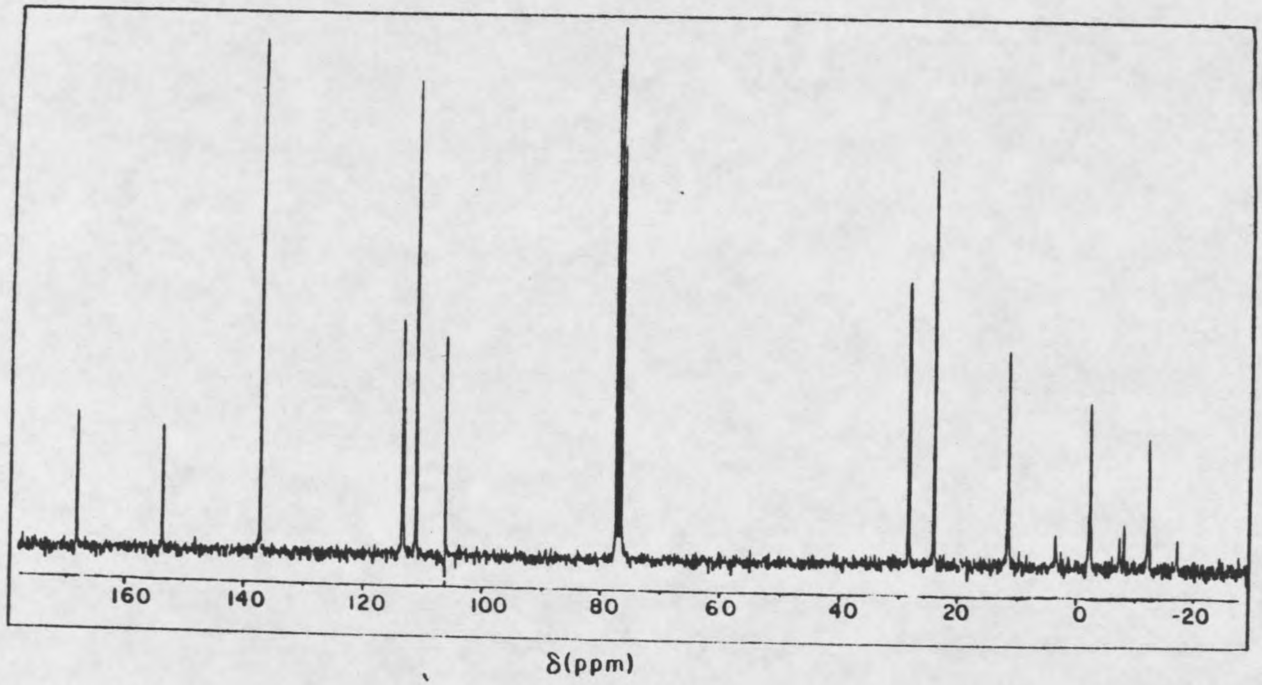


Figure 25. $^{13}C(^{1}H)$ NMR spectrum of $[Pt_2(CH_3)_4(mhp)_2((C_2H_5)_2S)]$.

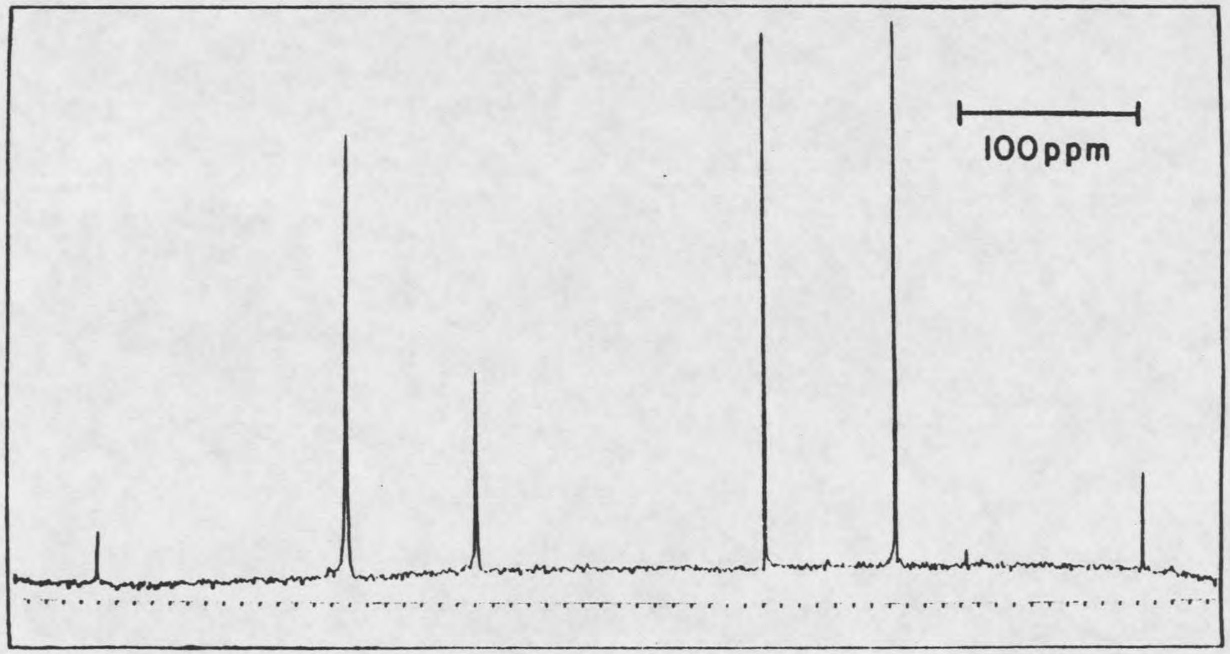


Figure 26. ^{195}Pt NMR spectrum of $[Pt_2(CH_3)_4(mhp)_2((C_2H_5)_2S)]$.

Table 35. $Pt_2(CH_3)_4(FHP)_2(Pyr)_2$ (head-to-tail dimer).

Resonance	(Mult.)	Assignment	Coupling Constants
Proton Assignments			
1.13	(3)	MeI	$^2J_{CH_3-Pt}$ 80.57Hz $^3J_{CH_3-Pt}$ 3.05Hz
1.61	(3)	MeII	$^2J_{CH_3-Pt}$ 72.63Hz $^3J_{CH_3Pt}$ 7.32Hz
5.69(d) 5.73		5H	
6.34 6.38	(d)	3H	
7.3	(Broad Mult)	4H	
7.45		β-Pyridine	
7.74	(3)	γ-Pyridine	
8.52	(4)	α-Pyridine	
Carbon-13 Assignments			
-14		MeI	$^1J_{CH_3-Pt}$ 661.54Hz $^2J_{CH_3-Pt}$
-7.32		MeII	$^1J_{CH_3-Pt}$ 744.24Hz $^2J_{CH_3-Pt}$ 27.56Hz
91.34 91.85		C_5	
112.63		C_3	$S-CH_2$
124.03		β-Pyridine	
138.8		γ-Pyridine	
140.49		C_4	
148.82		α-Pyridine	
164.67		C_6	
170.05		C_2	
Platinum-195 Spectra			
-2323	One Resonance Only	Equal Chemical Environment	

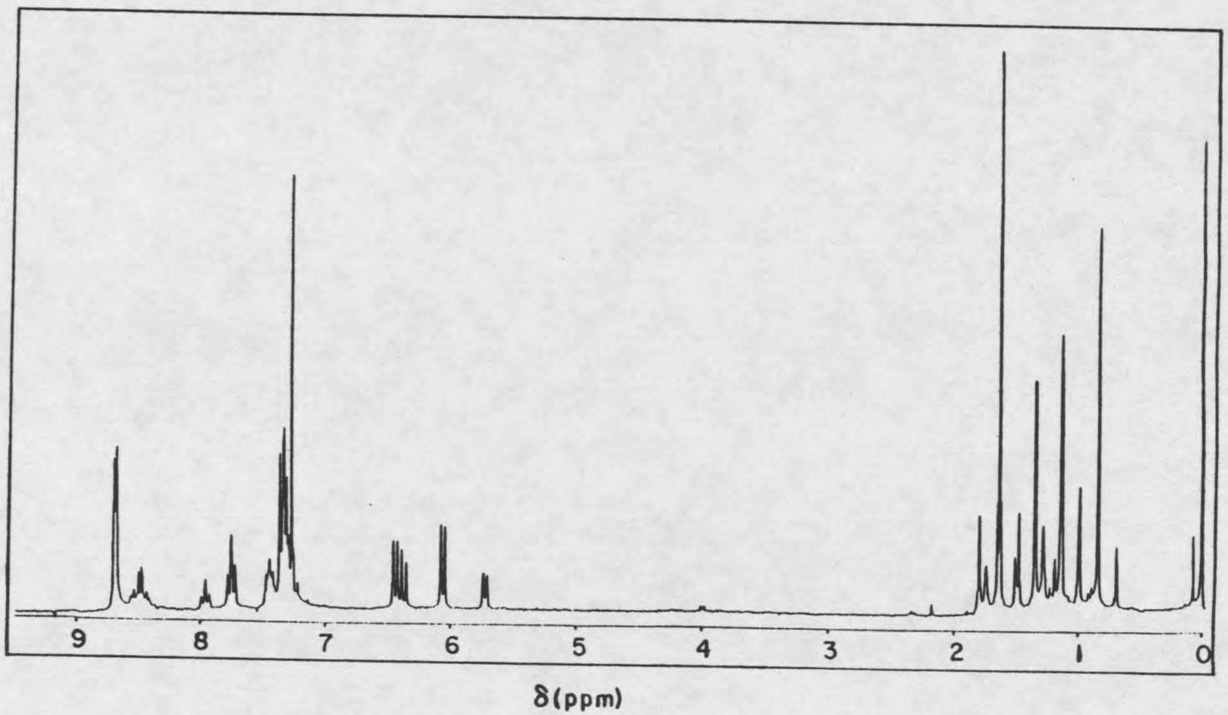


Figure 27. ^{1}H NMR spectrum of $[Pt_2(CH_3)_4(fhp)_2(pyr)_2]$.

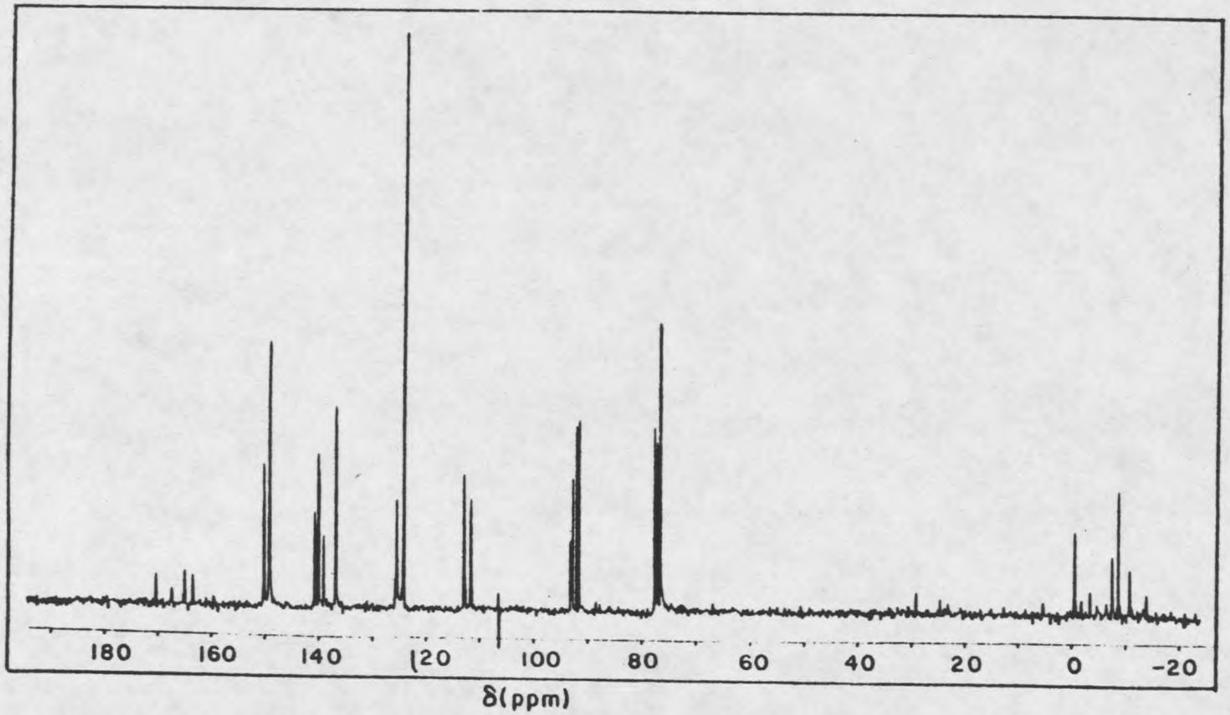


Figure 28. $^{13}C(^{1}H)$ NMR spectrum of $[Pt_2(CH_3)_4(fhp)_2(pyr)_2]$.

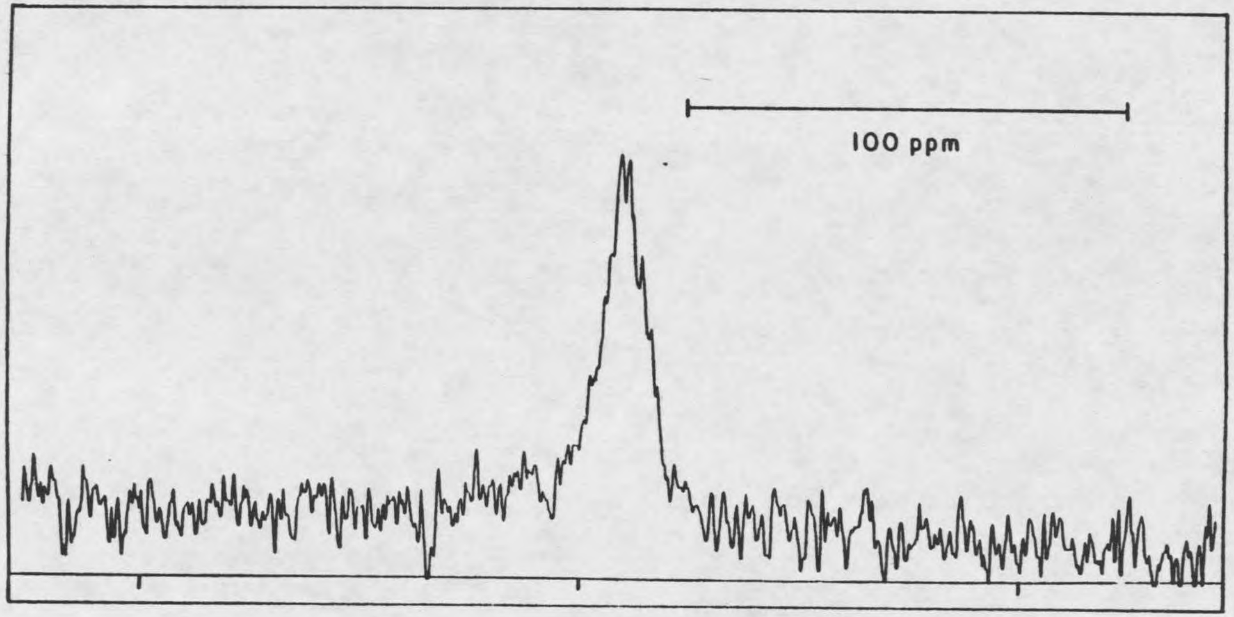


Figure 29. ^{195}Pt NMR spectrum of $[Pt_2(CH_3)_4(fhp)_2(pyr)_2]$.

Table 36. $Pt_2(CH_3)_4(chp)_2(pyr)_1$ (head-to-head dimer).

Resonance	(Mult.)	Assignment	Coupling Constants
Proton Assignments			
1.15	(t)	MeI	$^2J_{CH_3-Pt}$ 70.2Hz $^3J_{Pt-CH_3}$ 6.10Hz
1.46	(t)	MeII	$^2J_{CH_3-Pt}$ 79.65Hz
6.40	(d)	5H	
6.45	(d)	3H	
7.14	(t)	4H	
7.24		$CHCl_3$	
7.36		β-Pyridine	
7.88		γ-Pyridine	
8.40		α-Pyridine	
Carbon-13 Assignments			
-8.78	(t)	MeI	$^1J_{Pt-CH_3}$ 667.0Hz $^2J_{Pt-CH_3}$ 34.88Hz
-2.05	(t)	MeII	$^1J_{CH_3-Pt}$ 736.8Hz $^2J_{CH_3-Pt}$ 28.3Hz
110.62		C_5	
114.05		C_3	
125.31		β-Pyridine	
137.65		γ-Pyridine	
138.65		C_4	
150.02		C_6 + α-Pyridine	
168.91		C_2	
Platinum-195 Spectra			
-3016.7		Pt_1	12,353.5Hz
-1785.6		Pt_2	

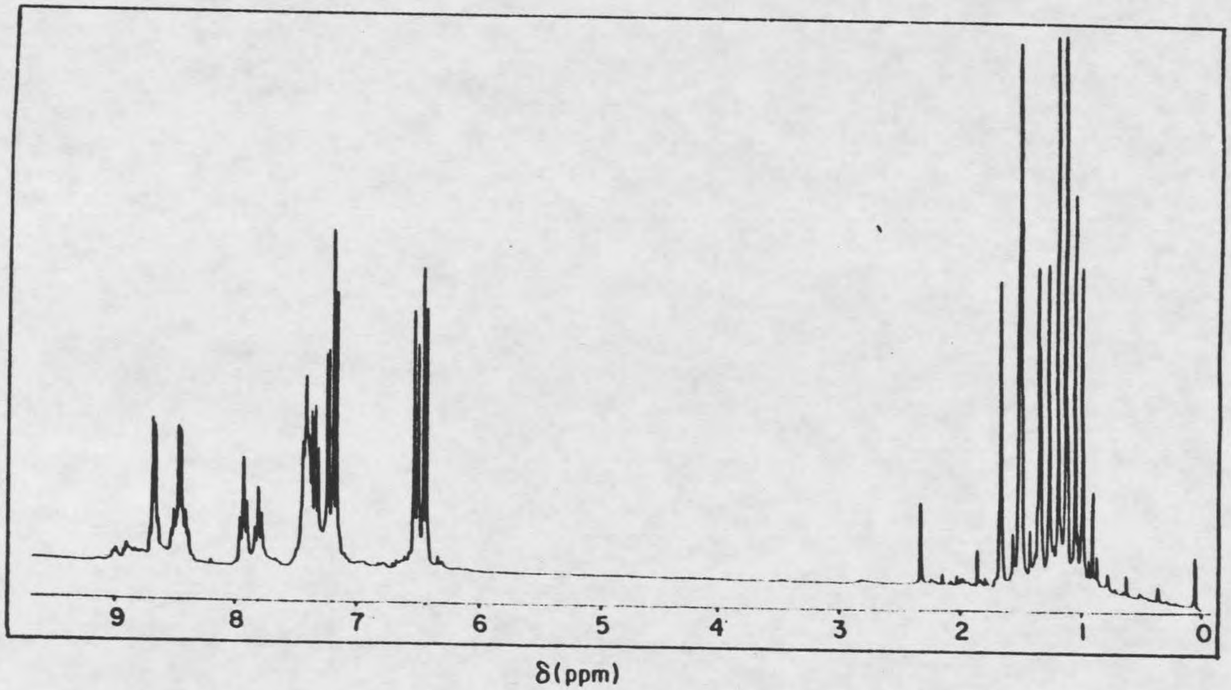


Figure 30. ^{1}H NMR spectrum of $[Pt_2(CH_3)_4(chp)_2(pyr)]$.

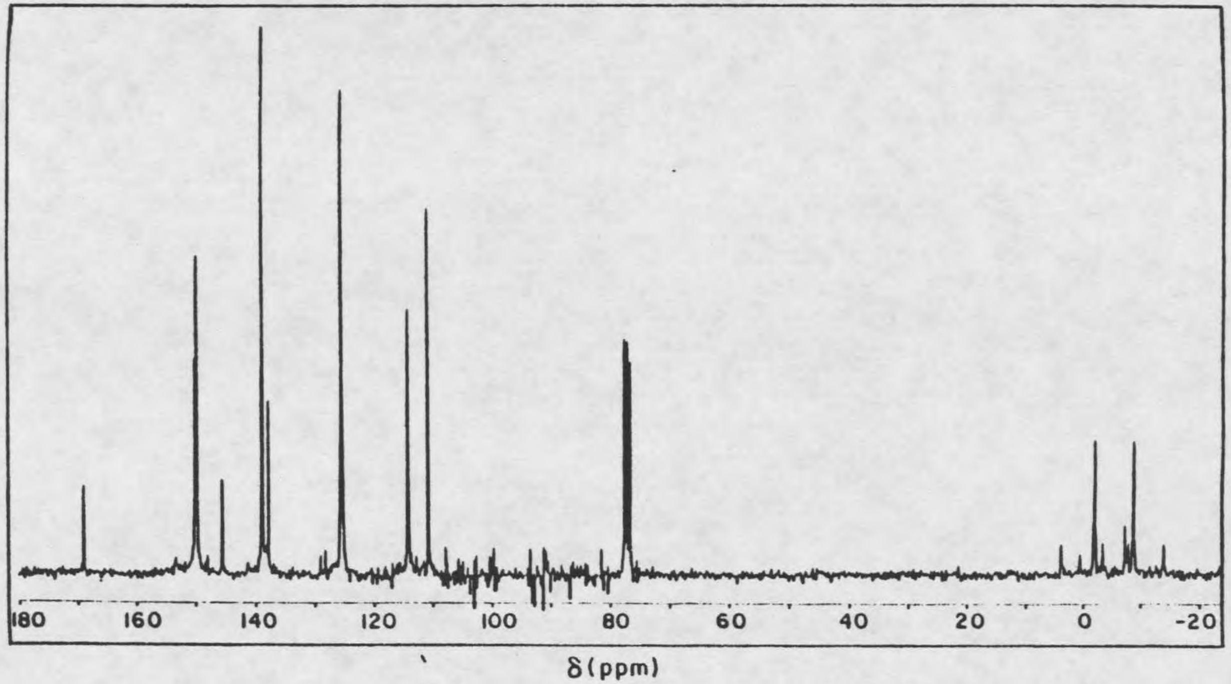


Figure 31. $^{13}C(^{1}H)$ NMR spectrum of $[Pt_2(CH_3)_4(chp)_2(pyr)]$.

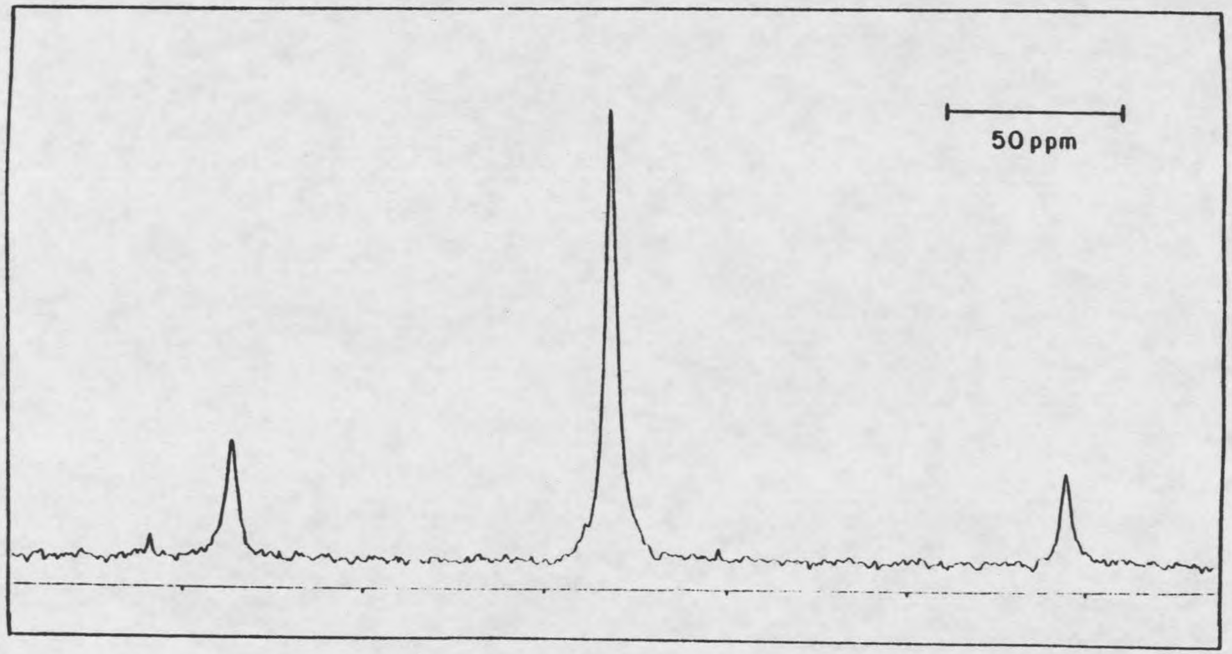


Figure 32. Upfield region of ^{195}Pt NMR spectrum of $[Pt_2(CH_3)_4(chp)_2(pyr)]$.

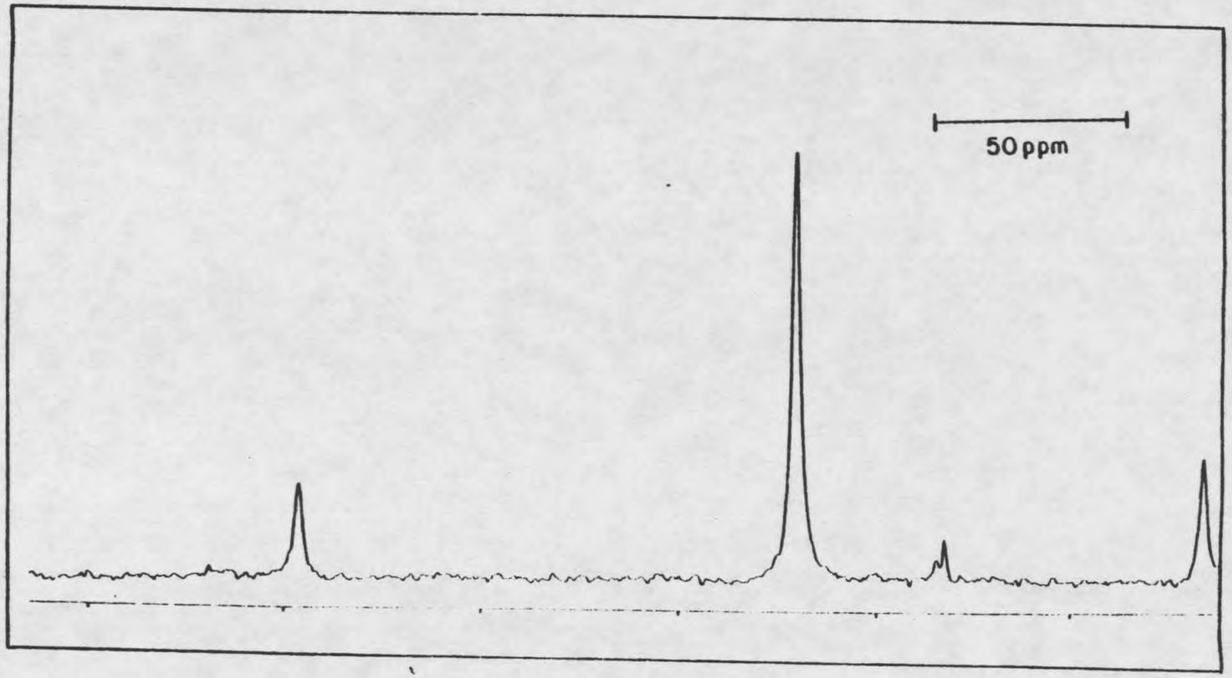


Figure 33. Downfield region of ^{195}Pt NMR spectrum of $[Pt_2(CH_3)_4(chp)_2(pyr)]$.

Table 37. $Pt_2(CH_3)_4(fhp)_2(Et_2S)_1$ (head-to-head dimer).

Resonance	(Mult.)	Assignment	Coupling Constants
Proton Assignments			
1.25	(t)	MeI	$^2J_{CH_3-Pt}$ 10.96Hz
1.36	(t)	MeII	$^2J_{CH_3-Pt}$ 15.35Hz
2.13		$S-CH_3$	
2.76		$S-CH_2$	
6.00(S)		5H	
6.34		3H	
7.27(q)		4H	
Carbon-13 Assignments			
-12.02	(t)	MeI	$^2J_{CH_3-Pt}$ 28.4Hz
-1.83	(t)	MeII	$^2J_{CH_3-Pt}$ 24.41Hz
11.37	(t)	$S-CH_3$	
28.45		$S-CH_2$	
92.44, 92.92	(d)	C_5	
111.23		C_3	
140.22		C_4	
159.40, 163.25	(d)	C_6	
167.13		C_2	
Platinum-195 Spectra			
-829		Pt_1	11230.7Hz
-640		Pt_2	

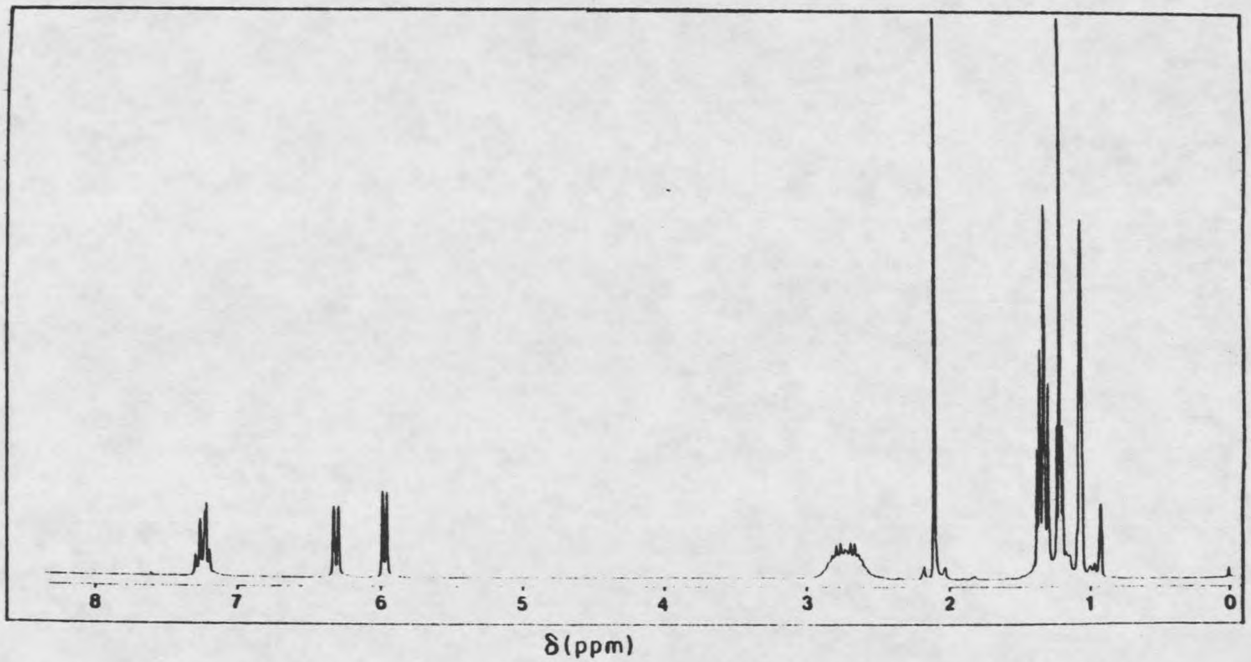


Figure 34. ^{1}H NMR spectrum of $[Pt_2(CH_3)_4(fhp)_2((C_2H_5)_2S)]$.

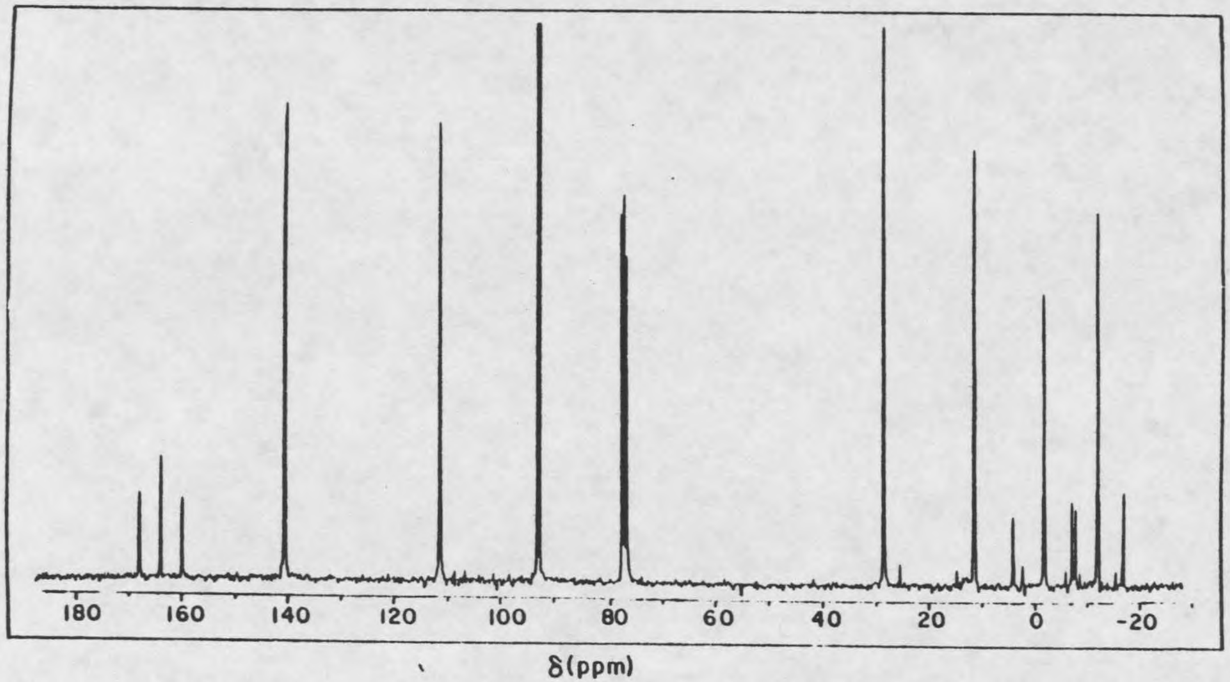


Figure 35. $^{13}C(^{1}H)$ NMR spectrum of $[Pt_2(CH_3)_4(fhp)_2((C_2H_5)_2S)]$.

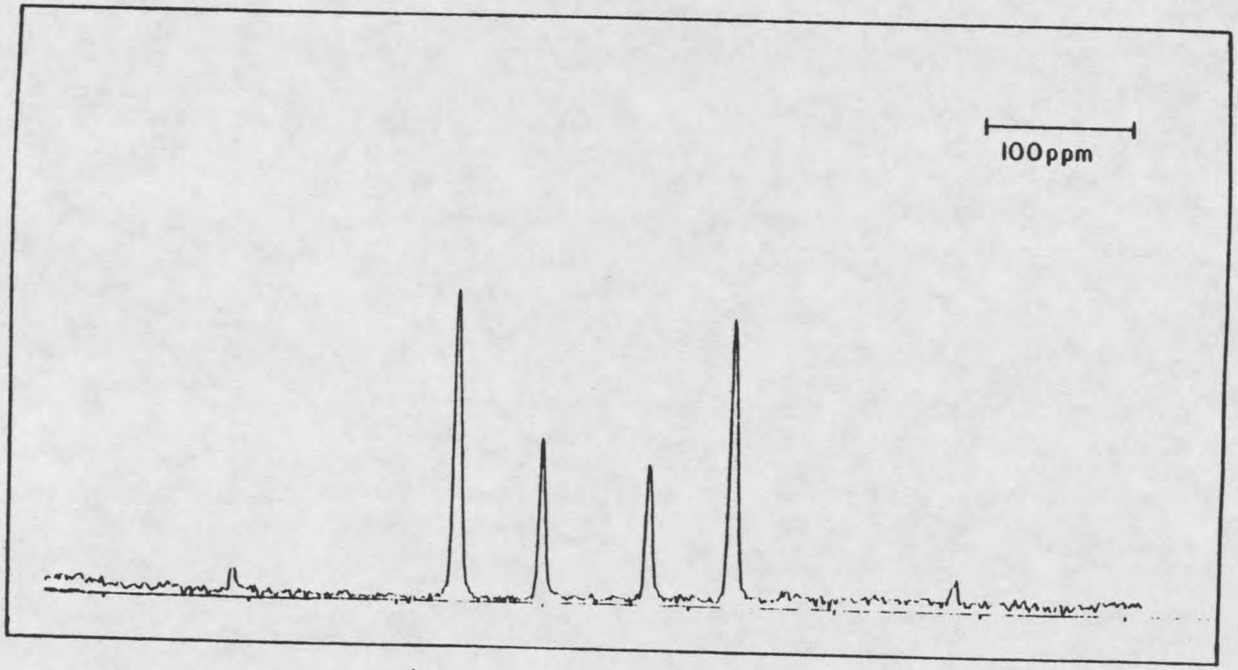


Figure 36. ^{195}Pt NMR spectrum of $[Pt_2(CH_3)_4(fhp)_2((C_2H_5)_2S)]$.

Table 38. $Pt_2(CH_3)_4(fhp)_2(pyr)_1$ (head-to-head dimer).

Resonance	(Mult.)	Assignment	Coupling Constants
Proton Assignments			
1.11	(t)	MeI	$^2JCH_3$-Pt 69.84Hz
1.77	(t)	MeII	$^2JCH_3$-Pt 79.34Hz
6.07	(t)	5H	
6.43	(d)	3H	
7.26	(t)	4H	
7.3		β-Pyridine	
7.8		γ-Pyridine	
8.46		α-Pyridine	
Carbon-13 Assignments			
-8.91	(t)	MeI	$^1JCH_3$-Pt 661.8Hz $^2JCH_3$-Pt 34.59Hz
-0.78	(t)	MeII	$^1JCH_3$-Pt 738.5Hz $^2JCH_3$-Pt 24.41Hz
+92.26		C_5	
93.07			
111.37		C_3	
125.41		β-Pyridine	
138.89		γ-Pyridine	
140.55		C_4	
149.96		α-Pyridine	
163.19		C_6	
167.17		C_2	
Platinum-195 Spectra			
-3123.0		Pt_1	11690.3Hz
-1740.1		Pt_2	11919.8Hz

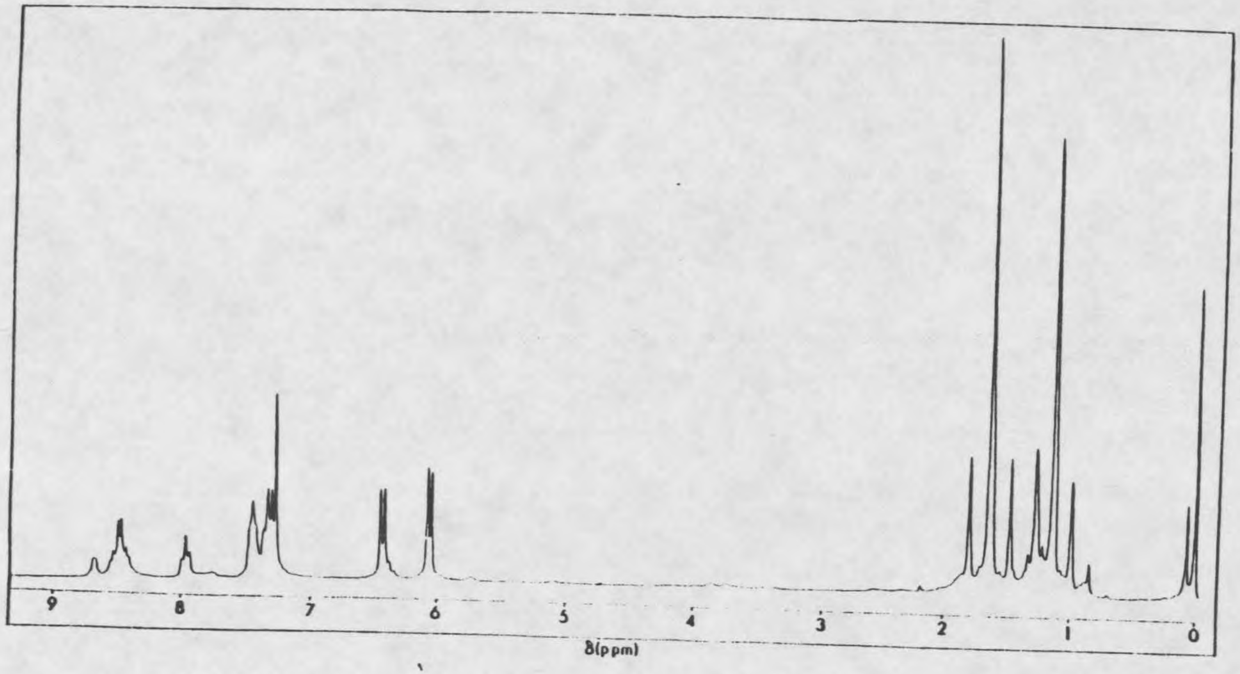


Figure 37. ^{1}H NMR spectrum of $[Pt_2(CH_3)_4(fhp)_2(pyr)]$.

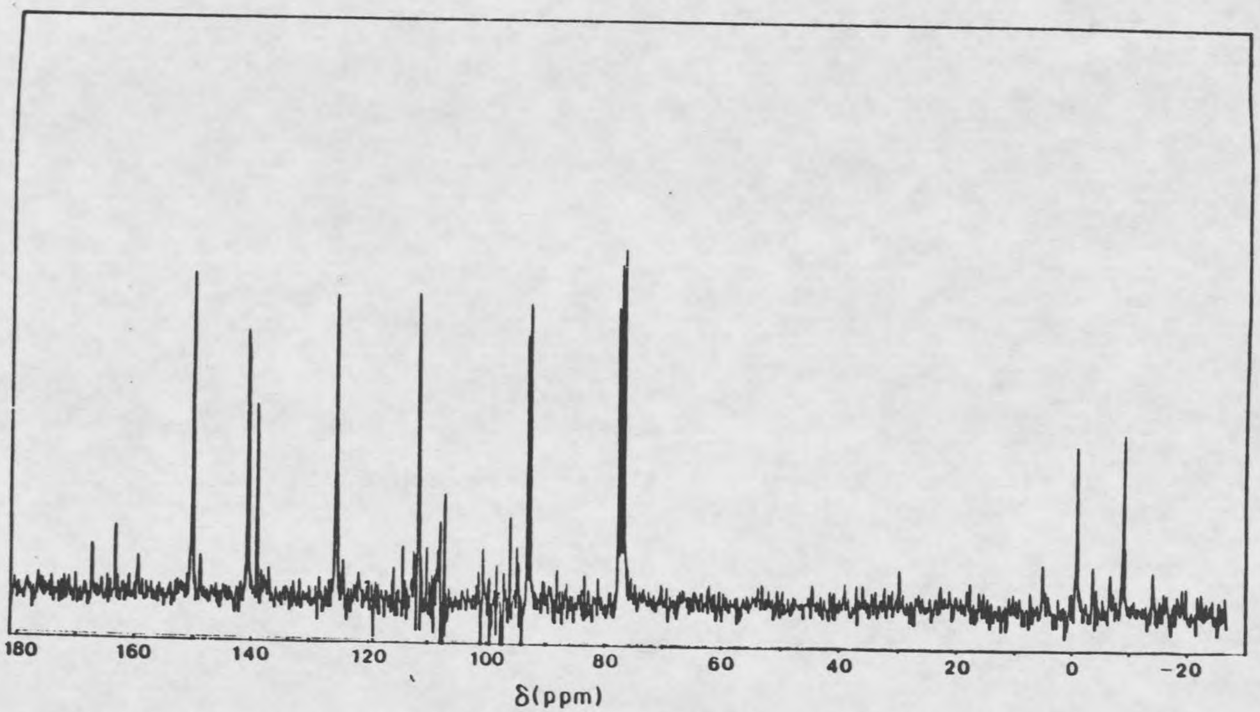


Figure 38. $^{13}C(^{1}H)$ NMR spectrum of $[Pt_2(CH_3)_4(fhp)_2(pyr)]$.

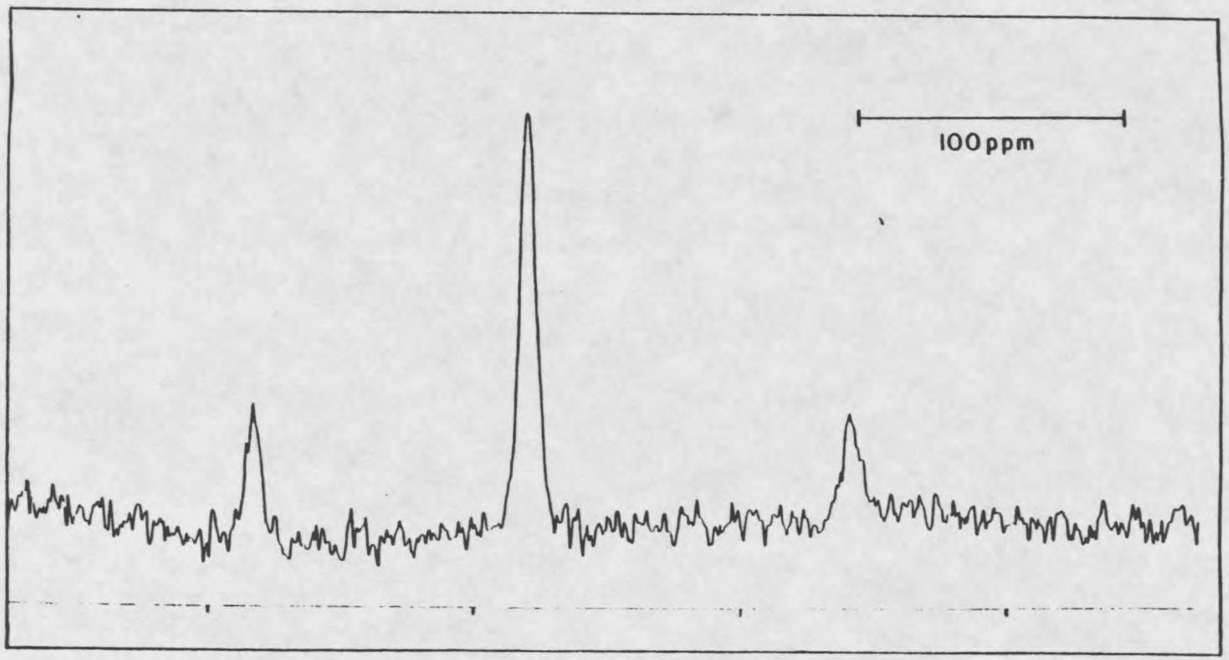


Figure 39. Upfield region of ^{195}Pt spectrum of $[Pt_2(CH_3)_4(fhp)_2(pyr)]$.

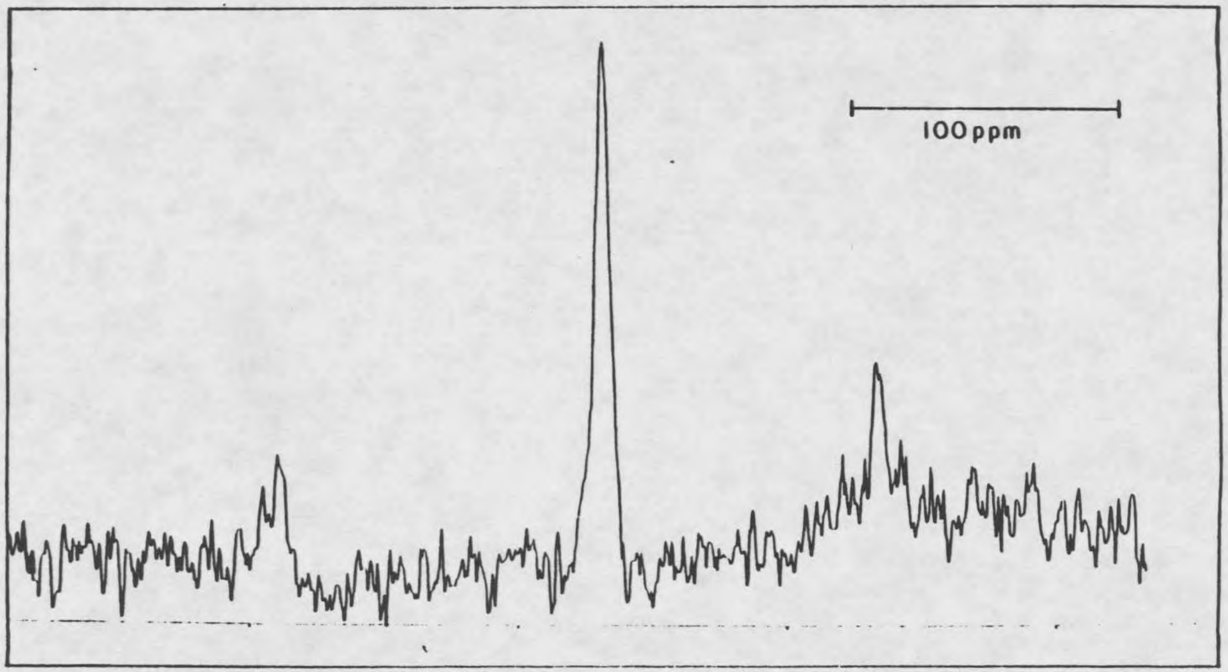


Figure 40. Downfield region of ^{195}Pt NMR spectrum of $[Pt_2(CH_3)_4(fhp)_2(pyr)]$.

Table 39. $Pt_2(CH_3)_4(hp)_2(pyr)_2$ (head-to-tail dimer) and $Pt_2(CH_3)_4(hp)_2(pyr)_1$ (head-to-head dimer).

Resonance	(Mult.)	Assignment	Coupling Constants
HEAD-TO-TAIL DIMER			
Proton Assignments			
0.64		MeI	$^2J_{CH_3-Pt}$ 69.97Hz
1.16		MeII	$^2J_{CH_3-Pt}$ 78.7Hz
			$^3J_{CH_3-Pt}$ 4.88Hz
5.72	(d)	5H	
7.22	(t)	4H	
7.40	(t)	β-Pyridine	
7.85	(Mult.)	γ-Pyridine	
8.70	(Mult.)	α-Pyridine	
Carbon-13 Assignments			
-9.88	(t)	MeI	J_{Pt-CH_3} 610.3Hz
			$^2J_{CH_3Pt}$ 29.59Hz
-4.15	(t)	MeII	$^1J_{PtCH_3}$ 739.8Hz
			$^2J_{CH_3Pt}$ 24.0Hz
110.28		C_5	
116.57		C_3	
124.12		β-Pyridine	
136.58		C_4	
138.14		γ-Pyridine	
144.31		C_6	
149.6	(d)	α-Pyridine	
169.17		C_2	
Platinum-195 Spectra			
-2894		Pt_1	10,823.6Hz

Table 39. (continued)

Resonance	(Mult.)	Assignment	Coupling Constants
HEAD-TO-HEAD DIMER			
Proton Assignments			
1.0		MeI	
1.56		MeII	
6.34		5H	
6.55		3H	
7.25		4H	
7.35		6H (OH pyr) (Ring Subs.)	
7.40		β-Pyridine	
7.80		γ-Pyridine	
8.50		α-Pyridine	
Carbon-13 Assignments			
-8.5	(t)	MeI	
-4.08	(t)	MeII	
110.33		C_5	
117.82		C_3	
127 128	(d)	β-Pyridine	
140		C_4	
138 141		γ-Pyridine	
147		C_6	
152 153		α-Pyridine	
172.53		C_2	
Platinum-195 Spectra			
-1894		Pt_1	$^1J_{Pt-Pt}$ 10823
-1792		Pt_2	

*Notes: #6 proton was not observed; the spectra shown are approximately 50:50 equilibrium mixtures of the head-to-head and head-to-tail complexes. The assignments for both complexes were made from this set of data.

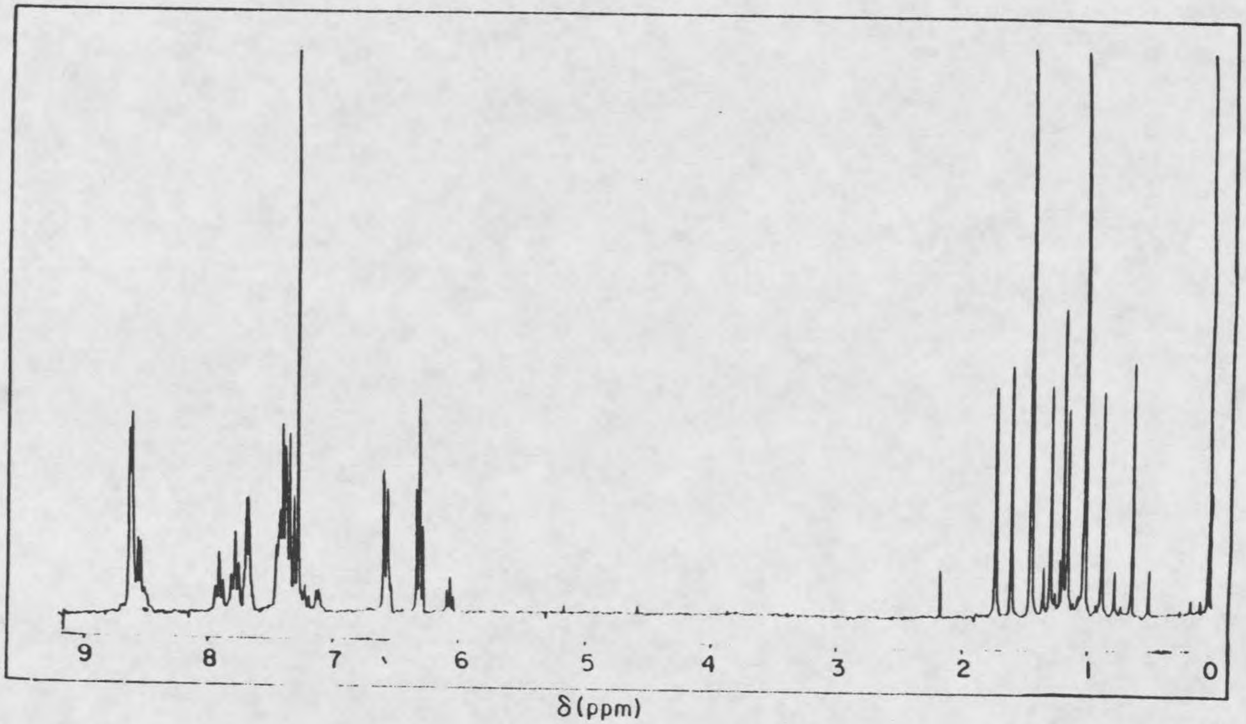


Figure 41. ^{1}H NMR spectrum of $[Pt_2(CH_3)_4(hp)_2(pyr)_2]$.

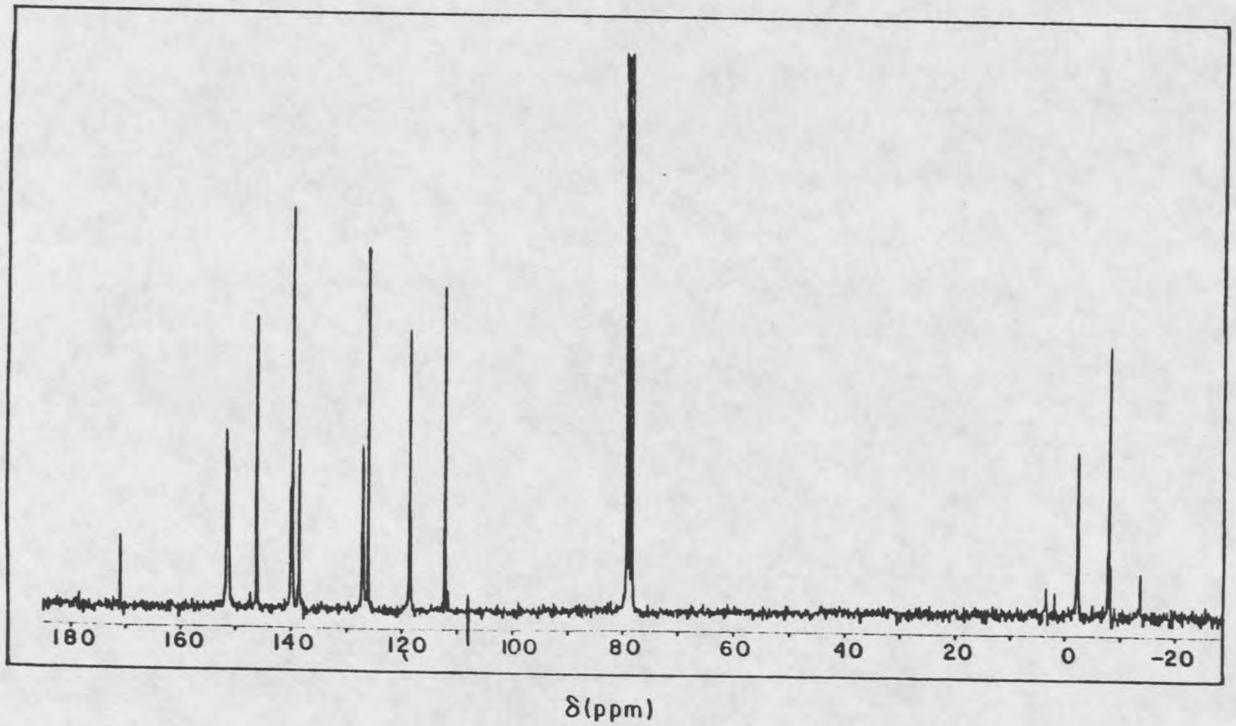


Figure 42. $^{13}C(^{1}H)$ NMR spectrum of $[Pt_2(CH_3)_4(hp)_2(pyr)_2]$.

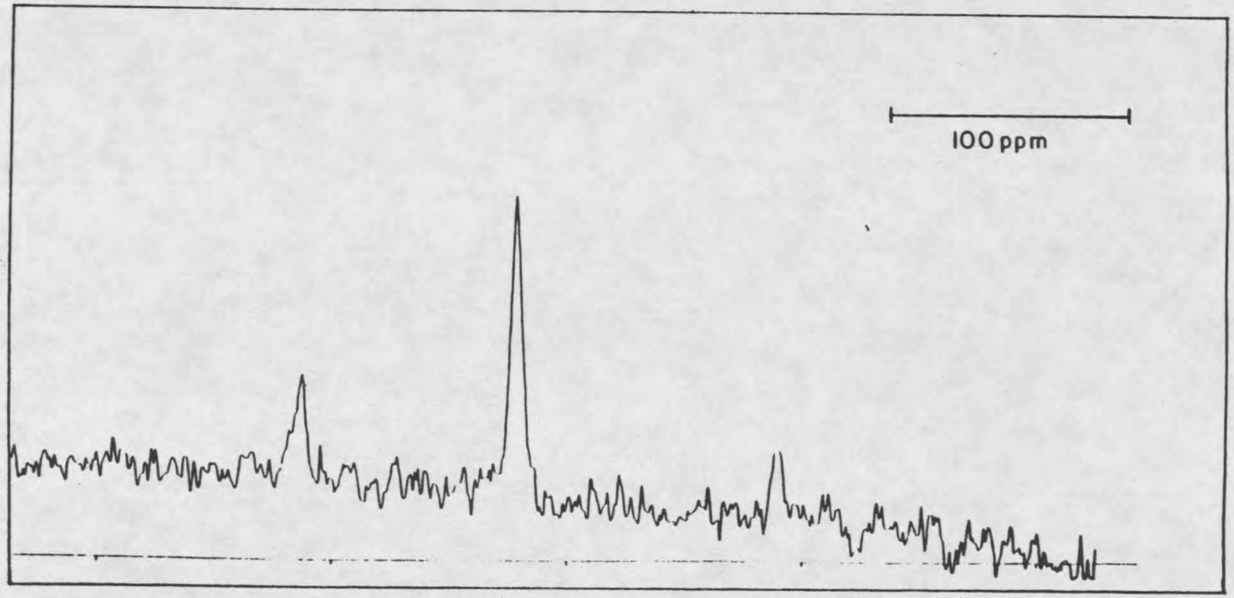


Figure 43. Upfield region of ^{195}Pt NMR spectrum of $[Pt_2(CH_3)_4(hp)_2(pyr)_2]$.

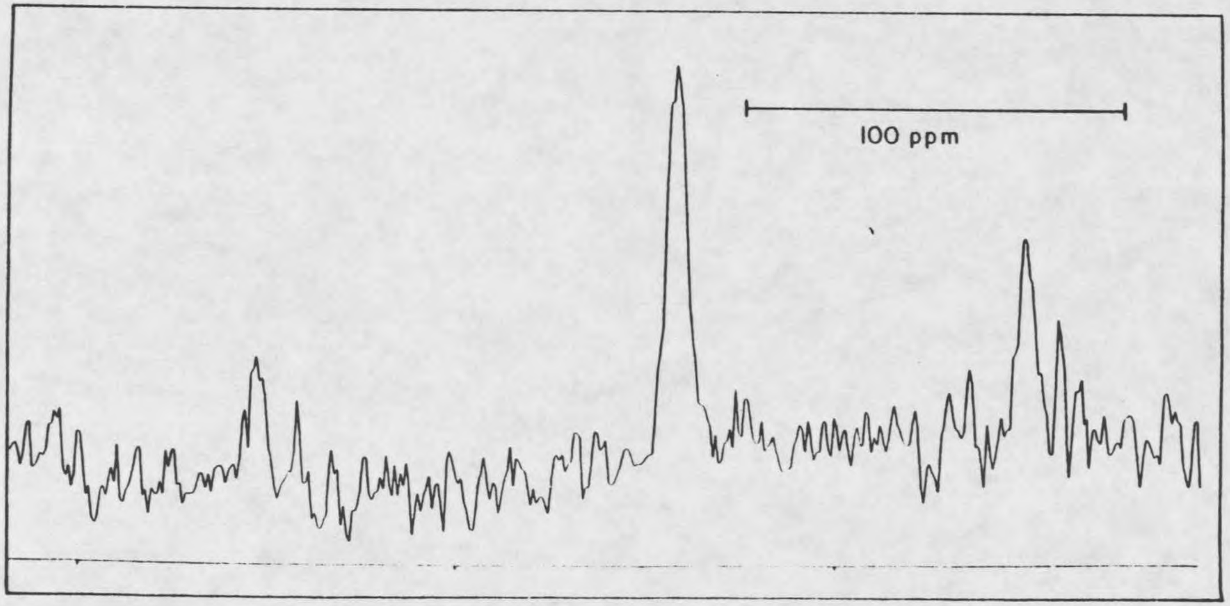


Figure 44. Downfield region of ^{195}Pt NMR spectrum of $[Pt_2(CH_3)_4(hp)_2(pyr)_2]$.

Infrared Spectral Results

The following tables present the observed infrared spectral frequencies, their relative intensities, and their assignments. Assignments have been made by comparison to other reported spectra for similar types of functional groups (63). The primary literature and a number of reference texts were also consulted.

Table 40. Infrared spectral results for $K[Pt(NO_2)_4(NO)(OH_2)]\cdot OH_2$, 1.

Band (cm^{-1})	Intensity	Assignment
1780	S (B)	ν OH_2
1654	S	ν NO (bent)
1423	S	νa NO_2
1320	S	νs NO_2
1260	S (B)	ν PO_4^{2-}
635	M	Pw NO_2

Table 41. Infrared spectral results for $K[Pt(NO_2)_2Cl_3(NO)]$, 2.

Band (cm^{-1})	Intensity	Assignment
1788	S	ν OH_2
1656	S	ν NO (bent)
1425	S	νa NO_2
1335	S	νs NO_2
1275	S (B)	ν PO_4^{2-}
635	M	Pw NO_2

Table 42. Infrared spectral results for $Pt_4(OAc)_6(CO)_2$, purple fraction, 6

Band (cm^{-1})	Intensity	Assignment
1910	M	ν CO Bridging
1684	S	νa Acetate Bridging
1604	S	νs Acetate Bridging
1419	S	νa Acetate Bridging
1300	S	νs Acetate Bridging
1051	S	Pr (CH_3) Acetate
1024	M	Pr (CH_3) Acetate
895	W	ν (C–C)
695	W	ν (O–C–O)
613	W	π CH_3 or π COO–

Table 43. Infrared spectral results for $Pt_4(OAc)_8$, blue fraction, **7**, **10**.

Band (cm^{-1})	Intensity	Assignment
1710	M	ν Acetic Acid
1565	VS	νa Bridging Acetate
1470	VS	νs Acetic Acid
1410	M	νs Bridging Acetate
1331	S	δ (CH_3)
1052	M	Pr Acetate (CH_3)
1022	M	Pr (CH_3) Acetate
667	M	ν (O–C–O)
618	M	π CH_3 or π COO–

Table 44. Infrared spectral results for $Pt_4(OAc)_8$, green fraction, 8.

Band (cm^{-1})	Intensity	Assignment
1717	M	ν Acetic Acid
1594	S	νa Acetate
1389	S	νs Acetate
1050	S	Pr (CH_3) Acetate
1029	M	Pr (CH_3) Acetate
620	W	π CH_3 or π COO–

Table 45. Infrared spectral results for reaction of Pt_4(OAc) blue and $NOBF_4$ or NO (gas) or HNO_3, two equivalents (purple solid), 12.

Band (cm^{-1})	Intensity	Assignment
1636	S	ν NO Bridging
1631	S	νa Acetate Bridging
1559	S	νs Acetate Bridging
1418	VS	νa Acetate Bridging
1385	VS	νs Bridging Terminal
1327	VS	NO Bridging Terminal (or NO_3 Bridging)
1270	S	
1100	M	ν BF_4 (in NBF_4 addition experiment)
1046	M	Pr (CH_3) Acetate
974	M	NO Bridging/Terminal
667	M	ν (O–CO) Acetate
617	W	π CH_3 or π COO–

Table 46. Infrared spectral results for reaction of $Pt_4(OAc)_8$ blue and KOCN, 10 and 20 equivalents, 14.

Band (cm^{-1})	Intensity	Assignment
2158	W	νa (NCO)
1724	M	NCO Bridging
1710	M	Acetic Acid
1658	M	νa Bridging Acetate
1609	VS	νs Bridging Acetate
1582	VS	νa Bridging Acetate
1400	VS	νs Bridging Acetate
1366	VS	νs (NCO)
1285S	S	KOCN (excess)
1166	S	
1050	S	Pr (CH_3) Acetate
1020	S	Pr (CH_3) Acetate
893	S	
696	M	
619	M	(NCO)
478	S	
455		

Table 47. Infrared spectral results for reaction of $Pt_4(OAc)_8$ blue and KSCN, 20 equivalents, 15.

Band (cm^{-1})	Intensity	Assignment
2126	Vs	ν SCN (Terminal)
2097	S	ν SCN (Terminal)
2053	Vs	ν KSCN (Excess)
1716	M	ν Acetic Acid
1562	Vs	ν C=O Potassium Acetate
1327	S	ν C-O Potassium Acetate
1100	S	ν C≡N Stretch
1019	M	Pr (CH_3) Potassium Acetate
748	W	KSCN (Excess)
470	W	KSCN (Excess)

Table 48. Infrared spectral results for reaction of $Pt_4(OAc)_8$ blue and eight equivalents KSCN H_2O insoluble fraction, 16.

Band (cm^{-1})	Intensity	Assignment
2168	S	ν (CN) Bridging Thiocyanate
2129	S	ν (CN)Bridging Thiocyanate
1619	W	νa (C=0) unidentate Acet.
1408	W	νs (C-0) unidentate Acet.
1039	W	Pr (CH_3)
1026	W	Pr (CH_3)
788	W	ν (CS) Thiocyanate
700	W	ν (CS) Thiocyanate
415	M	δ (SCN)

Table 49. Infrared spectral results for reaction of $Pt_4(OAc)_8$ blue and four equivalents KSCN H_2O soluble fraction, 17S.

Band (cm^{-1})	Intensity	Assignment
1576	S	νa Bridging Acetate
1409	S	νs Briding Acetate
1327	M	δ (CH_3)
1048	W	Pr (CH_3)
1017	W	Pr (CH_3)
651	W	π (CH_3) or π (COO)

Table 50. Infrared spectral results for reaction of $Pt_4(OAc)_8$ blue and four equivalents KSCN H_2O insoluble fraction, 17I, 18I.

Band (cm^{-1})	Intensity	Assignment
2169	S	ν (CN) Bridging Thiocyanate
2126	S	ν (CN) Bridging Thiocyanate
1297	S	νa Bridging Acetate
1569	S	νa Bridging Acetate
1412	S	νs Bridging Acetate
1369	S	νs Bridging Acetate
1319	S	δ (CH_3)
1041	W	Pr (CH_3) Acetate
1020	W	Pr (CH_3) Acetate
787	M	ν (CS) Thiocyanate
698	M	ν (CS) Thiocyanate
620	W	π (CH_3) or π (COO)
418	M	δ SCN

Table 51. Infrared spectral results for reaction of $Pt_4(OAc)_8$ blue and KSCN (two equivalents), 18S.

Band (cm^{-1})	Intensity	Assignment
2175	S	ν (CN) Bridging
1718	M	ν Acetic Acid
1632	S	νa Acetate Bridging
1576	S	νs Acetate Bridging
1410	S	νa Acetate Bridging
1374	S	νs Acetate Bridging
1323	M	ν (CH_3)
1100	S	ν ($C\equiv N$)
1050	M	Pr (CH_3) Acetate
1017	M	Pr (CH_3) Acetate
788	M	ν (CS) Thiocyanate
669	M	ν (O–C–O)
617	M	π CH_3 or π COO–

Table 52. Infrared spectral results for reaction of $Pt_4(OAc)_8$ blue and HC≡CH (gas), 19.

Band (cm^{-1})	Intensity	Assignment
2048	S	M–C≡CH
1707	M	ν acetic Acid
1686	M	νa Acetate Bridging
1580	VS	νs Acetate Bridging
1413	VS	νa Acetate Bridging
1341	W	νs Acetate Bridging
1182	M	
1138	M	
1050	M	Pr (CH_3) Acetate
1024	M	Pr (CH_3) Acetate
895	M	ν(C–C) Acetate
667	M	ν (O–C–O)
617	M	π CH_3 or π COO–

Table 53. Infrared spectral results for $Pt_4(OAc)_8$ blue and phenylacetylene, 20.

Band (cm^{-1})	Intensity	Assignment
2080	W	ν C≡C)
1574	S	νa Bridging Acetate
1419	S	νs Bridging Acetate
1333	S	
1106	M	ν Phenyl
1048	M	Pr (CH_3)
1027	M	Pr (CH_3)
760	W	ν Phenyl
699	W	ν (M–C)
659	W	ν (O–C–O), (M–C)
619	W	π (CH_3) or π (COO), (M–C)
467	W	ν (M–C)

Table 54. Infrared spectral results for reaction of $Pt_4(OAc)_8$ blue and PhC≡CPh, <u>21</u>.

Band (cm^{-1})	Intensity	Assignment
1709	M/W	ν Acetic Acid
1684	M	ν (C≡C)
1604	M	νa Bridging Acetate
1454	M	νs Bridging Acetate
1433	M	νa Bridging Acetate
1413	M	νa Bridging Acetate
1209	M	ν Phenyl
1180	S	ν Phenyl
1163	M	ν Phenyl
1048	M	Pr (CH_3)
1029	M	Pr (CH_3)
724	M	ν (O–C–O)
680	M	ν Pt–C and π (CH_3), π (COO)

Table 55. Infrared spectral results for reaction of $Pt_4(OAc)_8$ blue and (Ph_3P), 2 and 4 equivalents, <u>23</u>, <u>24</u>.

Band (cm^{-1})	Intensity	Assignment
1709	W	ν Acetic Acid
1653	M	νa Bridging Acetate
1570	S	νs Bridging Acetate
1542	S	νs Bridging Acetate
1436	S	νs Bridging Acetate & TPP
1329	S	δ (CH_3)
1100	M	ν TPP
1052	M	Pr (CH_3)
1022	S	Pr (CH_3)
741	M	ν TPP
695	M	δ (CH_3)
667	S	ν (O–C–O)
517	M	ν TPP
469	M	
435	S	ν TPP
420	S	ν TPP

Table 56. Infrared spectral results for reactions of $Pt_4(OAc)_8$ blue and HCN or KCN, two equivalents, 26.

Band (cm^{-1})	Intensity	Assignment
2201	W	ν M-C≡N Stretch
1714	M	ν Acetic Acid
1652	S	νa Acetate (Ionic)
1611	S	νa Acetate Bridging
1420	S	νs Acetate Bridging and Ionic Acetate
1372	S	νs (CN)
1100	M	ν (C≡N)
1048	M	Pr (CH_3)
1015	M	Pr (CH_3)
698	W	ν C≡N)
669	W	π (CH_3) or π (COO)
618	W	ν (C≡N)

Table 57. Infrared spectral results for $Pt_4(OAc)_8$ blue plus cyanamide, one and two equivalents, 27.

Band (cm^{-1})	Intensity	Assignment
2263	M	ν (C≡N)
2192	M	ν (C≡N)
2157	M	ν (C≡N)
1666	S	νa Briding Cyanamide
1627	S	νa Bridging Acetate
1560	S	νs Bridging Cyanamide
1447	S	νa Bridging Acetate
1290	W	
1164	W	Pr (NH_2) Cyanamide
1050	W	Pr (CH_3) Acetate
1024	W	Pr (CH_3) plus δ (NH_2)
784	W	
670	W	
576	W	

Table 58. Infrared spectral results for $Pt_4(OAc)_8$ blue with 8 equivalents acetamide, 28.

Band (cm^{-1})	Intensity	Assignment
1572	S	νs Acetamide
1414	S	νa Acetamide
1373	S	
1322	S	δ (CH_3)
1042	W	Pr (CH_3)
1020	W	Pr (CH_3)
718	W	ν N-H
696	W	δ (CH_3)
667	W	ν (O-C-N)
619	W	δ (CH_3) or π (C-O-N)

Table 59. Infrared spectral results for $Pt_4(OAc)_8$ blue with trifluoroacetic acid, 29.

Band (cm^{-1})	Intensity	Assignment
1709	M	ν Acetic Acid
1563	S	νa Bridging Acetate
1450	S	νa Bridging Acetate
1380	S	νs Briding Acetate
1337	M	νs Bridging Acetate
1198	M	ν CF_3
1152	M	ν CF_3
1049	W	Pr (CH_3)
1024	W	Pr (CH_3)
957	W	ν CF_3 (Free)
734	W	ν CF_3
720	W	ν (O-C-O)
690	W	δ (CH_3)
620	W	π (CH_3) or π (COO)

Table 60. Infrared spectral results for $Pt_4(OAc)_8$ blue with H_2SO_4, 30.

Band (cm^{-1})	Intensity	Assignment
1628	W	
1285	S	
1147	S	ν SO_4 Bridging
1040	W	ν SO_4 Bridging
1035	W	ν SO_4 Bridging
990	M	ν SO_4 Bridging
908	S	
673	M	
631	M	ν SO_4 Briding
617	W	ν SO_4^{2-}
587	M	ν SO_4 Bridging
502	W	

Table 61. Infrared spectral results for reaction of $Pt_4(OAc)_8$ blue and excess K_2SO_4, 31.

Band (cm^{-1})	Intensity	Assignment
1620	S	
1567	S	νa Bridging Acetate
1409	S	νs Bridging Acetate
1328	M	
1117	S	ν^s SO_4 Monodentate
1047	W	Pr CH_3 Acetate
1019	W	Pr CH_3 Acetate
730	W	
695	W	ν (O-C-O).
617	S	π CH_3 or π COO-

Electronic Spectral Results

Table 62 presents the results of the visible spectral investigations. The fact that each of the first group of blue complexes exhibits a bent nitrosyl ligand is supported by the correlation of the results which have already been presented. The results of the spectral work for the tetrameric systems which are presented also exhibit a good deal of correlation with each other; the results show three bands, each of which is suggestive that the symmetry about the metal atoms is the same. This suggestion lends support to the idea that the tetrameric structure of the complex is preserved for most of the complexes.

Table 62. Visible spectroscopic measurements.

Compound, Cmpd. No.	Absorbances (nm)			Solvent/Ref.
$KPt(NO_2)_4(NO)(OH_2)$, 1	615			$H_2O:H_3PO_4$/1:3
$K_2Pt(NO_2)_4 + NOBF_4$, 1	640			H_2O
$K_2Pt(NO_2)_4 + NOBF_4 + H^+$, 1	615			$H_2O:H_3PO_4$/1:3
"Wilkinson's Blue", 1	618			$H_2O:H_3Po_4$/1:3
$K_2Pt(NO_2)_4$ + NO(gas), 1	643			H_2O
$K_2Pt(NO_2)_4$ + NO(gas) + H^+, 1	616			$H_2O:H_3PO_4$/1:3
$K_2Pt(NO_2)_4 + H_3PO_4 + 3Cl^-$, 2	614			$H_2O:H_3PO_4$/1:3
$Pt_4(OAc)_8$ Blue, 7	700	592	431	HOAc
$Pt_4(OAc)_8$ Blue Pt(II), 10	700	605	431	HOAc
$Pt_4(OAc)_6(CO)_2\cdot 2HOAc$ (Purple Fract.), 6	700	595	431	HOAc
$Pt_4(OAc)_8$ Blue + Diphenylacetylene, 21	648	552	447	HOAc
$Pt_4(OAc)_8$ Blue + Phenylacetylene, 20	700	---	622	HOAC

Table 62. (continued)

Compound, Cmpd. No.	Absorbances (nm)			Solvent/Ref.
$Pt_4(OAc)_8$ Blue + $2HNO_3$, 12	582	525	428	HOAc
$Pt_4(OAc)_8$ + $4HNO_3$, 12	587	517	418	HOAc
$Pt_4(OAc)_8$ Blue + Triphenylphosphine, 22, 23, 24	677	——	385	HOAc
$Pt_4(OAc)_8$ Blue + 2KSCN H_2O Sol., 18S	675	585	380	HOAc
$Pt_4(OAc)_8$ Blue + 2KSCN H_2O Insol., 18I	705	613	395	HOAc
$Pt_4(OAc)_8$ Blue + 4KSCN H_2O Insol., 17I	695	590	395	HOAc
$Pt_4(OAc)_8$ Blue + 4KSCN H_2O Insol. + Heat, 17I	705	618	385	HOAc
$Pt_4(OAc)_8$ Blue + 4KSCN H_2O Sol., 17S	663	590	540	HOAc
$Pt_4(OAc)_8$ Blue + 4KSCN H_2O Sol. + Heat 30 Min., 17S	685	590	390	HOAc
$Pt_4(OAc)_8$ Blue + 4KSCN H_2O Sol. + Heat 60 Min., 17S	630	540	390	HOAc
$Pt_4(OAc)_8$ + 8 eq, Acetamide, 28	700	540	380	HOAc

Total Ligands Per Metal Cluster Determinations

Using ^{1}H nuclear magnetic resonance as was previously described in Methods and Materials (Chapter 3), we have been able to destroy the complexes and determine the number of ligands (acetates) present on each of the complexes described in the Table 63. Several complexes have an exceptionally large amount of acetate present per complex. We suggest that these complexes actually are composed mostly of potassium acetate which resulted from the addition of various potassium salts and the consequent substitution of ligands. These experiments add support to the elemental analytic and infrared spectral results.

Results of Elemental Analyses of Selected Compounds

The results of elemental analyses for selected compounds are presented in Table 64. Some of the results do not correlate well with our initial formulations of several of the complexes. However, as is observed in the Discussion, the results do shed some light upon the composition of the compounds.

Table 63. Determination of total ligands per cluster by ^{1}H NMR.

Compound, Cmpd. No.	Moles of Sample	Solvent	Moles MeOH	Moles HOD Initial
$Pt_4(OAc)_8$ Blue, 7	3.8×10^{-5}	$CDCl_3$	7.4×10^{-5}	1.74×10^{-5}
$Pt_4(OAc)_6(CO)_2 \cdot 2HOAc$, 6	3.8×10^{-6}	D_2O	1.24×10^{-4}	9.8×10^{-5}
$Pt_4(OAc)_6(NO)_2 \cdot 2HOAc$, 12	3.8×10^{-6}	D_2O	7.41×10^{-5}	9.7×10^{-5}
$Pt_4(OAc)_8$ Blue + 8 KSCN H_2O Insol., 16I	3.8×10^{-6}	DCl	7.41×10^{-5}	7.72×10^{-5}
$Pt_4(OAc)_8$ Blue + 8 KSCN H_2O Sol., 16S	3.8×10^{-6}	DCl	7.41×10^{-5}	7.72×10^{-5}
$Pt_4(OAc)_8$ Blue + 4 KSCN H_2O Insol., 17I	3.8×10^{-6}	DCl	7.41×10^{-5}	7.72×10^{-5}
$Pt_4(OAc)_8$ Blue + 2 KSCN H_2O Insol., 18I	3.8×10^{-6}	DCl	1.24×10^{-5}	9.26×10^{-5}
$Pt_4(OAc)_8$ Blue + 2 KSCN H_2O Sol., 18S	3.8×10^{-6}	DCl	1.24×10^{-5}	9.26×10^{-5}
$Pt_4(OAc)_8$ Blue + 8 Acetamide, 28	3.8×10^{-6}	DCl	1.24×10^{-5}	9.26×10^{-5}
$Pt_4(OAc)_8$ Blue + 8 Hydroxypyridine, 32	3.8×10^{-6}	DCl	1.24×10^{-5}	9.26×10^{-5}

Table 63. (continued)

Compound, Cmpd. No.	Moles HOD Final	Moles H^+	Moles $(OAc)^-$
$Pt_4(OAc)_8$ Blue, 7	9.07×10^{-6}	8.28×10^{-6}	3.98×10^{-5}
$Pt_4(OAc)_6(CO)_2 \cdot 2HOAc$, 6	8.3×10^{-6}	8.3×10^{-6}	3.34×10^{-5}
$Pt_4(OAc)_6(NO)_2 \cdot 2HOAc$, 12	8.07×10^{-6}	1.15×10^{-6}	3.57×10^{-5}
$Pt_4(OAc)_8$ Blue + 8 KSCN H_2O Insol., 16I	8.63×10^{-5}	9.1×10^{-6}	5.3×10^{-6}
$Pt_4(OAc)_8$ Blue + 8 KSCN H_2O Sol., 16S	8.32×10^{-5}	5.9×10^{-6}	4.69×10^{-5}
$Pt_4(OAc)_8$ Blue + 4 KSCN H_2O Insol., 17I	7.9×10^{-5}	1.8×10^{-6}	1.23×10^{-5}
$Pt_4(OAc)_8$ Blue + 2 KSCN H_2O Insol., 18I	8.53×10^{-5}	-7.3×10^{-6}	2.07×10^{-5}
$Pt_4(OAc)_8$ Blue + 2 KSCN H_2O Sol., 18S	8.53×10^{-5}	1.7×10^{-5}	5.93×10^{-5}
$Pt_4(OAc)_8$ Blue + 8 Acetamide, 28	9.45×10^{-5}	—	—
$Pt_4(OAc)_8$ Blue + 8 Hydroxypyridine, 32	9.43×10^{-5}	0	0

Table 63. (continued)

Compound, Cmpd. No.	Ratios (Moles H^+/Moles Cluster) Found	Calculated	Ratios (Moles OAc/Moles Cluster) Found	Calculated
$Pt_4(OAc)_8$ Blue, 7	2.1	2	10.2	10
$Pt_4(OAc)_6(CO)_2 \cdot 2HOAc$, 6	2.1	2	5.9	6
$Pt_4(OAc)_6(NO)_2 \cdot 2HOAc$, 12	3.4	2	7.1	6
$Pt_4(OAc)_8$ Blue + 8 KSCN H_2O Insol., 16I	2.4	0	1.4	1.4
$Pt_4(OAc)_8$ Blue + 8 KSCN H_2O Sol., 16S	1.6	2	12.3	10
$Pt_4(OAc)_8$ Blue + 4 KSCN H_2O Insol., 17I	0.5	0	3.3	4
$Pt_4(OAc)_8$ Blue + 2 KSCN H_2O Insol., 18I	-1.92	0	4.9	4
$Pt_4(OAc)_8$ Blue + 2 KSCN H_2O Sol., 18S	4.5	4	14.2	14
$Pt_4(OAc)_8$ Blue + 8 Acetamide, 28	2	0	8.3	8
$Pt_4(OAc)_8$ Blue + 8 Hydroxypyridine, 32	0	0	0	0

Table 64. Results of elemental analyses.

Compound, Cmpd. No.	% Pt Found	% Pt Calculated	% C Found	% C Calculated
$Pt_4(OAc)_8$ Blue, 7	64.0	62.3		15.34
$Pt_4(OAc)_6(CO)_2 \cdot 4HOAc$, 6	60.0	59.78	19.71	19.31
$Pt_4(OAc)_6(CO)_2 \cdot 2HOAc$, 6	60.0	59.78	18.60	16.56
$Pt_4(OAc)_6(NO)_2 \cdot 2HOAc$, 12	59.3	59.5	16.34	14.65
$Pt_4(OAc)_8$ Blue + 8 KSCN H_2O Insol., 16I	74	73	8.95	7.7
$Pt_4(OAc)_8$ Blue + 8 KSCN H_2O Sol., 16S	63	56.9	18.66	17.7
$Pt_4(OAc)_8$ Blue + 4 KSCN H_2O Insol., 17I	68.6	65.8	10.95	12.12
$Pt_4(OAc)_8$ Blue + 2 KSCN H_2O Sol., 18S	60.0	62.3	16.00	15.34
$Pt_4(OAc)_8$ Blue + 2 KSCN H_2O Insol., 18I	65.93	65.8	10.98	12.12
$Pt_4(OAc)_8$ Blue + 2 [PhC $C(C_6H_5)$], 20	58.3	58.4	24.19	25.1
$Pt_4(OAc)_8$ Blue + 8 Acetamide, 28	39.1	39.9	25.8	24.6
$Pt_4(OAc)_8$ Blue + 8 Hydroxypyridine, 32	40.0	38.9	33.77	33.53
$K_2PtCl_4 \cdot H_2O$, blank (Pt analysis only)	43.4	45.2	—	—

Table 64. (continued)

Compound, Cmpd. No.	% H Found	% H Calculated	% N Found	% N Calculated
$Pt_4(OAc)_8$ Blue, 7		1.92	—	—
$Pt_4(OAc)_6(CO)_2 \cdot 4HOAc$, 6	2.73	2.68	—	—
$Pt_4(OAc)_6(CO)_2 \cdot 2HOAc$, 6	2.97	1.60	—	—
$Pt_4(OAc)_6(NO)_2 \cdot 2HOAc$, 12	2.30	2.00	1.81	1.80
$Pt_4(OAc)_8$ Blue + 8 KSCN H_2O Insol., 16I	0.44	0	8.07	9.0
$Pt_4(OAc)_8$ Blue + 8 KSCN H_2O Sol., 16S	1.70	1.90	1.90	2.04
$Pt_4(OAc)_8$ Blue + 4 KSCN H_2O Insol., 17I	1.09	1.01	4.28	4.70
$Pt_4(OAc)_8$ Blue + 2 KSCN H_2O Sol., 18S	2.37	1.92	0.47	—
$Pt_4(OAc)_8$ Blue + 2 KSCN H_2O Insol., 18I	1.05	1.01	4.05	4.70
$Pt_4(OAc)_8$ Blue + 2 [PhC $C(C_6H_5)$], 20	2.42	2.20	0	0
$Pt_4(OAc)_8$ Blue + 8 Acetamide, 28	3.00	3.07	2.55	2.86
$Pt_4(OAc)_8$ Blue + 8 Hydroxypyridine, 32	2.79	2.81	4.91	5.51
$K_2PtCl_4 \cdot H_2O$, blank (Pt analysis only)	—	—	—	—

Table 64. (continued)

Compound, Cmpd. No.	Empirical Formula
$Pt_4(OAc)_8$ Blue, 7	$Pt(OAc)_2$
$Pt_4(OAc)_6(CO)_2 \cdot 4HOAc$, 6	$Pt_2(OAc)_3(CO) \cdot 2HOAc$
$Pt_4(OAc)_6(CO)_2 \cdot 2HOAc$, 6	$Pt_2(OAc)_3(CO) \cdot HOAc$
$Pt_4(OAc)_6(NO)_2 \cdot 2HOAc$, 12	$Pt_2(OAc)_3(NO) \cdot HOAc$
$Pt_4(OAc)_8$ Blue + 8 KSCN H_2O Insol., 16I	$Pt(SCN)_2 \cdot 0.7HOAc$
$Pt_4(OAc)_8$ Blue + 8 KSCN H_2O Sol., 16S	$Pt_2(OAc)_3(SCN) \cdot 2HOAc$
$Pt_4(OAc)_8$ Blue + 4 KSCN H_2O Insol., 17I	$Pt(OAc)(SCN)$
$Pt_4(OAc)_8$ Blue + 2 KSCN H_2O Sol., 18S	$Pt(OAc)_2 \cdot 0.13SCN$
$Pt_4(OAc)_8$ Blue + 2 KSCN H_2O Insol., 18I	$Pt_2(OAc)_2(SCN) \cdot HOAc$
$Pt_4(OAc)_8$ Blue + 2 [PhC $C(C_6H_5)$], 20	$Pt_2(OAc)_3(PhX\ CH)_1$
$Pt_4(OAc)_8$ Blue + 8 Acetamide, 28	$[Pt(OAc)_3(NOCCH_{31}] \cdot HOAc$
$Pt_4(OAc)_8$ Blue + 8 Hydroxypyridine, 32	$[Pt(C_5H_4ON)_2(O_2C_2H_3)_2]$
$K_2PtCl_4 \cdot H_2O$, blank (Pt analysis only)	$K_2PtCl_4 \cdot H_2O$

DISCUSSION

This discussion covers three general areas. First the bent nitrosyl compounds and the derivatives will be covered, then the NMR investigations involved with the dimeric platinum(III) species, and, finally, the systematic chemistry of the tetrameric acetate species and their derivatives.

Both structures of the bent nitrosyl complexes display features that are characteristic of complexes with strongly-bent nitrosyl groups. In the terminology of Enemark and Feltham, they fall into the class [MNO] and are best represented as complexes of NO. The N(3)-O(3) distance, 1.19(3), and Pt-N(3)-O(3) angle, 110(2)°, for 2 are within the ranges reported for other [MNO] complexes with bent nitrosyl ligands, as are the Pt-N(5)-O(5) angles for the three disordered O(5) positions in the structure of 1, the weighted average being 125°. The nitrosyl Pt-N distances for the two structures are slightly larger but not significantly longer than the nitrite Pt-N distances. Both structures illustrate the trans bond lengthening effect of the bent nitrosyl groups (64). In the structure of 1 the Pt-O distance for the water ligand is 2.37(1) Å, about 0.3 Å longer than expected. The Pt-Cl distance for Cl(3) in the structure of 2 is 2.562(5) Å, which is about 0.25 Å longer than the other Pt-Cl distances in the complex. We are aware of no other crystallographic structures of mononuclear platinum nitrosyl complexes.

Suppositions based on Raman spectra suggest that for the tetra nitrite-platinate(II) ion in solution, the nitrite groups are perpendicular to the coordination plane around the platinum (65). In 1, 2, and in the crystal structure of $K_2Pt(NO_2)_4 \cdot H_2O$ (65) the nitrite moieties are neither perpendicular nor coplanar with the platinum coordination planes; for the compounds in the solid state, back bonding must be minimal between the platinum and nitrite groups. Crystal-packing effects in the solids may outweigh any additional bonding that might be present in solution. The O(6)-O(7) distance of 2.76 Å in the structure of $K[Pt(NO_2)_4(NO)(H_2O)] \cdot H_2O$ indicates hydrogen bonding between the water ligand and the lattice water molecule.

Although both compounds are too reactive to obtain satisfactory elemental analyses by conventional methods, the structure determination of $K[Pt(NO_2)_2(NO)Cl_3]$ allows an unambiguous identification of 2 as a six-coordinate platinum(IV) complex. However, since hydrogen atoms could not be located in the structure of the blue compound, the formulation $K[Pt(NO_2)_4(NO)(H_2O)] \cdot H_2O$ cannot be established from x-ray data alone. Valences of +2, +3, or +4 could be assigned to the platinum, and each can be logically defended by assuming an appropriate number of protons on the water and nitrosyl ligands. Whether the nitrosyl group has been correctly identified, given the rotational disorder described earlier might also be questioned; the structure of 2 supports the identification of the nitrosyl ligand in 1, as does the observation of an intense infrared band at 1655 cm^{-1} for the solution containing 1. The band is assigned to the NO stretching and is in the appropriate region for the stretching of bent nitrosyl groups (66). A six-coordinate platinum(II) complex with small inorganic ligands seems unlikely, and solutions of the compound are diamagnetic. Therefore the assignment of the +4 oxidation state to the platinum in 1 is most reasonable. Since hydrogen atom positions could not be located, these considerations and the requirements of charge balance favor the formulation $K[Pt(NO_2)(NO)(H_2O)]\cdot H_2O$. An alternative formulation with a protonated nitrosyl group and either an OH^- ligand or an OH^- counter ion seem rather unlikely in 10 M phosphoric acid. The blue color is likely to be the consequence of a charge transfer band arrising from the transfer of the lone pair electrons on the nitrogen to the platinum ions (31,32).

Blue solutions that contain 1, or a very similar complex, can be prepared by other means. Some years ago Wilkinson et al. (67) dissolved $K_2Pt(NO_2)_4$ in aqueous nitric acid to form a blue solution with an absorption maximum at 607 nm, a figure in agreement with the maximum we found for the solution containing 1 in the reaction of $K_2Pt(NO_2)_4$ with phosphoric acid. Because the solutions were reacting continuously, extinction coefficients could not be measured accurately but were comparable. We have also reacted $K_2Pt(NO_2)_4$ with $NOBF_4$ in water (pH = 7) which rapidly forms a blue solution with a maximum at 625 nm. Addition of a small amount of concentrated H_3PO_4 immediately shifts the maximum to 607 nm. Again, the extinction coefficient is comparable to those of Wilkinson's nitric acid solutions (67) and the phosphoric acid solutions containing 1.

Finally, it is worth commenting that our interest in the structure of 1, aside from its unusual color, stems from the fact that it is present in systems that eventually lead to compounds which exhibit some of the shortest known platinum-platinum bonds. However, no evidence has yet been advanced that 1 is an intermediate in platinum-platinum bond formation, though if a single deep blue crystal of 1 is placed in concentrated phosphoric acid and heated, a red solution exhibiting the same visible absorption spectrum as the dimeric product is produced. Nonetheless, some simple stoichiometric considerations demand that there be at least one other platinum complex present in the reaction mixture containing 1.

Stoichiometric balance of this type has been studied by several groups (38,39). They have suggested that the rate determining step in the generation of the complexes is the protonation of the nitrite species. The proton could be considered to assist in the displacement of a nitrosyl ligand. Rapid protonation of the resulting hydroxy intermediate would then follow to give a platinum(II) species (33) (Figure 45). At this point we then would suggest that the nitrosyl ion oxidatively adds to one of the

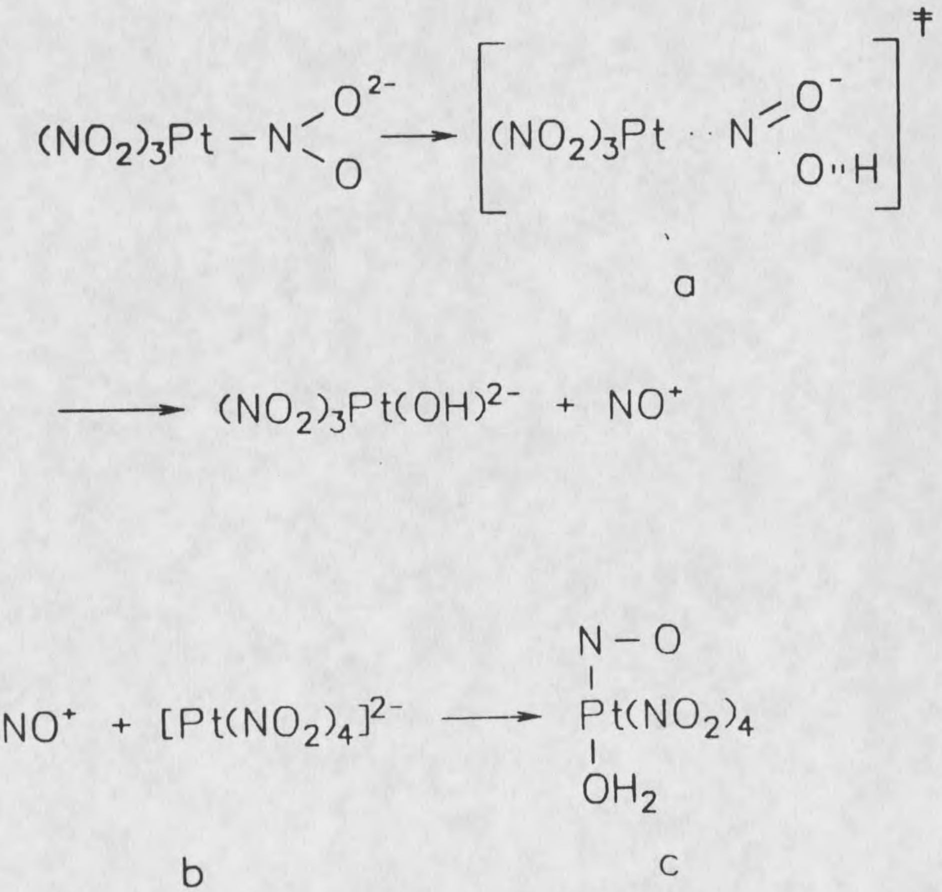


Figure 45. Hypothetical mechanism for the generation of a nitrosyl complex. a) The protonation of the nitrito-group; b) displacement of the NO group; c) our proposed oxidative addition of the NO ligand to the platinum(II) species (33).

platinum(II) species in solution, thence giving the resulting nitrosyl complex (Step c of Figure 45). ESCA data obtained from the dried blue powder reaction mixture shows the presence of two platinum species. The 4f(7/2) binding energies for the two species were found to be 72.9 eV and 75.2 eV, respectively. The signal intensities suggest an approximate 1:1 mixture of the two platinum species. The origin of the two sets of platinum 4f(7/2),(5/2) doublets has been assigned to the presence of two different platinum species, one in the platinum(II) oxidation state and the other in the platinum(IV) oxidation state.

Our observations correlate with each other and suggest a possible mechanism for the initial step in platinum-platinum bond formation. Such a mechanism would possibly require the presence of <u>both</u> platinum(IV) and platinum(II) oxidation states in solution prior to the formation of the metal-metal bond. With the first step which we have described, both such species do indeed exist in solution. Hypothetically the ligands (SO_4^{2-} or HPO_4^{2-}) would attach to the metal ions, and a mixed valence platinum(IV)-platinum(II) species would form. The sharing of a pair of electrons from the platinum ions would give an oxidation state of platinum(III), along with the short platinum-platinum bond. Our spectrophotometric studies have also shown that the "green" species (Figure 1) is mainly a mixture of the "blue" species and the "yellow" species.

The structure of <u>3</u> was determined because we felt that the crystals had potential for giving further information about later steps in platinum-platinum bond formation. It was also hoped that the bent nitrosyl group had been maintained, and even stabilized, with the additional electron density offered by the chloride ions. From the structure, one can observe that the NO ligand has been substituted by a chloride ion to give the more stable tetrachloro species. The structure is unique.

Once again, in an effort to stabilize the bent nitrosyl blue complex, an electron-rich species, Br^-, was added to the blue solution containing <u>1</u>. As the solution slowly became a dark red color, some reddish brown gas was given off. The gas could have been either Br_2 or some NO gas. The dark red crystals which resulted gave the <u>trans</u> dibromo-tetranitrito-platinum(IV) species, <u>4</u>. The Br^- apparently oxidatively added to the tetranitrito species, giving the resulting platinum(IV) complex. The <u>trans</u> dibromo structure was initially determined by a group of Russian workers (78). However, the structure determination which was published had a relatively high R value of 8.57%, and only the heavy atoms in the structure were located. In our structure, the bond distances and angles for the heavy atoms are comparable; however, the lighter atoms (N and O) have been located and refined as well, with the resulting R being somewhat lower (R = 6.10%). Therefore, the structure is presented here primarily because it is an improved structure over the initial determination. To our knowledge, this is the only improved structure of the complex with the lighter atoms located and refined.

The structure of compound 5 is somewhat more difficult to explain. The cis-dichloro-diphosphite platinum(II) offers an interesting view of some phosphorus chemistry. Additionally, the complex lends evidence for the presence of both platinum(II) and platinum(IV) being in solution at the same time. The source of the phosphite groups probably stems from the well-understood decomposition of pyrophosphoric acid in aqueous ortho phosphoric acid media at elevated temperatures (77). The phosphite groups then are able to bond with the platinum through ligand exchange reactions, giving the structure shown in Figure 14. To our knowledge, the structure which has been described is unique.

In the NMR studies of the α-oxopyridonate-bridged dimeric platinum(III) complexes, a number of interesting points for discussion are found. The chemical shift and coupling constant data for the complexes are found in Tables 32-38. Protons on the α-pyridonate ligands can be assigned by comparison of the unsubstituted complex with the complexes which are substituted in the six-position. The protons on carbons 3 and 4 are a doublet and a multiplet, respectively, while the carbon 5 resonance is a doublet for the OH ligand and a multiplet for substituted cases. (See Figure 16 for the molecular numbering scheme.)

All of the complexes exhibit two methyl resonances, each of which is split by two- and-three-bond coupling to each platinum-195 atom. The head-to-head complexes exhibit two electronically identical methyls on the platinum ions; the head-to-tail complexes exhibit a pair of different methyls on each of the platinum ions. Therefore a different methyl resonance results for each of the methyls on the singular platinum ion. Careful examination of Figure 46 suggests that the two methyls on the opposite platinum type (II) ion are also different, yet each matches one of the other methyls on the platinum type (I) ion. One pair of methyls is trans to a nitrogen, the other pair is trans to an oxygen; thus one sees two resonances for the methyls in the head-to-tail case. To clarify the point, in a hypothetical generation of a monosubstituted head-to-tail complex, all of the methyls would be in different electronic environments, and three methyl resonances would result.

Assignment of the methyls of the head-to-head complex was achieved using the Nuclear Overhauser Enhancement (N.O.E.) experiment (68). Decoupling of the downfield methyl group resonances gave energy transfer and an observed enhancement of the pyridine α-protons. In head-to-tail compounds, irradiations for each of the two methyl resonances gave identical enhancements of the pyridine α-protons. The carbon-13 spectra were initially assigned by comparing observations of six-fluoroinated pyridines found in the literature (69,70). Coupling constants and chemical shifts were found to be quite comparable. Proton-carbon correlation NMR spectroscopic observations confirmed the initial assignments which are presented (71).

The platinum-195 NMR spectra exhibit some extremely interesting information. The coupling constants between the platinum ions are

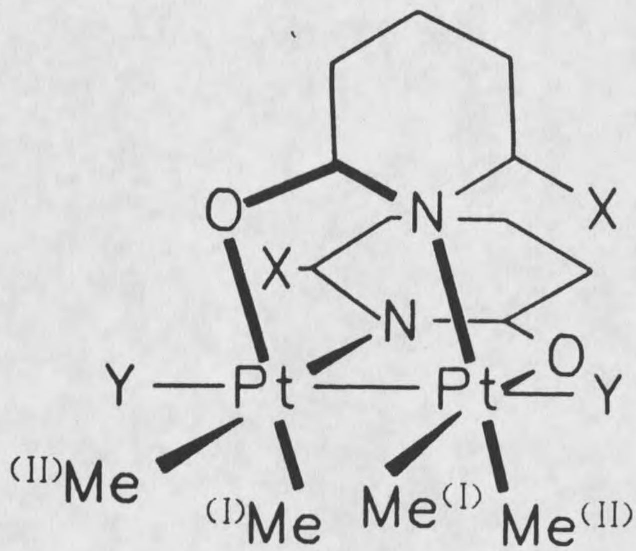


Figure 46. Head-to-tail dimeric platinum(III) arrangement showing the two types (I and II) of methyls on opposite platinum ions.

much larger than any previously observed in dimeric platinum species. Hitherto, the largest coupling constants observed were in the range of 3000-6000 Hz; in these cases we observed 10,000-12,000 Hz couplings.) The very large coupling constants result in AB-like spectra, despite the more than 100 ppm separation of the two platinum resonances. Due to the rather close proximity of the two platinum ions one observes the higher order type of spectrum. Each half of the AB splitting pattern has a major peak located at the weighted center of the pattern; such a peak results from a spin 1/2 platinum-195 being attached to a platinum-195 isotope with no spin. The "wings" found in the AB type of splitting pattern result from the splitting of a spin 1/2 platinum-195 by a second platinum-195 spin 1/2 nucleus in like manner as for the spin 1/2-no-spin case. Since the platinum-195 spin 1/2 nucleus is only 33.3% abundant, 33.3% of the intensity will be found in the AB "wings," while the remaining 66.7% of the intensity is found in the large central peak of the AB pattern.

This relatively interesting and somewhat involved group of NMR experiments has confirmed the solution-state structure of a series of platinum(III)-platinum(III) bonded species. Not only have we noted that the compound remains as a dimeric complex while in solution, but other studies in our laboratory indicated that the compound can be made to undergo some interesting reaction chemistry. Investigations of such chemistries continue in our laboratory.

The d^7-d^7 electronic configuration has been questioned by several workers in transition metal chemistry. For some time the suggestion has existed that the d^6-d^8 configuration would be a significantly better means of describing such complexes. Therefore each of the complexes would become a mixed valence species, and the d^7-d^7 configuration for platinum would not be appropriate. A number of experiments which would demonstrate such a mixed valence complex could be suggested. The primary requirements of this type of experiment would be that the experiment examine the valence level electrons of the platinum atom. One example of an experiment which meets this need is Electron Spectroscopy for Chemical Analysis (ESCA) or X-ray Photoelectron Spectroscopy (XPS).

Because the energies of the photoelectrons which are ejected by the x-ray beam in the ESCA experiment are directly proportional to the strength of binding of the electrons within the atomic orbitals, the ESCA experiment should give a very good gauge of the oxidation state of the metal ion. Generally it is observed that there is approximately a 1.1 eV chemical shift in the 4f(7/2) platinum signal per unit change in oxidation state. Therefore one would expect the following:

a) d^6-d^8 case two sets of well-separated (3.2 eV) 4f(7/2),(5/2) electron peaks, one pair at the appropriate chemical shift for platinum(IV), and one pair for platinum(II).

b) d^7-d^7 case a single set of 4f(7/2),(5/2) peaks found at an intermediate chemical shift to the platinum(II) and platinum(IV) peaks.

As one observes from the results already presented (Table 31), the platinum 4f(7/2),(5/2) chemical shifts reside at values intermediate to the chemical shifts for platinum(II) and platinum(IV). Such a result suggests a single oxidation state for the complexes which we observed. Thus the d^7-d^7 configuration of platinum(III) appears to be supported as a singular oxidation state.

The tetrameric species which were at one time characterized as being relatively unreactive have certainly been found to have some very exciting and unique chemistries. There are a number of aspects concerning the complexes' chemistry which bear discussion. The areas the following section cover are synthetic procedures, structure, reactivity, NMR efforts, ESCA studies, infrared studies, and elemental analyses.

Synthetic Procedures

The compound $[PtCl_4]\cdot H_2O$ has proven a useful starting material for the synthesis of a group of tetraplatinum complexes of the general type shown in Figure 4. The work by Davidson and Triggs suggested that the bridging ligand could be almost any carboxalate ion. From this work an isolation and purificxation scheme which gives very pure $Pt_4(OAc)_8$ Blue has resulted. This work has also generalized this chemistry further by demonstrating that the ligands may be of the 2-hydroxypyridine (α-oxopyridinato) or amide types as well.

The synthesis of the octakis-carboxylato species 7 proceeds quite smoothly so long as the reaction conditions are regulated carefully. The separation scheme which was worked out in this investigation gives a much purified blue compound. The other fractions (yellow 9, green 8, and purple 6) have also been characterized during the course of this work. The yellow 9 proved to be left-over starting material, as was demonstrated chemically; the green 8 appears to be a tetranuclear species which is probably composed simply of blue fraction which has lost excess acetic acid, Figure 6. Finally, the purple fraction 6 is composed of the dicarbonyl complex exhibiting both symmetric and asymmetric bridging ligands, which will be discussed later. Each of the four fractions has been analyzed by chemical and analytical methods, as is evident in the Results section. Generally we find in each case that slight variations in reaction conditions (e.g., reduction time, reduction temperature, formic acid concentration, and silver concentrations) give varying yields of complex. Remarkably, the complexes formed in this reaction are some of the most insoluble species encountered by this author to date, despite the presence of organic ligands in the compounds. We found that if a trace of acid ion was present, the compounds were highly, soluble in nearly any solvent; however, in the absence of acid ions, the complexes were nearly completely insoluble. Such insolubility simply could be regarded as the need for solvate formation or the need to form hydride complexes in solution. There was no evidence found for the formation of metal hydrides in this investigation; therefore, the thought that solvate formation is the principle force dictating the solubility of the compounds is most probable. Hence, the reactions of the tetrameric Blue compound 7 with varying ligands were carried out in glacial acetic acid. Efforts to perform reactions in other solvents without acid ions generally proved futile in that platinum metal generally resulted. Due to the complexes' extreme insolubility, single crystal growth proved to be quite a challenge and has resulted in only one major structure which will be discussed shortly.

Generally the reactions of the $Pt_4(OAc)_8$ Blue complex were performed with stoichiometric amounts of ligand being added. In most cases (SCN^- excepted), the resulting complexes seemed to give the substitutions around the tetrameric square. This synthetic strategy has some serious drawbacks. Most significantly, the fact that work is carried out under acidic conditions makes most basic ligands unavailable for the synthesis. The ligands used in this investigation were chosen for their ability to stand up under acid conditions (KCN excepted) as described above. Despite their drawbacks, the synthetic approaches taken here have shed some light upon an entirely new type of chemistry for the tetrameric system of platinum.

Reactivity Studies

Systematic reactivity studies of $Pt_4(OAc)_8$ Blue with a variety of different reagents shows that the complex can be induced to undergo reactions that give an equal variety of results. As with nearly all platinum complexes, the most facile reactions appear to be ligand substitutions. The systematic approach used here has allowed us to carefully examine the compounds and their reactivity, and possibly to suggest the structural changes which each complex is undergoing. The nuclearity of the complexes was gained from elemental analysis as well as from the visible spectral data. Generally, structural data were suggested by infrared spectroscopy, and much of the suggested information rests heavily upon the infrared spectra. Electrochemical studies, Raman spectral studies, and further ESCA studies would be very useful in determining the electrochemistry of the complexes and would give more understanding of the solution state structure, as well as helping to examine more clearly the oxidation state of the metal centers. Additionally, gaining an understanding of the necessity for having the complex in acidic media would be most useful.

Structural Studies

The structural studies for each of the complexes have consisted of trying to grow single crystals of sufficient quality for x-ray diffraction studies. Infrared spectroscopy and visible spectroscopy have also proven extremely powerful tools in understanding the solid state structures of the complexes. Many of the proposed structures, however, remain to be proven by x-ray diffraction. Two structures are of significant interest in this investigation. The first one is the octakis-acetate (or $Pt_4(OAc)_8$ Blue) complex since it is essentially a starting point for most of the reactivity studies. The structure was determined by Skapski et al. (49) and was found to consist of four platinum ions which lie in a perfect, nearly planar square. Each of the platinum ions is separated by 2.5 Å from its nearest neighboring platinum ion. Each edge of the square is bridged by two acetate ions, thus resulting in the "$Pt_4(OAc)_8$" (Figure 4) composition which has been used so freely in this dissertation. Some of the other interesting features of the complex lie in discussing the bonding in the cluster.

When considering the $Pt_4(OAc)_8$ cluster, the oxidation state of the four platinum ions can be logically defended as +2 or +3. In either case, the net result of a pseudo-octahedral platinum ion is somewhat interesting. Since the metal ions are very close to each other and the color of the complex is a deep blue, metal-metal bonding ("interaction" at the very least) is assumed. A discussion of the bonding in the metal cluster is difficult at the very least. If the metal ions are considered to exist in the +2 oxidation state (d^8 configuration) as is suggested in the literature, then how are metal-metal bonds obtained? One answer to this question has been suggested by Professor Cotton (72) who notes that the platinum-platinum bonds could be explained if one unpairs one electron pair on each of the metal atoms. Then each metal atom would donate one of the electrons to each of its two metal bonds. The net result of such an unpairing-repairing of the electrons would still give a d^8 ion, yet allow for platinum-platinum bonding. Such an explanation would work quite well and possibly even explain some of the solubility difficulties. An alternative explanation for the question would be to consider each of the platinum ions as a +3 ion (d^7 configuration). In the d^7 configuration each metal ion would have a single electron to share with the other metal ions. Thus there would be a total of four "skeletal" electrons per metal cluster. At this point there is a significant problem with charge balance; the cluster would have a net change of +4. However the charge balance problem could relatively easily be resolved by allowing four hydride ions each to contribute an electron to each of the platinum-platinum bonds, thus giving charge neutrality to the cluster and fulfilling the need for counter ions which are not observed in the crystal structure. Such an approach could hypothetically then have "d^7" ions and a cluster with four Pt(III) ions in it. Some parts of the data collected in the course of this investigation lend support to each of the above possible explanations for platinum-platinum bonding.

There certainly is no simple explanation of the bonding in the $Pt_4(OAc)_8$ cluster. The next structure only makes matters more difficult to understand. Compound <u>6</u> exhibits bridging carbonyl ligands, a pair of asymmetric acetate ions, and two pairs of symmetric acetate ions. The side of the rectangle with the asymmetric ligands lacks a metal-metal bond where the CO has inserted into the metal-metal bond, while the short sides of the rectangle have retained their metal-metal bonds. Note that the structure of the complex has gone from a nearly perfectly square, planar system to a distorted, rectangular complex as is shown in Figure 16. The platinum-platinum bonds have reached what is considered a maximum length for what may be called a bond. The electronic configuration has become somewhat more difficult to describe; oxidation states of +1.5, +2, or +3 each can be suggested.

The simplest description of the bonding would be to consider the platinum ions as +1.5 and allow the CO groups to contribute an electron to each of the metal atoms, thus resulting in a charge neutral species; however, the loss of a net 0.5 electrons per platinum ion (a total of 2.0 electrons per cluster) is distressing when considering this explanation. The alternative arguments for oxidation states of +2 and +3 each require invoking hydride ions and seem relatively unlikely in light of our proton NMR spectral data, which will be discussed shortly. However, the possibility of hydride ions being involved in these complexes or in any of their structural analogues, which will also be discussed shortly, should not be completely dismissed.

Two additional comments are warranted here; a structural analogue to the dicarbonyl complex has been reported in the literature, and a question exists concerning the source of CO in the complex. Let us first examine the structural analogue question. The complex reported in the literature was made using the original synthesis of the complex which was described in the Introduction (Chapter 1). Since excesses of nitric and formic acids were both present in the hot solutions during the reduction process, the presence of a considerable amount of CO and NO in solution would not be unusual. Thus either one could well have inserted into the metal-metal bond and given the suggested isostructural dinitrosyl complex

(44). Yet another possible explanation is that the complex was mischaracterized and actually was the dicarbonyl with a pair of nitric acids in the crystalline lattice, instead of the suggested acetic acids, thus giving what the authors claimed as "an appropriate" elemental analysis. Our structure of the dicarbonyl certainly had no source of nitrogen, and shows no nitrogen by elemental analysis. Therefore, we have concluded that the characterization of the complex as a dicarbonylhexaacetatotetraplatinate is correct. The second issue mentioned earlier, that of the CO source, is one which is a bit subtle and is answered by the well-known dehydration of formic acid in acidic media (73). The dehydration reaction has been shown to take place in the presence of acetic acid and result in the in situ generation of CO gas. A number of structural analogues to the dicarbonyl have been synthesized and will be presented in the following portions of this discussion.

NMR Studies

The NMR studies of the tetrameric platinum systems have been directed in two ways: a) application of nuclear magnetic resonance techniques in the "normal" fashion for determining solution state structural details by ^{1}H, ^{13}C, ^{195}Pt spectral investigations; and b) application of ^{1}H nuclear magnetic resonance to determine the total number of ligands per cluster. Some aspects of these studies have been quite enlightening, while others have proven quite mystifying. Each of the above points will be discussed.

The best insight into the composition of these complexes comes from relatively unusual application of ^{1}H NMR spectroscopy for the determination of the total number of ligands present on each cluster. The experimental details have already been described in the Materials and Methods portion of Chapter 3. The spectra did not appear exciting, since there were only three peaks to be examined--the HOD peak, the methyl alcohol internal standard peak, and the methyl peak from the acetate ions on the complexes. Nonetheless, the information contained in the spectra certainly has proven valuable in this investigation. For the cases of compounds **6**, **7**, **12**, **16I**, **16S**, **17I**, **18I**, **18S**, **28** and **32**, this application of ^{1}H NMR spectroscopy proved critical in suggesting the actual composition of the complex. Combining the information from elemental analysis and this technique, a great deal can be learned about the complexes, including the number of crystalline lattice acetic acid molecules present in each of the clusters.

In the case of the isostructural dicarbonyl and dinitrosyl complexes, the total number of ligands and lattice acetic acids were determined and found to correlate with elemental analysis; for each of the other proposed structures similar determinations have been made and are shown in Table 63.

The first part of the NMR studies, using ^{1}H, ^{13}C, and ^{195}Pt NMR techniques to explore the structural details of the tetrameric species, proved to be somewhat disappointing. The complex appears to be almost perfectly suited to nuclear magnetic resonance studies.

There are four platinum ions, there are carbon atoms within one or two bond distances of the platinum atoms, and the protons in the system certainly could give some interesting structural details, especially if there should be some sort of hydrogen bonding, hydrides or other structural interaction within the system. The symmetry of the cluster also lends itself to NMR studies since the symmetry should simplify exactly what one observes in the spectrum.

The expected observation in the ^{1}H spectrum would be three electronically distinct types of methyls--those signals arising from the equatorial acetate ions, signals arising from axial methyl ions, and free acetic acid methyls. In the ^{13}C spectrum signals arise from the methyl carbons of the axial and equatorial acetate ions, and the carboxylate carbons plus platinum carbon couplings should be evident. Finally, the ^{195}Pt spectrum should exhibit one large platinum resonance arising from the four electronically equivalent platinum atoms. However, due to the 33% natural abundance of the spin 1/2 nucleus of platinum and the close proximity of the platinum atoms, a complex splitting pattern would be observed instead. Such a group of possibilities for the $Pt_4(OAc)_8$ Blue complex alone is enticing in the number of possibilities for gaining insight into the solution-state structural details of the complex; the implications for complexes in which the symmetry has been broken upon addition of ligands is staggering. However, in all eleven cases--6, 7, 12, 19, 21, 23, 24, 27, 28, 29, 32--for which NMR investigations have been attempted, no platinum resonnances, nor any resonances for atoms directly bonded to the platinum atoms were observed. The one exception to the above statement was the octakistrifluoroacetato-tetraplatinum(II) complex (29), for which a single very poorly-resolved ^{13}C spectrum was observed for the carboxylate carbon. Some platinum couplings were possibly observed; however, no definite conclusion could be drawn from the spectrum due to the extremely poor signal to noise ratio. Additionally, the low solubility and/or acid proton requirement of the complexes made such investigations difficult. The proton spectra of all of the complexes were broad and poorly resolved. Finally, no ^{195}Pt spectral resonances could be located over a 1.5 MHz scanning range.

There exist a number of possible explanations for such a unique group of difficulties to exist in a system that seems perfect for NMR studies. A few of the possibilities will be suggested here, with the recognition that there are probably a number of additional explanations for not observing the spectra. The simplest explanation would be that the complexes are fluxional (74) in solution. The result of fluxionality in molecules like the tetrameric species described here would entail loss of structural information in the form of NMR spectral broadening. However, the fact that the NMR spectra exhibit no temperature dependence eliminates this explanation. Another possible explanation would involve second order Zeeman effect paramagnetism in the complex arising from low lying excited states stemming from the rather unusual bonding found in the complexes. Yet another possible explanation lies in the relaxation properties of platinum.

Chemical shift anisotropy (C.S.A.) is the mechanism by which platinum relaxes (75). If the mechanism were the only reason for our unusually broad spectra, then one should not be able to observe any platinum NMR spectra. Generally, species for which C.S.A. is the primary mechanism for relaxation show a temperature dependence. Since we observe no temperature dependence, this is probably not a reasonable explanation for our difficulties in observing NMR spectra. A final possible explanation for the lack of NMR signals stems from possible aligomer formation in solution, and therefore exceptionally large molecules. If the molecule is too large, the nuclear spin relaxation times will be shortened so much that the NMR signals are virtually undetectable (75). The fact that our solution concentrations are so terribly great in order to observe any NMR signals certainly makes such an explanation plausible. At this point, this author feels that the effect which has been observed is most probably due to the low lying excited state/secondary Zeeman effect explanation.

ESCA Studies

The results of the Electron Spectroscopy for Chemical Analysis studies are summarized in Table 31. Some insight into the oxidation state of the metal ions has been gained through these studies.

The ESCA technique has also provided a means for quality control of our synthetic products by enabling observation of trace impurities such as silver and/or chloride ions. Approximate concentrations of impurities were gauged by the relative intensity of the impurity signals. Elemental analyses were performed to substantiate the findings in the ESCA experiments.

The chemical shifts for the tetrameric platinum species were found to be reasonably constant. The chemical shifts were generally higher than those normally expected for platinum(II), but were still within the expected range. Ligand shifts were most likely responsible for the high numeric values which were observed. Generally, the platinum 4f(7/2),(5/2) signals were well-resolved and remained quite stable for each sample, even over extended periods in the vacuum chamber. Two exceptions were noted--both the dinitrosyl complex <u>12</u> and the dicarbonyl complex <u>6</u> gave initial signals which were approximately 1 eV lower than that normally found for platinum(II). After approximately 30 or 40 minutes in the vacuum chamber, an additional Pt 4f(7/2),(5/2) pair of signals had appeared. The signals were of approximately equal intensity. Then, after 4 to 20 hours of exposure to the vacuum, the signals at higher binding energy dominated the spectrum. It was also found that by dosing the samples with CO gas, the signals which were at lower binding energy could be caused to reappear in approximately the same intensity as the higher binding energy pair of signals. Upon removal from the vacuum, the solid's color was noted to have changed from purple to green. This sort of behavior suggests two possible mechanisms.

The first, and potentially the most practical explanation, involves simply pumping the acetic acid out of the crystalline lattice, thereby causing a change in the chemical environment around the platinum ions and resulting in a shift to an apparently higher binding energy. If the acetic acids were in some way sharing electrons with the ligands of the cluster (for which we have no evidence either by NMR or crystallography), such a shift would be expected. Once again the question of the metal's actual oxidation state eludes this investigation. The second mechanism which could possibly have been functioning would involve the lattice acetic acids protonating the NO or CO ligands, resulting in loss of the NO or CO ligands and the direct replacement of each NO or CO ligand by the resulting acetate ions. The resulting complex would then give the same binding energies which were observed for the other tetrameric species. A detailed examination of each of the samples with careful "sputtering" of the surfaces and subsequent observation of the spectra gave no indication of other ligands or other experimental complications in the measurements discussed above.

Overall, the ESCA data suggest an oxidation state of platinum (1.5) for the NO and CO complexes (in spite off the electron count difficulties which are encountered with such formulations. Additionally, the evidence favors direct destruction and formation of the complexes under ultra-high vacuum conditions. Finally, the data suggest an oxidation state of platinum(II) for most of the other tetrameric species.

Infrared Spectral Studies

The results of the infrared spectral studies have already been presented in Tables 40-61. The infrared studies have proven to be critical in this portion of the investigation; they have given considerable insight into the possible structural details of the various synthetic products presented here. This portion of the discussion will be given by ligand with some possible structural information suggested for the major groups of compounds which were synthesized. Before proceeding, however, the details involved in the infrared experiments shall be briefly discussed.

The Fourier Transform spectrometer which was used for obtaining spectral data upon the tetrameric species needed constant attention to its alignment in order to obtain satisfactory spectral results. Additionally, observations revealed that inclusion of a clean (no sample) KBr window in the laser beam at the time of taking the background scans, the signal-to-noise ratio of the recorded spectra was markedly improved (approximately 3 times). Finally, as sound infrared spectroscopy procedures dictate, keeping the KBr itself, the window press and the mortar and pestle scrupulously clean and dry certainly improved the quality of the spectra obtained for this investigation.

The spectra obtained for this investigation have supplied a significant portion of the proposed structural details, since NMR and x-ray crystallographic results proved difficult to obtain for each of the complexes. Therefore a brief discussion (ligand by ligand) of the assignments made in the Results portion of the thesis is in order; finally, proposed structures appear at the end of this discussion.

For the octakisacetato and the octakistrifluoroacetato compounds 7 and 29, one pair of symmetric and asymmetric (νs and νa) acetate absorptions were regularly observed at 1565 and 1410 cm^{-1}. Generally, each of the absorptions was moderate-to-strong and reasonably sharp. The absorptions remained remarkably sharp throughout the investigations. The normal rocking modes for the methyl and trifluoromethyl groups were observed, along with the other δ-and π deformation modes. In only one instance did the acetate absorptions significantly interfere with the spectral details of the C≡C stretching mode of the $HC{\equiv}C(C_6H_5)$ derivative of $PT_4(OAc)_8$ Blue.

For the compounds 19–21, the acetylene derivatives of the $Pt_4(OAc)_8$ Blue, making both the trifluoro and ordinary actato derivatives proved useful because it allowed the unequivocal assignment of the acetylenic C≡C stretch as a bridging species since the trifluoroacetate groups give a much simpler and somewhat less intense pair of acetate stretches. Comparison of both sharpness of the stretches and total integrated area of the 1430 stretch indicated a second band being present, which was assigned to the C≡C stretch.

The carbonyl derivative compound 7 was the first accurately characterized complex in this portion of the study, and the infrared spectrum proved to be very useful for structural confirmation. The complex has already been discussed in the x-ray crystallographic portion of this discussion; nonetheless a few notes are appropriate here. Using the infrared spectrum we were able to assign both symmetric and asymmetric carboxylate stretches which were supportive of the x-ray crystallography. Not only were the carboxylate stretches assigned but the bridging carbonyl stretches at 1610 cm^{-1} were also made, giving significant support to the x-ray crystallographic structure. The structural analogue of the dicarbonyl, the dinitrosyl complex, was assigned in a like manner. The bridging NO stretch was found to be somewhat lower in the spectrum than expected at 1385 cm^{-1}. However there are two carboxylate species present, and thus it is proposed that the nitrosyl is bridging the metals. The possibility of the above compound having a nitrate bridge has been ruled out by elemental analysis.

The thiocyanate species were probably some of the most carefully examined complexes in this discussion. Due to the distinct ionic thiocyanate C≡N stretches at 2050 cm^{-1}, we were able to discern quickly the species which were bridging metal centers from ordinary ionic species. Notably, upon bridging two metal centers, the C≡N stretching frequency increases by about 100 cm^{-1} giving distinct stretches at about 2130, 2100 and 697 cm^{-1}. Chatt and

Duncanson (80) have suggested that such a shift is due to back bonding from the metal centers at each end of the thiocyanate bridge. The complex formed when 20 equivalents of KSCN were added to the $Pt_4(OAc)_8$ Blue complex was identified solely by infrared spectroscopy as potassium tetrathiocyanatoplatinate(II). The other complexes were assigned by a combination of infrared, elemental analysis, and visible spectroscopy.

One group of compounds which proved difficult to assign by nearly any method was the triphenylphosphine derivatives of $Pt_4(OAc)_8$ Blue compounds 22-24. These compounds were found to have a distinct infrared spectrum which exhibits two types of acetate ions and possibly coordination of the phosphorus to the metal (given only by shifts in the phenyl-phosphorus stretches). As more triphenylphosphine is added, (going from two to four equivalents), the second type of carboxylate stretches disappear (asymmetric) leaving only one species of apparently symmetric carboxylate ligands. A parallel loss of color is also noted when going from the two equivalents to four equivalents complexes; the color goes from a deep green to a bright yellow color. Such a color change is suggestive that the metal-metal bonds have been broken with a possible mononuclear platinum-triphenylphosphine-carboxylato species resulting (46). This particular group of reactions bear further investigation.

When the α-oxopyridinate ligand, hydroxypyridine, was added to the $Pt_4(OAc)_8$ Blue complex, a rather complex deepening of the solution color which ultimately gives rise to a purple solution (32) takes place. The reaction was carried out with only eight equivalents of the ligand per mole of the complex. The infrared data are complex and somewhat difficult to interpret. NMR studies and elemental analyses suggest that compound 32 is an octakis-oxopyridinato complex with acetate ions present for charge balance. This group of complexes bears further investigation.

The complex that results when eight equivalents of acetamide are added to $Pt_4(OAc)_8$ Blue has approximately the same color as the starting material. The infrared results are shown in Table 58. The stretches at 1572 and 1414 cm^{-1} are indicative of the presence of bridging acetamide ligands. Considering the similarities between the acetate ion and the acetamide ion, the above results would seem reasonable for a bridging acetamide. Therefore this investigation suggests that the bridging acetate ions have been exchanged for acetamide ligands. The lack of color change indicates that the metal-metal bonds may have been preserved, and as a direct result, the tetrameric structure may also be preserved.

Finally, when concentrated H_2SO_4 is added to $Pt_4(OAc)_8$ Blue, an almost instantaneous change in solution color is observed. The initially deep blue solution becomes a dark brown color. No precipitates were observed to form, and as the deep brown solution is heated, the deep red color described previously results. The deep red or bright yellow colored solid which results gives an infrared spectrum which is appropriate for a sulfate bridged species (23). The addition of K_2SO_4 to the deep blue solution containing $Pt_4(OAc)_8$

apparently gives no reaction. The reaction with K_2SO_4 bears further investigation.

Elemental Analytic Studies

The analysis of the tetrameric complexes has proven somewhat complicated. Each time that light atoms (C, H, N, etc.) were analyzed by Galbraith Labs, the results generally fitted the proposed compounds. However, when platinum analyses were requested, the results were invariably 10%-45% lower than expected. When questioned about their method of analysis, Galbraith responded that they submitted the samples to an acid hydrolysis and then used Inductively Coupled Plasma Atomic Absorption (ICPAA) for analysis. The method seems to be an appropriate approach for the analysis of the heavy metals. Nonetheless, the question remained, "Why are our samples so low in their percent Pt and so accurate for the light atoms?". The only explanation we suggest is that the platinum-platinum bonded clusters were not breaking up under their conditions. Further evidence for the "toughness" of the species comes from our platinum analyses in which some of the complexes required boiling in aqua regia to perform the analysis. Questions of purity and dryness of the microcrystalline powders of the complexes were addressed, too. Generally the purity and dryness were not found to be significant problems. We found that if the complexes were placed in formic acid and boiled for two to three hours, the clusters were reduced to platinum metal, and upon careful drying the yield of metal gave accurate analyses for platinum. This method was also tried for standards (e.g., K_2PtCl_4, $PtCl_2$, $PtCl_4^{2-}$, $PtCl_6^{2-}$) and found to be quite accurate (±1.5%). Therefore all of the platinum analyses which appear in this dissertation were carried out in our laboratory. The complexes for which analyses were obtained were purified from the reaction products, and thus we feel that the results presented earlier are reasonable. In Table 65 we suggest the formulas for the complexes which were made in this portion of the investigation.

Proposed Structures

This final portion of the discussion suggests the possible structures for all of the derivatives of the various platinum species presented in this dissertation. Since it was not possible to obtain single crystals of many of the compounds for x-ray crystal analysis, it is necessary to depend upon the structures which are known, and which we have found, as bases for the inferences which lead to the following group of proposed structures. These structures represent the combination of infrared spectroscopic, elemental analytical, visible spectroscopic, and chemical reactivity information, all of which have been presented earlier in this discussion.

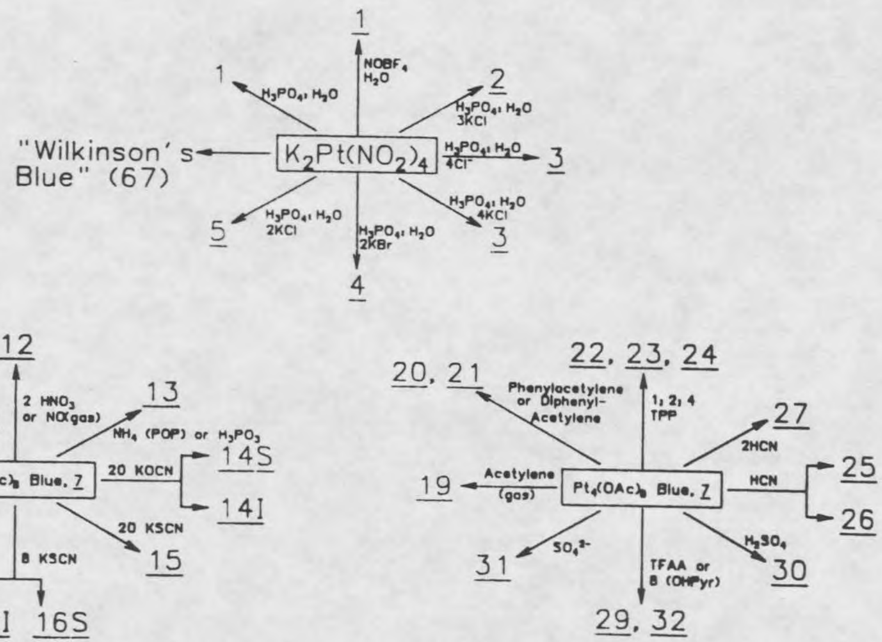


Figure 47. Synthesis of the derivative species and their compound numbers as presented in this discussion.

Table 65. Proposed formulae, supporting data, and proposed structures for all of the platinum complexes presented.

Compound Number	Empirical Formula	Proposed Formula
1	$K_2[Pt(NO_2)_4(NO)(OH_2)]\cdot OH_2$	same
2	$K_2[Pt(NO_2)_2(Cl)_3(NO)]$	same
3	$K_2[Pt(NO_2)_2(Cl)_4]$	same
4	$K_2[Pt(NO_2)_4(Br)_2]$	same
5	$K_2[Pt(NO_2)_2(PO_3)_2]$	same
6	$[Pt_2(OAc)_3(CO)]\cdot HOAc$	$[Pt_4(OAc)_6(CO)_2]\cdot 2HOAc$
7	$Pt(OAc)_2\cdot 2HOAc, \cdot 4HOAc$	$[Pt_4(OAc)_8]\cdot 2, \cdot 4HOAc$
8	$Pt(OAc)_2$	$[Pt_4(OAc)_8]$
10	$Pt(OAc)_2$	$[Pt_4(OAc)_8]$
12	$[Pt(OAc)_3(NO)]\cdot 0.5HOAc$	$[Pt_4(OAc)_6(NO)_2]\cdot 2HOAc$
13	$[Pt(POP)_2]$	$[Pt_2(POP)_4]$
15	$[Pt(SCN)_4]$	same
16I	$[Pt(SCN)_2]\cdot 0.7HOAc$	$[Pt_4(SCN)_8]\cdot 7HOAc$
16S	$[Pt_2(OAc)_3(SCN)]\cdot 2HOAc$	$[Pt_4(OAc)_6(SCN)_2]\cdot 4HOAc$
17I	$[Pt(OAc)(SCN)]$	$[Pt_4(OAc)_4(SCN)_4]$
17S	$K(OAc)$	same
18S	$[Pt(OAc)_2]\cdot 0.13SCN$	$[Pt_4(OAc)_8]\cdot 0.7HOAc$
18I	$[Pt_2(OAc)_2(SCN)_2]\cdot HOAc$	$[Pt_2(OAc)_2(SCN)_2\cdot HOAc$
18I	$[Pt_2(OAc)_2(SCN)_2]\cdot HOAc$	$[Pt_4(OAc)_4(SCN)_4]\cdot 2HOAc$
19	$[Pt_2(OAc)_3(HC{\equiv}CH)]$	$[Pt_4(OAc)_6(HC{\equiv}CH)_2]$
20	$[Pt_2(OAc)_3(HC{\equiv}CH)(C_6H_5)]\cdot HOAc$	$[Pt_4(OAc)_6(HC{\equiv}CH)(C_6H_5)_2]\cdot 2HOAc$
21	$[Pt_2(OAc)_3\{(C_6H_5)C{\equiv}C(C_6H_5)\}]$	$[Pt_4(OAc)_6\{(C_6H_5)_2C{\equiv}C\}_2]$
22,23,24	$[Pt_4(OAc)_7(Ph_3P)]$	- - - - -
27	$[Pt_4(OAc)_6(NCN)_2]$	- - - - -
28	$[Pt(OAc)_3(H_2NOCCH_3)]\cdot HOAc$	$[Pt_2(OAc)_6(H_2NOCCH_3)_2]\cdot 2HOAc$
29	$Pt(O_2C_2F_3)_2$	$Pt_4(O_2C_2F_3)_8$
30	$[Pt(SO_4)_2]$	$[Pt_2(SO_4)_4]$
32	$[Pt(OHPyr)_2(OAc)_2]$	$[Pt_4(OHPyr)_8(OAc)_8]$

Table 65. (continued)

Compound Number	X-Ray	I.R.	Vis.
1	X	X	X
2	X	X	X
3	X		
4	X		
5	X		
6	X	X	X
7		X	X
8		X	X
10		X	X
12		X	X
13			X
15		X	X
16I		X	X
16S		X	X
17I		X	X
17S		X	X
18S		X	X
18I		X	X
18I		X	X
19		X	X
20		X	X
21		X	X
22,23,24		X	X
27		X	X
28		X	X
29		X	X
30		X	X
32		X	X

Table 65. (continued)

Compound Number	^{1}H/Lig.	Elemental Analysis	ESCA
1			X
2			
3			
4			
5			
6	X	X	X
7	X	X	X
8	X	X	
10	X		
12	X	X	X
13			
15	X		
16I	X	X	
16S	X	X	
17I	X	X	
17S	X		
18S	X	X	
18I	X	X	
18I	X	X	
19	X		
20		X	
21			
22,23,24			
27			
28	X	X	
29	X		
30			
32		X	

Table 65. (continued)

Compound Number	Proposed Structure
1	Bent Nitrosyl, Monomer
2	Bent Nitrosyl, Monomer
3	Tetrachloro, Monomer
4	Dibromo, Monomer
5	Diphosphite, Monomer
6	Dicarbonyl, Tetramer
7	Octakis-Acetato-Tetramer
8	Octakis-Acetato-Tetramer
10	Octakis-Acetato-Tetramer
12	Dinitrosyl, Tetramer
13	Diphosphite Pt(II) Dimer
15	Tetrathiocyanate Pt(II), Monomer
16I	Octakis-Thiocyanato-Tetramer
16S	Bisthiocyanato-Tetramer
17I	Mixed Thiocyanate-Acetate Dimer/ Tetramer
17S	Potassium Acetate
18S	Octakis-Acetato-Tetramer
18I	Bisthiocyanato-Tetramer
18I	Bisthiocyanato-Tetramer
19	Diacetylide Tetramer
20	Bis-Phenylacetylide, Tetramer
21	Bis-Phenylacetylide, Tetramer
22, 23, 24	- - - - -
27	- - - - -
28	Diacetamido-Tetramer
29	Octakis-Trifluoroacetate-Tetramer
30	Tetrasulfato-Dimer
32	Octakis-Hydroxypyridinato-Tetramer

SUMMARY

Man's fascination with platinum has evolved somewhat from a primary use of the metal in ornaments such as jewelry to the chemical and physical applications which we see today. Though the Spanish once threw the "platina" back into the South American rivers, man now searches for the platinum metals in more and more remote parts of our world; we have been able to increasingly benefit from the presence of such elements in our world. The number of applications for the metals in the chemical industry seem boundless, only through careful investigation of the chemical properties of platinum and its associated metals will mankind continue to benefit from the materials which can be made from the element.

This investigation has been concerned with the formation and breaking of chemical platinum-platinum bonds. The first portion was concerned with the initial steps in the formation of platinum-platinum bonds while the second area of study examined a group of complexes and their in-solution structures. Finally, the third part of the problem dealt with the systematic substitution chemistry of a group of tetrameric platinum-platinum bonded compounds which are initially metal-metal bonded, but whose bonds can be broken using appropriate ligands.

The bent nitrosyl complexes have provided a glimpse at the first step in the reactions leading to platinum-platinum bond formation.

Due to the high reactivity of the species, one must exercise caution in exposing the compounds to air and moisture. The valences of the metal ions can certainly be debated; however our results indicate that the complex is in the +4 state. Other synthetic methods for the generation of the bent nitrosyl complexes suggested that the compounds are not too uncommon, but that due to their reactivity they are exceptionally hard to isolate. Finally, one might comment upon the presence of the platinum(IV) complex as a precursor to the formation of platinum-platinum bonds: the possibility exists that a mixed valence dimeric precursor is present. However, the details of the mechanism and actual oxidation state of the metal centers remain to be revealed.

Our investigations of the α-oxopyridinato platinum(III) complexes have yielded some unusual in-solution structural observations. The higher order platinum NMR spectral results certainly were interesting in light of the seemingly not so large difference in the electronic environment about the platinum ions. This observation probably is indication of just how sensitive the platinum chemical shifts are to small electronic perturbances induced by the ligands around the ion. The question of mixed valence d^6-d^8 electronic configuration or d^7-d^7 electronic configurations has a direct bearing upon the first portion of this dissertation, as well as upon the final sections. The question of a mixed valence cluster has been addressed here and quite probably ruled out based upon ESCA data. Therefore, the oxidation state of +3 is reasonable for platinum clusters and certainly is useful in explaining the bonding between metal ions.

In the final portion of this dissertation the synthesis, purification, analysis, and characterization of a group of tetrameric platinum clusters has been pursued. The synthesis suggested by Davidson and Triggs has been modified to allow the purification of the complexes. Using the $Pt_4(OAc)_8$ Blue fraction obtained in the modified synthesis, a number of synthetic analogues have been made. One should note that the reaction conditions used in this study are one of its unique aspects. Additionally the syntheses have shown the complex to undergo a number of interesting reactions some even yielding platinum(III) species. The results of this portion of the investigation have allowed generalization of the reactions of platinum to form tetrameric species with not only carboxylato species but also with amido and α-oxopyridinato ligands. Finally, a simpler synthesis of the tetrameric compound was found using platinum(II) as a starting material. Some modification of the method is warranted and certainly bears closer investigation.

Thus, the investigation of this particular group of platinum clusters has given some insight into the formation, in-solution structure, and reactivity of platinum-platinum bonded clusters. The number of additional avenues which could be pursued is nearly limitless, and it is hoped that additional systematic synthetic efforts in this area will follow from this work.

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APPENDIX

F_o F_c Tables for Compounds <u>1</u> - <u>6</u>

Table 66. F_o F_c Tables for $K[Pt(NO_2)_4(NO)H_2O]\cdot H_2O$, 1, F(obs), F(calc) and σ_F ($-\sigma_F$ indicates omitted data).

H	K	L	$10F_o$	$10F_c$	10σ
1	0	0	1291	1313	33
2	0	0	343	370	7
3	0	0	253	275	17
4	0	0	375	382	7
5	0	0	470	500	35
6	0	0	700	738	14
7	0	0	368	374	16
8	0	0	291	289	10
9	0	0	121	131	16
-9	1	0	219	233	12
-8	1	0	245	251	10
-7	1	0	63	32	-29
-6	1	0	131	107	11
-5	1	0	561	594	25
-4	1	0	1085	1096	10
-3	1	0	853	843	29
-2	1	0	876	904	16
-1	1	0	474	407	19
1	1	0	694	639	4
2	1	0	351	389	6
3	1	0	561	563	11
4	1	0	944	972	24
5	1	0	419	454	12
6	1	0	178	197	10
7	1	0	77	86	16
8	1	0	233	235	9
9	1	0	237	220	11
-9	2	0	141	150	22
-8	2	0	236	264	11
-7	2	0	371	388	10
-6	2	0	437	451	11
-5	2	0	457	457	13
-4	2	0	342	338	18
-3	2	0	391	397	15
-2	2	0	440	438	23
-1	2	0	996	963	33
0	2	0	1682	1544	20
1	2	0	970	981	13
2	2	0	645	615	7
3	2	0	115	107	8
4	2	0	348	330	8
5	2	0	737	729	18
6	2	0	626	627	41
7	2	0	322	325	9
8	2	0	305	305	9
9	2	0	58	69	-28
-9	3	0	191	204	16
-8	3	0	178	164	18
-7	3	0	57	35	-52
-6	3	0	163	148	-41
-5	3	0	859	780	52
-4	3	0	721	748	39
-3	3	0	914	886	45
-2	3	0	1163	1101	36
-1	3	0	296	259	21
0	3	0	75	37	-17
1	3	0	1420	1414	10
2	3	0	860	859	14
3	3	0	893	924	8
4	3	0	1016	1041	11
5	3	0	360	345	15
6	3	0	155	137	20
7	3	0	201	180	9
8	3	0	212	199	15
9	3	0	254	235	10
-9	4	0	165	152	28
-8	4	0	256	230	26
-7	4	0	555	465	25
-6	4	0	425	426	17
-5	4	0	470	452	58
-4	4	0	145	123	13
-3	4	0	384	389	22
-2	4	0	533	520	10
-1	4	0	1189	1103	37
0	4	0	979	955	28
1	4	0	989	1015	7
2	4	0	428	414	16
3	4	0	130	125	9
4	4	0	220	207	10
5	4	0	529	517	20

H	K	L	$10F_o$	$10F_c$	10σ
6	4	0	449	437	12
7	4	0	373	396	14
8	4	0	216	216	20
9	4	0	29	37	−55
−9	5	0	189	181	32
−8	5	0	94	89	−52
−7	5	0	61	14	−57
−6	5	0	211	206	14
−5	5	0	447	441	21
−4	5	0	508	504	10
−3	5	0	683	671	47
−2	5	0	513	457	16
−1	5	0	385	371	9
0	5	0	253	256	13
1	5	0	636	649	8
2	5	0	623	604	23
3	5	0	889	887	9
4	5	0	471	470	10
5	5	0	317	307	11
6	5	0	25	58	−48
7	5	0	209	195	27
8	5	0	196	189	10
9	5	0	263	245	18
−9	6	0	181	115	−46
−8	6	0	236	216	23
−7	6	0	354	342	24
−6	6	0	280	274	27
−5	6	0	281	264	21
−4	6	0	80	79	−29
−3	6	0	210	213	11
−2	6	0	651	624	38
−1	6	0	1238	1223	53
0	6	0	693	696	23
1	6	0	600	613	10
2	6	0	244	242	9
3	6	0	51	53	−26
4	6	0	323	337	7
5	6	0	566	580	12
6	6	0	410	405	24
7	6	0	308	319	17
8	6	0	120	135	−30
−8	7	0	37	40	−70
−7	7	0	73	10	−33
−6	7	0	224	236	12
−5	7	0	398	393	16
−4	7	0	573	567	29
−3	7	0	621	599	35
−2	7	0	370	355	13
−1	7	0	236	214	19
0	7	0	300	304	9
1	7	0	396	420	20
2	7	0	572	590	11
3	7	0	604	589	11
4	7	0	350	366	13
5	7	0	258	267	10
6	7	0	61	37	−22
7	7	0	125	122	14
8	7	0	179	177	11
−8	8	0	169	190	−42
−7	8	0	189	195	18
−6	8	0	247	249	10
−5	8	0	176	177	11
−4	8	0	67	55	−26
−3	8	0	182	158	9
−2	8	0	444	429	22
−1	8	0	429	422	30
0	8	0	497	507	41
1	8	0	434	443	12
2	8	0	108	114	−26
3	8	0	63	38	−18
4	8	0	335	360	15
5	8	0	323	333	10
6	8	0	301	295	10
7	8	0	257	250	10
−7	9	0	71	45	−34
−6	9	0	184	188	12
−5	9	0	249	251	12
−4	9	0	401	396	25
−3	9	0	344	344	15
−2	9	0	221	223	13
−1	9	0	58	44	−28
0	9	0	313	316	31
1	9	0	392	403	30
2	9	0	503	527	10
3	9	0	395	418	9
4	9	0	257	261	17
5	9	0	122	119	13
6	9	0	66	58	−31
−6	10	0	165	169	15
−5	10	0	112	79	16
−4	10	0	28	36	−53
−3	10	0	199	198	10
−2	10	0	350	360	20
−1	10	0	366	369	11

H	K	L	$10F_o$	$10F_c$	10σ
0	10	0	435	437	35
1	10	0	206	225	19
2	10	0	61	65	-24
3	10	0	94	68	-26
4	10	0	197	210	11
5	10	0	227	239	26
6	10	0	278	274	11
-5	11	0	183	177	19
-4	11	0	264	262	10
-3	11	0	203	204	13
-2	11	0	150	149	21
-1	11	0	75	28	-29
0	11	0	128	126	13
1	11	0	222	242	23
2	11	0	332	334	19
3	11	0	211	227	13
4	11	0	192	191	24
5	11	0	75	58	-31
-4	12	0	30	23	-56
-3	12	0	158	168	18
-2	12	0	241	241	24
-1	12	0	224	235	15
0	12	0	222	231	11
1	12	0	138	132	-33
2	12	0	43	38	-38
3	12	0	103	110	18
-1	13	0	54	42	-33
0	13	0	113	102	18
1	13	0	189	207	12
-1	-13	1	116	141	25
0	-13	1	170	173	18
1	-13	1	166	185	19
-3	-12	1	255	267	15
-2	-12	1	256	281	14
-1	-12	1	234	233	15
0	-12	1	114	120	22
1	-12	1	53	26	-45
2	-12	1	87	105	-28
3	-12	1	201	220	16
4	-12	1	169	198	20
-5	-11	1	243	260	16
-4	-11	1	162	165	16
-3	-11	1	75	64	-27
-2	-11	1	57	55	-35
-1	-11	1	200	215	15
0	-11	1	181	220	16
1	-11	1	307	327	14

H	K	L	$10F_o$	$10F_c$	10σ
2	-11	1	230	251	15
3	-11	1	118	132	23
4	-11	1	31	27	-82
5	-11	1	111	89	24
-6	-10	1	29	5	-78
-5	-10	1	112	108	21
-4	-10	1	191	193	14
-3	-10	1	328	350	14
-2	-10	1	329	324	11
-1	-10	1	300	317	12
0	-10	1	97	127	-22
1	-10	1	68	50	-31
2	-10	1	171	211	17
3	-10	1	313	345	13
4	-10	1	258	275	14
5	-10	1	191	243	17
6	-10	1	74	115	-39
-7	-9	1	230	221	15
-6	-9	1	305	292	14
-5	-9	1	270	291	14
-4	-9	1	195	179	13
-3	-9	1	125	123	15
-2	-9	1	195	201	12
-1	-9	1	385	402	11
0	-9	1	495	518	13
1	-9	1	531	536	13
2	-9	1	313	317	12
3	-9	1	185	226	15
4	-9	1	28	15	-74
5	-9	1	137	144	20
6	-9	1	173	194	20
7	-9	1	208	214	21
-7	-8	1	174	146	15
-6	-8	1	50	42	-38
-5	-8	1	132	130	16
-4	-8	1	434	426	13
-3	-8	1	517	529	13
-2	-8	1	514	505	12
-1	-8	1	475	475	12
0	-8	1	42	74	-36
1	-8	1	24	31	-65
2	-8	1	342	373	12
3	-8	1	390	434	12
4	-8	1	313	332	13
5	-8	1	347	353	13
6	-8	1	71	126	-44
7	-8	1	35	33	-94

H	K	L	$10F_o$	$10F_c$	10σ
-8	-7	1	178	172	15
-7	-7	1	229	229	13
-6	-7	1	382	366	12
-5	-7	1	336	355	12
-4	-7	1	252	263	11
-3	-7	1	100	118	18
-2	-7	1	383	373	12
-1	-7	1	417	423	11
0	-7	1	573	594	16
1	-7	1	594	609	16
2	-7	1	547	525	12
3	-7	1	249	263	12
4	-7	1	122	130	18
5	-7	1	183	172	16
6	-7	1	319	342	17
7	-7	1	234	268	24
8	-7	1	128	182	-46
-8	-6	1	212	214	15
-7	-6	1	123	102	17
-6	-6	1	87	85	-21
-5	-6	1	336	318	11
-4	-6	1	557	583	15
-3	-6	1	636	630	14
-2	-6	1	916	915	13
-1	-6	1	414	404	10
0	-6	1	100	89	17
1	-6	1	172	158	12
2	-6	1	679	708	15
3	-6	1	621	661	18
4	-6	1	602	631	14
5	-6	1	308	337	14
6	-6	1	140	156	27
7	-6	1	119	24	-42
8	-6	1	54	136	-143
-9	-5	1	81	89	-30
-8	-5	1	217	202	13
-7	-5	1	385	361	12
-6	-5	1	656	637	19
-5	-5	1	380	374	12
-4	-5	1	334	316	11
-3	-5	1	38	34	-36
-2	-5	1	492	451	13
-1	-5	1	667	675	11
0	-5	1	1136	1166	11
1	-5	1	673	685	12
2	-5	1	530	547	15
3	-5	1	180	174	14
4	-5	1	197	186	17
5	-5	1	168	179	24
6	-5	1	368	437	22
7	-5	1	357	339	32
8	-5	1	264	239	28
9	-5	1	93	105	-110
-9	-4	1	252	211	14
-8	-4	1	257	243	12
-7	-4	1	90	61	-20
-6	-4	1	23	44	-62
-5	-4	1	396	375	11
-4	-4	1	553	564	14
-3	-4	1	630	649	12
-2	-4	1	1015	1019	10
-1	-4	1	431	402	11
0	-4	1	241	246	10
1	-4	1	297	298	10
2	-4	1	582	593	13
3	-4	1	786	842	16
4	-4	1	847	924	23
5	-4	1	303	347	26
6	-4	1	265	272	30
7	-4	1	62	56	-164
8	-4	1	150	193	-55
9	-4	1	113	166	-62
-9	-3	1	131	129	18
-8	-3	1	214	217	12
-7	-3	1	491	472	13
-6	-3	1	513	500	11
-5	-3	1	471	457	10
-4	-3	1	419	402	13
-3	-3	1	234	230	8
-2	-3	1	635	604	10
-1	-3	1	2142	2000	9
0	-3	1	1293	1286	8
1	-3	1	614	650	10
2	-3	1	904	898	12
3	-3	1	32	31	-86
4	-3	1	217	262	40
5	-3	1	603	536	35
6	-3	1	433	428	27
7	-3	1	304	335	24
8	-3	1	249	297	27
9	-3	1	41	77	-108
-9	-2	1	249	249	13
-8	-2	1	217	200	12
-7	-2	1	25	47	-66

H	K	L	$10F_o$	$10F_c$	10σ
-6	-2	1	126	114	13
-5	-2	1	741	744	13
-4	-2	1	776	761	11
-3	-2	1	887	861	10
-2	-2	1	1040	1096	9
-1	-2	1	493	481	8
0	-2	1	290	263	10
1	-2	1	465	475	12
2	-2	1	574	577	19
3	-2	1	921	920	24
4	-2	1	894	999	26
5	-2	1	380	448	26
6	-2	1	182	201	22
7	-2	1	36	124	-95
8	-2	1	158	192	25
9	-2	1	204	236	22
-9	-1	1	119	138	19
-8	-1	1	224	233	12
-7	-1	1	525	504	13
-6	-1	1	574	542	15
-5	-1	1	656	657	13
-4	-1	1	244	252	8
-3	-1	1	265	294	8
-2	-1	1	375	372	9
-1	-1	1	1564	1643	8
0	-1	1	1420	1366	7
1	-1	1	1295	1375	16
2	-1	1	522	547	23
3	-1	1	185	113	20
4	-1	1	219	245	15
5	-1	1	656	716	20
6	-1	1	387	412	13
7	-1	1	415	457	15
8	-1	1	277	293	15
9	-1	1	92	69	-33
-10	0	1	199	175	15
-9	0	1	270	264	12
-8	0	1	144	124	14
-7	0	1	65	59	-25
-6	0	1	333	336	12
-5	0	1	496	533	15
-4	0	1	639	663	12
-3	0	1	1468	1424	9
-2	0	1	468	499	9
-1	0	1	767	774	8
0	0	1	372	283	12
1	0	1	767	807	10
2	0	1	746	771	11
3	0	1	1392	1487	11
4	0	1	667	684	14
5	0	1	495	505	12
6	0	1	104	127	22
7	0	1	136	148	19
8	0	1	202	193	17
9	0	1	287	291	16
-10	1	1	88	52	-27
-9	1	1	110	122	21
-8	1	1	337	333	11
-7	1	1	534	544	13
-6	1	1	497	503	16
-5	1	1	517	523	14
-4	1	1	89	101	14
-3	1	1	273	274	9
-2	1	1	891	977	21
-1	1	1	1743	1725	7
0	1	1	1402	1464	7
2	1	1	209	190	9
3	1	1	70	89	-16
4	1	1	303	289	11
5	1	1	641	649	15
6	1	1	507	545	13
7	1	1	429	439	12
8	1	1	196	192	16
9	1	1	134	95	20
-9	2	1	211	216	16
-8	2	1	112	125	18
-7	2	1	75	65	-24
-6	2	1	309	321	12
-5	2	1	457	442	12
-4	2	1	724	771	18
-3	2	1	1209	1125	10
-2	2	1	756	719	8
-1	2	1	598	573	7
0	2	1	369	404	8
1	2	1	396	401	9
2	2	1	1131	1132	9
3	2	1	1138	1192	10
4	2	1	650	670	13
5	2	1	565	573	16
6	2	1	85	44	-21
7	2	1	144	140	15
8	2	1	255	247	13
9	2	1	268	267	16
-9	3	1	129	116	21

Table 66. (continued)

H	K	L	$10F_o$	$10F_c$	10σ
-8	3	1	298	335	15
-7	3	1	309	334	15
-6	3	1	441	489	18
-5	3	1	394	382	22
-4	3	1	23	10	-62
-3	3	1	282	274	9
-2	3	1	1599	1525	8
-1	3	1	743	682	8
0	3	1	965	930	8
1	3	1	1249	1303	8
2	3	1	316	303	8
3	3	1	60	9	-19
4	3	1	599	613	13
5	3	1	492	471	11
6	3	1	471	473	13
7	3	1	377	400	13
8	3	1	189	173	17
9	3	1	98	81	-27
-9	4	1	170	139	22
-8	4	1	152	127	31
-7	4	1	125	44	-54
-6	4	1	425	361	14
-5	4	1	569	524	18
-4	4	1	792	767	13
-3	4	1	809	749	11
-2	4	1	866	799	10
-1	4	1	220	219	9
0	4	1	403	389	11
1	4	1	695	660	10
2	4	1	999	988	10
3	4	1	720	740	12
4	4	1	623	633	14
5	4	1	287	264	11
6	4	1	77	52	-23
7	4	1	143	127	16
8	4	1	297	278	14
9	4	1	211	220	18
-9	5	1	165	144	-44
-8	5	1	278	272	26
-7	5	1	399	328	16
-6	5	1	454	435	12
-5	5	1	201	202	12
-4	5	1	71	38	-23
-3	5	1	290	287	10
-2	5	1	822	756	11
-1	5	1	805	767	11
0	5	1	1070	1032	10
1	5	1	500	504	13
2	5	1	259	273	9
3	5	1	92	114	19
4	5	1	464	473	11
5	5	1	427	426	13
6	5	1	592	557	13
7	5	1	317	300	13
8	5	1	138	153	20
-9	6	1	71	106	-66
-8	6	1	36	86	-95
-7	6	1	123	105	20
-6	6	1	188	184	13
-5	6	1	451	434	13
-4	6	1	749	701	15
-3	6	1	458	430	17
-2	6	1	533	496	14
-1	6	1	57	14	-24
0	6	1	266	254	9
1	6	1	603	595	16
2	6	1	818	857	13
3	6	1	545	541	16
4	6	1	522	523	11
5	6	1	175	185	13
6	6	1	48	12	-41
7	6	1	170	147	15
8	6	1	231	232	16
-8	7	1	216	199	17
-7	7	1	287	260	13
-6	7	1	260	268	13
-5	7	1	175	155	13
-4	7	1	34	19	-44
-3	7	1	427	393	12
-2	7	1	576	526	15
-1	7	1	781	739	14
0	7	1	680	656	14
1	7	1	320	323	13
2	7	1	213	218	11
3	7	1	179	175	12
4	7	1	331	345	12
5	7	1	446	451	14
6	7	1	338	350	15
7	7	1	180	177	15
8	7	1	107	131	-25
-8	8	1	57	36	-44
-7	8	1	76	84	-31
-6	8	1	173	166	15
-5	8	1	409	398	12

H	K	L	$10F_o$	$10F_c$	10σ
-4	8	1	479	448	14
-3	8	1	379	356	14
-2	8	1	192	183	12
-1	8	1	23	32	-62
0	8	1	146	159	15
1	8	1	612	563	23
2	8	1	485	488	12
3	8	1	421	440	14
4	8	1	360	365	12
5	8	1	94	69	-21
6	8	1	72	29	-29
7	8	1	175	168	17
-7	9	1	202	188	16
-6	9	1	161	155	16
-5	9	1	98	114	-23
-4	9	1	57	50	-32
-3	9	1	328	315	13
-2	9	1	262	289	14
-1	9	1	519	506	13
0	9	1	559	537	13
1	9	1	323	319	12
2	9	1	25	50	-66
3	9	1	198	195	13
4	9	1	224	234	13
5	9	1	324	328	13
6	9	1	268	262	14
-6	10	1	164	157	18
-5	10	1	282	272	14
-4	10	1	293	303	14
-3	10	1	328	297	12
-2	10	1	90	89	-22
-1	10	1	65	29	-26
0	10	1	227	218	14
1	10	1	408	379	13
2	10	1	292	308	12
3	10	1	315	311	13
4	10	1	145	165	18
5	10	1	75	60	-30
-5	11	1	77	64	-29
-4	11	1	83	77	-26
-3	11	1	202	179	15
-2	11	1	248	249	15
-1	11	1	320	320	13
0	11	1	267	244	13
1	11	1	172	172	15
2	11	1	42	20	-46
3	11	1	113	111	22
4	11	1	171	194	17
-4	12	1	197	192	15
-3	12	1	156	167	18
-2	12	1	74	50	-30
-1	12	1	57	22	-37
0	12	1	170	172	16
1	12	1	276	256	13
2	12	1	278	255	13
3	12	1	217	218	17
-1	13	1	193	184	16
0	13	1	161	162	18
0	-13	2	31	69	-83
1	-13	2	59	9	-44
-3	-12	2	61	53	-36
-2	-12	2	84	98	-28
-1	-12	2	150	157	19
0	-12	2	247	262	15
1	-12	2	232	251	16
2	-12	2	182	202	18
3	-12	2	130	120	24
4	-12	2	69	6	-41
-5	-11	2	59	106	-39
-4	-11	2	224	251	15
-3	-11	2	263	262	13
-2	-11	2	287	312	14
-1	-11	2	147	187	19
0	-11	2	109	86	22
1	-11	2	29	51	-77
2	-11	2	202	214	15
3	-11	2	177	193	17
4	-11	2	221	245	18
5	-11	2	174	162	18
-6	-10	2	239	263	16
-5	-10	2	198	213	16
-4	-10	2	188	183	15
-3	-10	2	46	9	-42
-2	-10	2	123	125	18
-1	-10	2	228	233	12
0	-10	2	404	435	13
1	-10	2	392	402	14
2	-10	2	299	309	13
3	-10	2	157	108	16
4	-10	2	60	7	-43
5	-10	2	119	120	24
6	-10	2	179	201	22
-7	-9	2	86	65	-26
-6	-9	2	28	6	-74

Table 66. (continued)

H	K	L	$10F_o$	$10F_c$	10σ
-5	-9	2	199	182	15
-4	-9	2	308	315	12
-3	-9	2	439	461	14
-2	-9	2	463	484	13
-1	-9	2	251	274	12
0	-9	2	158	181	15
1	-9	2	186	189	14
2	-9	2	302	322	13
3	-9	2	284	320	14
4	-9	2	358	363	14
5	-9	2	192	217	18
6	-9	2	119	139	-28
7	-9	2	37	4	-100
-7	-8	2	294	297	14
-6	-8	2	273	288	13
-5	-8	2	270	264	12
-4	-8	2	262	280	12
-3	-8	2	35	42	-46
-2	-8	2	177	191	12
-1	-8	2	535	539	12
0	-8	2	487	502	12
1	-8	2	388	398	15
2	-8	2	417	419	12
3	-8	2	78	82	-27
4	-8	2	28	13	-76
5	-8	2	221	239	18
6	-8	2	245	263	19
7	-8	2	209	204	24
-8	-7	2	173	159	15
-7	-7	2	59	88	-36
-6	-7	2	25	28	-66
-5	-7	2	318	327	12
-4	-7	2	415	432	12
-3	-7	2	631	628	16
-2	-7	2	535	548	16
-1	-7	2	334	340	11
0	-7	2	110	101	18
1	-7	2	278	294	13
2	-7	2	409	440	14
3	-7	2	608	655	14
4	-7	2	467	466	13
5	-7	2	277	321	16
6	-7	2	117	159	-35
7	-7	2	118	55	-43
8	-7	2	151	88	-42
-8	-6	2	176	184	14
-7	-6	2	352	352	13
-6	-6	2	406	386	11
-5	-6	2	484	475	12
-4	-6	2	155	168	12
-3	-6	2	84	56	-20
-2	-6	2	376	347	11
-1	-6	2	839	859	13
0	-6	2	686	694	14
1	-6	2	765	825	15
2	-6	2	510	535	12
3	-6	2	124	130	21
4	-6	2	108	91	-25
5	-6	2	312	331	18
6	-6	2	258	277	21
7	-6	2	283	313	31
8	-6	2	208	200	32
-9	-5	2	257	230	14
-8	-5	2	154	150	15
-7	-5	2	133	128	15
-6	-5	2	164	169	13
-5	-5	2	420	402	12
-4	-5	2	461	466	16
-3	-5	2	901	927	13
-2	-5	2	637	650	13
-1	-5	2	538	519	13
0	-5	2	86	70	16
1	-5	2	340	337	12
2	-5	2	386	378	13
3	-5	2	928	966	18
4	-5	2	489	485	15
5	-5	2	277	314	20
6	-5	2	118	126	-55
7	-5	2	75	70	-70
8	-5	2	128	134	-40
9	-5	2	256	201	37
-9	-4	2	76	83	-32
-8	-4	2	277	274	12
-7	-4	2	432	439	14
-6	-4	2	480	486	12
-5	-4	2	450	431	11
-4	-4	2	69	40	-20
-3	-4	2	43	26	-29
-2	-4	2	618	590	12
-1	-4	2	1155	1107	10
0	-4	2	1089	1098	11
1	-4	2	716	699	13
2	-4	2	233	242	14
3	-4	2	260	294	19

H	K	L	$10F_o$	$10F_c$	10σ
4	-4	2	367	370	19
5	-4	2	465	416	24
6	-4	2	405	411	21
7	-4	2	465	437	31
8	-4	2	214	183	44
9	-4	2	198	105	41
-9	-3	2	221	206	14
-8	-3	2	143	155	15
-7	-3	2	91	87	19
-6	-3	2	244	237	10
-5	-3	2	371	379	11
-4	-3	2	908	887	12
-3	-3	2	929	950	11
-2	-3	2	1014	1092	10
-1	-3	2	869	904	10
0	-3	2	461	449	12
1	-3	2	352	308	11
2	-3	2	858	845	17
3	-3	2	1146	1162	23
4	-3	2	787	781	21
5	-3	2	537	473	33
6	-3	2	54	60	-144
7	-3	2	47	51	-127
8	-3	2	173	207	-39
9	-3	2	227	211	29
-9	-2	2	113	108	19
-8	-2	2	366	370	12
-7	-2	2	400	396	13
-6	-2	2	579	587	15
-5	-2	2	561	583	14
-4	-2	2	21	87	-57
-3	-2	2	141	165	10
-2	-2	2	1168	1239	9
-1	-2	2	1025	938	9
0	-2	2	795	671	11
1	-2	2	913	926	14
2	-2	2	498	470	21
3	-2	2	228	250	49
4	-2	2	475	553	30
5	-2	2	373	414	24
6	-2	2	363	417	21
7	-2	2	378	403	19
8	-2	2	193	205	25
9	-2	2	115	102	-37
-10	-1	2	216	209	15
-9	-1	2	187	178	13
-8	-1	2	220	208	12
-7	-1	2	24	1	-64
-6	-1	2	323	318	10
-5	-1	2	484	503	14
-4	-1	2	834	839	12
-3	-1	2	659	603	11
-2	-1	2	1176	1189	9
-1	-1	2	330	304	14
0	-1	2	493	421	16
1	-1	2	672	638	25
2	-1	2	1234	1459	26
3	-1	2	760	871	25
4	-1	2	848	933	23
5	-1	2	275	310	18
6	-1	2	88	21	-35
7	-1	2	91	78	-32
8	-1	2	282	309	18
9	-1	2	206	211	22
-10	0	2	66	21	-34
-9	0	2	183	173	13
-8	0	2	322	315	11
-7	0	2	483	468	12
-6	0	2	659	654	14
-5	0	2	237	234	11
-4	0	2	204	210	10
-3	0	2	507	519	12
-2	0	2	1170	1151	11
-1	0	2	1288	1267	16
0	0	2	1393	1761	19
1	0	2	757	921	20
2	0	2	722	801	15
3	0	2	79	28	-26
4	0	2	426	457	14
5	0	2	391	440	16
6	0	2	576	640	15
7	0	2	350	396	17
8	0	2	251	245	17
9	0	2	34	62	-91
-10	1	2	210	202	15
-9	1	2	163	179	16
-8	1	2	199	193	12
-7	1	2	63	83	-25
-6	1	2	292	272	10
-5	1	2	525	546	14
-4	1	2	937	1009	13
-3	1	2	1130	1083	15
-2	1	2	1173	1208	32
-1	1	2	164	164	24

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
0	1	2	251	225	11	8	3	2	224	242	17
1	1	2	524	543	11	9	3	2	230	230	19
2	1	2	1289	1354	11	-9	4	2	197	188	17
3	1	2	848	902	13	-8	4	2	241	247	19
4	1	2	618	637	15	-7	4	2	489	435	18
5	1	2	221	222	13	-6	4	2	471	453	12
6	1	2	27	75	-73	-5	4	2	305	296	10
7	1	2	189	174	16	-4	4	2	78	62	17
8	1	2	301	289	14	-3	4	2	527	499	12
9	1	2	212	206	18	-2	4	2	848	762	10
-10	2	2	66	32	-35	-1	4	2	1203	1123	9
-9	2	2	207	199	14	0	4	2	917	893	10
-8	2	2	251	275	13	1	4	2	725	741	11
-7	2	2	444	488	13	2	4	2	280	287	10
-6	2	2	435	460	12	3	4	2	301	307	12
-5	2	2	144	127	14	4	4	2	375	385	12
-4	2	2	148	174	-38	5	4	2	482	493	12
-3	2	2	586	533	18	6	4	2	382	376	12
-2	2	2	875	829	11	7	4	2	363	345	12
-1	2	2	1387	1307	8	8	4	2	147	162	21
0	2	2	490	537	10	-9	5	2	197	155	38
1	2	2	260	259	9	-8	5	2	36	29	-96
2	2	2	763	811	11	-7	5	2	75	63	-28
3	2	2	340	349	11	-6	5	2	316	305	12
4	2	2	389	408	12	-5	5	2	549	553	17
5	2	2	648	633	16	-4	5	2	423	401	11
6	2	2	558	575	13	-3	5	2	652	590	13
7	2	2	284	304	14	-2	5	2	291	277	10
8	2	2	256	241	16	-1	5	2	92	84	14
9	2	2	68	8	-43	0	5	2	418	388	13
-9	3	2	166	166	15	1	5	2	647	663	12
-8	3	2	85	86	-21	2	5	2	503	515	13
-7	3	2	78	64	-21	3	5	2	868	848	14
-6	3	2	270	272	11	4	5	2	385	370	13
-5	3	2	791	773	15	5	5	2	165	162	14
-4	3	2	604	597	13	6	5	2	27	30	-72
-3	3	2	1059	1013	10	7	5	2	249	238	14
-2	3	2	915	865	9	8	5	2	207	218	18
-1	3	2	78	52	12	-9	6	2	139	129	26
0	3	2	200	196	9	-8	6	2	248	232	15
1	3	2	1023	1075	9	-7	6	2	303	299	13
2	3	2	1097	1108	10	-6	6	2	266	240	11
3	3	2	1141	1140	12	-5	6	2	262	230	10
4	3	2	666	693	14	-4	6	2	192	181	11
5	3	2	168	179	14	-3	6	2	285	282	10
6	3	2	72	54	-26	-2	6	2	737	697	13
7	3	2	248	240	13	-1	6	2	1183	1137	12

Table 66. (continued)

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
0	6	2	740	738	13	-1	9	2	51	56	-34
1	6	2	512	504	15	0	9	2	399	369	12
2	6	2	67	17	-23	1	9	2	467	410	14
3	6	2	205	193	11	2	9	2	507	486	14
4	6	2	449	444	13	3	9	2	372	362	13
5	6	2	548	552	13	4	9	2	241	220	13
6	6	2	346	356	14	5	9	2	28	55	-74
7	6	2	272	270	16	6	9	2	96	102	-28
8	6	2	110	85	23	-6	10	2	134	149	19
-8	7	2	29	8	-76	-5	10	2	27	14	-71
-7	7	2	102	71	22	-4	10	2	104	101	20
-6	7	2	299	289	12	-3	10	2	261	240	13
-5	7	2	490	464	13	-2	10	2	398	376	13
-4	7	2	609	568	16	-1	10	2	416	394	13
-3	7	2	442	422	12	0	10	2	410	388	13
-2	7	2	192	189	11	1	10	2	131	134	17
-1	7	2	89	49	18	2	10	2	26	20	-70
0	7	2	379	379	12	3	10	2	165	142	15
1	7	2	461	462	11	4	10	2	238	247	14
2	7	2	565	557	15	5	10	2	238	230	15
3	7	2	556	526	12	-5	11	2	172	188	17
4	7	2	310	304	13	-4	11	2	197	215	16
5	7	2	171	168	15	-3	11	2	152	152	17
6	7	2	98	96	-24	-2	11	2	95	101	-25
7	7	2	149	152	18	-1	11	2	95	84	-24
-8	8	2	204	193	15	0	11	2	186	180	16
-7	8	2	212	196	15	1	11	2	255	236	13
-6	8	2	206	192	14	2	11	2	308	289	14
-5	8	2	143	117	13	3	11	2	198	202	16
-4	8	2	133	119	13	4	11	2	121	147	23
-3	8	2	223	208	12	-4	12	2	92	65	-25
-2	8	2	479	470	12	-3	12	2	209	177	16
-1	8	2	516	471	12	-2	12	2	239	244	15
0	8	2	498	460	13	-1	12	2	267	248	14
1	8	2	338	318	11	0	12	2	213	192	14
2	8	2	52	29	-31	1	12	2	55	62	-41
3	8	2	159	146	14	2	12	2	45	20	-49
4	8	2	407	405	13	3	12	2	140	147	22
5	8	2	343	334	14	-1	13	2	58	78	-42
6	8	2	240	245	14	-3	-12	3	262	275	15
7	8	2	187	186	18	-2	-12	3	217	227	15
-7	9	2	49	81	-47	-1	-12	3	165	178	18
-6	9	2	239	229	14	0	-12	3	30	75	-80
-5	9	2	271	266	14	1	-12	3	31	86	-84
-4	9	2	389	367	12	2	-12	3	122	134	23
-3	9	2	292	248	11	3	-12	3	177	207	20
-2	9	2	132	132	16	-5	-11	3	229	238	16

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
-4	-11	3	106	135	-24	3	-8	3	347	398	15
-3	-11	3	69	12	-31	4	-8	3	290	310	15
-2	-11	3	75	107	-32	5	-8	3	260	283	18
-1	-11	3	210	235	16	6	-8	3	77	73	-51
0	-11	3	224	246	15	7	-8	3	43	13	-115
1	-11	3	317	334	15	-8	-7	3	207	211	15
2	-11	3	178	193	18	-7	-7	3	265	244	13
3	-11	3	97	75	-29	-6	-7	3	311	319	12
4	-11	3	33	11	-88	-5	-7	3	282	276	12
5	-11	3	112	122	-29	-4	-7	3	144	171	14
-6	-10	3	33	54	-87	-3	-7	3	53	29	-29
-5	-10	3	163	156	17	-2	-7	3	429	443	13
-4	-10	3	221	243	14	-1	-7	3	442	440	13
-3	-10	3	336	354	13	0	-7	3	498	514	12
-2	-10	3	237	254	13	1	-7	3	509	527	13
-1	-10	3	207	209	14	2	-7	3	384	422	13
0	-10	3	27	43	-71	3	-7	3	57	97	-42
1	-10	3	149	127	17	4	-7	3	203	219	18
2	-10	3	247	256	14	5	-7	3	182	234	23
3	-10	3	304	322	15	6	-7	3	291	319	23
4	-10	3	212	236	20	7	-7	3	258	247	29
5	-10	3	170	204	23	8	-7	3	190	141	38
6	-10	3	53	75	-68	-8	-6	3	181	177	16
-7	-9	3	219	224	15	-7	-6	3	27	22	-72
-6	-9	3	266	271	13	-6	-6	3	132	144	14
-5	-9	3	252	248	13	-5	-6	3	335	355	11
-4	-9	3	108	117	19	-4	-6	3	650	676	16
-3	-9	3	39	42	-47	-3	-6	3	609	631	16
-2	-9	3	272	287	13	-2	-6	3	704	739	15
-1	-9	3	381	411	12	-1	-6	3	244	248	12
0	-9	3	469	509	15	0	-6	3	40	60	-47
1	-9	3	532	547	15	1	-6	3	295	302	13
2	-9	3	213	237	15	2	-6	3	832	879	18
3	-9	3	105	120	-25	3	-6	3	568	589	16
4	-9	3	32	89	-84	4	-6	3	483	506	16
5	-9	3	150	170	24	5	-6	3	258	288	22
6	-9	3	167	211	27	6	-6	3	44	69	-117
-7	-8	3	104	87	21	7	-6	3	47	24	-126
-6	-8	3	107	103	21	8	-6	3	192	173	27
-5	-8	3	169	175	15	-9	-5	3	167	134	18
-4	-8	3	450	486	14	-8	-5	3	256	259	14
-3	-8	3	513	552	13	-7	-5	3	369	368	13
-2	-8	3	426	436	13	-6	-5	3	567	558	12
-1	-8	3	310	312	12	-5	-5	3	318	314	11
0	-8	3	81	34	-23	-4	-5	3	212	219	11
1	-8	3	96	102	-22	-3	-5	3	277	286	11
2	-8	3	396	432	13	-2	-5	3	578	538	15

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
-1	-5	3	550	532	15	9	-3	3	92	35	-68
0	-5	3	1030	1050	13	-9	-2	3	227	230	14
1	-5	3	632	618	16	-8	-2	3	152	154	15
2	-5	3	474	489	15	-7	-2	3	81	56	-22
3	-5	3	36	8	-95	-6	-2	3	202	194	11
4	-5	3	183	185	26	-5	-2	3	734	762	14
5	-5	3	275	264	26	-4	-2	3	910	908	13
6	-5	3	519	456	18	-3	-2	3	1212	1207	12
7	-5	3	239	269	24	-2	-2	3	761	772	12
8	-5	3	184	204	28	-1	-2	3	127	130	14
-9	-4	3	230	203	15	0	-2	3	202	180	16
-8	-4	3	195	194	13	1	-2	3	1364	1244	18
-7	-4	3	91	40	19	2	-2	3	950	906	21
-6	-4	3	103	120	16	3	-2	3	817	815	25
-5	-4	3	355	361	12	4	-2	3	587	630	26
-4	-4	3	629	625	14	5	-2	3	180	266	-43
-3	-4	3	811	820	13	6	-2	3	156	96	35
-2	-4	3	629	663	13	7	-2	3	134	222	-41
-1	-4	3	147	184	13	8	-2	3	153	170	-35
0	-4	3	148	140	14	9	-2	3	168	215	33
1	-4	3	647	624	16	-10	-1	3	29	45	-76
2	-4	3	797	816	19	-9	-1	3	171	171	14
3	-4	3	726	759	18	-8	-1	3	307	306	11
4	-4	3	669	576	20	-7	-1	3	486	490	13
5	-4	3	254	231	20	-6	-1	3	356	358	12
6	-4	3	140	131	-33	-5	-1	3	515	496	15
7	-4	3	124	131	-60	-4	-1	3	107	106	16
8	-4	3	183	190	-52	-3	-1	3	552	523	13
9	-4	3	178	167	-45	-2	-1	3	690	668	13
-9	-3	3	166	167	15	-1	-1	3	396	401	13
-8	-3	3	254	273	13	0	-1	3	720	567	22
-7	-3	3	465	472	13	1	-1	3	1942	1716	20
-6	-3	3	366	378	10	2	-1	3	286	320	26
-5	-3	3	312	319	10	3	-1	3	208	208	27
-4	-3	3	271	270	10	4	-1	3	245	249	25
-3	-3	3	640	673	13	5	-1	3	556	613	21
-2	-3	3	708	727	12	6	-1	3	397	455	18
-1	-3	3	1045	1035	12	7	-1	3	386	432	18
0	-3	3	1336	1245	12	8	-1	3	162	187	28
1	-3	3	859	810	16	9	-1	3	89	22	-46
2	-3	3	586	559	17	-10	0	3	172	155	17
3	-3	3	226	171	34	-9	0	3	221	219	13
4	-3	3	243	203	24	-8	0	3	101	88	17
5	-3	3	546	515	25	-7	0	3	57	28	-28
6	-3	3	562	565	26	-6	0	3	375	382	12
7	-3	3	274	299	31	-5	0	3	577	607	15
8	-3	3	205	220	37	-4	0	3	718	784	15

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
-3	0	3	1308	1266	14	4	2	3	407	439	14
-2	0	3	524	460	14	5	2	3	348	376	13
-1	0	3	405	359	21	6	2	3	127	128	19
0	0	3	376	419	28	7	2	3	192	191	17
1	0	3	1449	1643	19	8	2	3	278	270	16
2	0	3	1039	1199	18	9	2	3	223	227	19
3	0	3	879	967	19	-9	3	3	152	156	16
4	0	3	448	475	17	-8	3	3	318	328	12
5	0	3	295	308	15	-7	3	3	341	327	12
6	0	3	32	3	-86	-6	3	3	417	423	20
7	0	3	273	246	16	-5	3	3	229	218	23
8	0	3	187	216	22	-4	3	3	197	205	17
9	0	3	229	248	21	-3	3	3	381	371	11
-10	1	3	83	98	-28	-2	3	3	1179	1117	11
-9	1	3	171	170	14	-1	3	3	1254	1213	10
-8	1	3	360	370	13	0	3	3	1050	1035	11
-7	1	3	541	551	13	1	3	3	514	552	13
-6	1	3	352	382	11	2	3	3	39	33	-36
-5	1	3	362	345	14	3	3	3	184	182	13
-4	1	3	156	168	19	4	3	3	656	662	16
-3	1	3	563	444	18	5	3	3	521	516	13
-2	1	3	925	1073	33	6	3	3	427	426	13
-1	1	3	1226	1532	18	7	3	3	340	317	14
0	1	3	741	829	15	8	3	3	99	111	-29
1	1	3	875	955	14	-9	4	3	114	105	20
2	1	3	110	112	20	-8	4	3	90	42	-25
3	1	3	114	38	21	-7	4	3	95	123	-42
4	1	3	372	368	16	-6	4	3	441	445	12
5	1	3	618	627	14	-5	4	3	592	580	17
6	1	3	491	492	16	-4	4	3	822	767	14
7	1	3	389	420	17	-3	4	3	523	520	14
8	1	3	130	116	27	-2	4	3	403	405	13
9	1	3	71	36	-46	-1	4	3	86	56	16
-10	2	3	202	193	15	0	4	3	630	619	12
-9	2	3	163	166	14	1	4	3	577	573	12
-8	2	3	25	67	-66	2	4	3	849	872	12
-7	2	3	24	19	-64	3	4	3	705	710	14
-6	2	3	357	361	12	4	4	3	510	504	12
-5	2	3	530	463	18	5	4	3	138	154	16
-4	2	3	799	941	27	6	4	3	136	118	17
-3	2	3	639	724	17	7	4	3	171	173	17
-2	2	3	381	377	13	8	4	3	281	289	16
-1	2	3	560	544	13	-9	5	3	183	174	29
0	2	3	420	425	13	-8	5	3	283	276	13
1	2	3	488	482	13	-7	5	3	309	290	11
2	2	3	1157	1216	12	-6	5	3	405	418	13
3	2	3	890	875	15	-5	5	3	112	114	15

Table 66. (continued)

H	K	L	$10F_o$	$10F_c$	10σ
-4	5	3	102	94	16
-3	5	3	431	383	10
-2	5	3	617	597	13
-1	5	3	809	796	13
0	5	3	1164	1138	12
1	5	3	257	240	10
2	5	3	66	49	-24
3	5	3	235	235	13
4	5	3	485	498	13
5	5	3	368	384	13
6	5	3	489	460	12
7	5	3	232	233	16
8	5	3	104	97	-28
-9	6	3	112	84	20
-8	6	3	27	35	-71
-7	6	3	169	158	15
-6	6	3	219	244	13
-5	6	3	416	441	13
-4	6	3	545	522	16
-3	6	3	403	364	11
-2	6	3	385	369	11
-1	6	3	225	178	11
0	6	3	456	468	16
1	6	3	598	581	15
2	6	3	645	671	15
3	6	3	533	530	19
4	6	3	428	402	13
5	6	3	27	44	-71
6	6	3	109	90	24
7	6	3	220	197	15
8	6	3	242	235	18
-8	7	3	205	212	15
-7	7	3	244	246	13
-6	7	3	201	209	13
-5	7	3	59	37	-26
-4	7	3	124	123	16
-3	7	3	497	466	12
-2	7	3	636	621	15
-1	7	3	717	687	15
0	7	3	492	499	16
1	7	3	168	163	12
2	7	3	51	72	-31
3	7	3	295	274	11
4	7	3	391	376	12
5	7	3	396	398	13
6	7	3	306	301	15
7	7	3	114	141	-27

H	K	L	$10F_o$	$10F_c$	10σ
-8	8	3	28	11	-75
-7	8	3	121	122	20
-6	8	3	210	210	13
-5	8	3	409	388	12
-4	8	3	335	330	12
-3	8	3	320	308	12
-2	8	3	208	210	12
-1	8	3	116	110	16
0	8	3	235	231	11
1	8	3	574	519	12
2	8	3	508	469	13
3	8	3	436	420	15
4	8	3	280	266	13
5	8	3	40	9	-52
6	8	3	99	74	-26
-7	9	3	172	193	17
-6	9	3	96	113	-23
-5	9	3	27	24	-71
-4	9	3	129	112	16
-3	9	3	346	317	12
-2	9	3	415	395	11
-1	9	3	503	478	14
0	9	3	330	305	13
1	9	3	175	164	14
2	9	3	27	33	-71
3	9	3	278	262	14
4	9	3	281	267	14
5	9	3	286	279	16
6	9	3	184	199	18
-6	10	3	170	195	16
-5	10	3	232	248	14
-4	10	3	225	219	13
-3	10	3	248	229	14
-2	10	3	69	56	-29
-1	10	3	144	121	16
0	10	3	275	264	13
1	10	3	359	343	13
2	10	3	312	305	13
3	10	3	314	294	14
4	10	3	119	112	20
5	10	3	78	2	-32
-5	11	3	28	5	-75
-4	11	3	107	111	24
-3	11	3	211	186	15
-2	11	3	305	289	14
-1	11	3	331	323	13
0	11	3	205	167	15

H	K	L	10F$_o$	10F$_c$	10σ	H	K	L	10F$_o$	10F$_c$	10σ
1	11	3	99	92	-24	0	-9	4	82	40	-25
2	11	3	85	57	-30	1	-9	4	242	258	14
3	11	3	157	153	19	2	-9	4	293	314	15
4	11	3	208	208	16	3	-9	4	287	333	17
-4	12	3	145	147	19	4	-9	4	283	315	18
-3	12	3	128	123	21	5	-9	4	119	143	-34
-2	12	3	29	13	-76	6	-9	4	91	99	-49
-1	12	3	108	81	24	-7	-8	4	281	288	15
0	12	3	208	191	18	-6	-8	4	257	274	13
1	12	3	219	217	17	-5	-8	4	202	222	14
2	12	3	230	223	16	-4	-8	4	139	150	15
-3	-12	4	43	1	-56	-3	-8	4	131	145	16
-2	-12	4	113	138	-26	-2	-8	4	249	245	13
-1	-12	4	189	197	17	-1	-8	4	530	555	15
0	-12	4	260	276	16	0	-8	4	478	507	15
1	-12	4	192	207	19	1	-8	4	352	375	15
2	-12	4	136	149	26	2	-8	4	270	299	16
3	-12	4	96	68	-34	3	-8	4	31	7	-82
-5	-11	4	136	154	23	4	-8	4	85	97	-39
-4	-11	4	227	276	16	5	-8	4	214	250	22
-3	-11	4	219	241	16	6	-8	4	246	248	24
-2	-11	4	234	263	16	7	-8	4	186	191	34
-1	-11	4	81	132	-33	-8	-7	4	117	112	19
0	-11	4	30	26	-80	-7	-7	4	27	31	-71
1	-11	4	75	86	-35	-6	-7	4	61	78	-30
2	-11	4	195	222	19	-5	-7	4	369	370	12
3	-11	4	165	204	22	-4	-7	4	442	454	14
4	-11	4	189	219	22	-3	-7	4	523	548	13
-6	-10	4	244	245	16	-2	-7	4	407	436	14
-5	-10	4	166	186	18	-1	-7	4	203	231	14
-4	-10	4	129	125	19	0	-7	4	27	25	-72
-3	-10	4	69	42	-29	1	-7	4	361	398	13
-2	-10	4	128	155	19	2	-7	4	400	416	15
-1	-10	4	247	269	14	3	-7	4	485	530	15
0	-10	4	370	415	16	4	-7	4	392	403	17
1	-10	4	299	326	16	5	-7	4	196	212	26
2	-10	4	231	239	17	6	-7	4	108	90	-51
3	-10	4	32	29	-85	7	-7	4	118	91	-58
4	-10	4	35	75	-93	-8	-6	4	192	206	16
5	-10	4	156	134	25	-7	-6	4	330	316	12
-7	-9	4	29	16	-78	-6	-6	4	297	305	12
-6	-9	4	73	57	-29	-5	-6	4	392	408	11
-5	-9	4	237	243	14	-4	-6	4	24	41	-65
-4	-9	4	309	316	12	-3	-6	4	240	220	12
-3	-9	4	370	400	14	-2	-6	4	386	386	14
-2	-9	4	344	396	15	-1	-6	4	764	777	18
-1	-9	4	113	143	20	0	-6	4	578	586	19

H	K	L	$10F_o$	$10F_c$	10σ
1	-6	4	744	753	19
2	-6	4	322	318	17
3	-6	4	111	20	-29
4	-6	4	173	167	25
5	-6	4	418	415	21
6	-6	4	275	254	26
7	-6	4	294	274	19
8	-6	4	156	140	25
-9	-5	4	202	204	16
-8	-5	4	51	93	-41
-7	-5	4	25	29	-67
-6	-5	4	267	268	12
-5	-5	4	500	491	12
-4	-5	4	571	580	16
-3	-5	4	746	755	16
-2	-5	4	380	381	13
-1	-5	4	321	353	12
0	-5	4	271	237	14
1	-5	4	590	591	14
2	-5	4	578	578	17
3	-5	4	596	610	20
4	-5	4	321	351	21
5	-5	4	342	297	21
6	-5	4	70	15	-53
7	-5	4	128	97	-30
8	-5	4	120	147	-38
-9	-4	4	98	126	-26
-8	-4	4	300	299	12
-7	-4	4	388	393	12
-6	-4	4	373	384	11
-5	-4	4	347	356	11
-4	-4	4	58	8	-30
-3	-4	4	176	168	13
-2	-4	4	544	527	16
-1	-4	4	803	831	15
0	-4	4	1070	1053	16
1	-4	4	840	795	18
2	-4	4	131	149	-37
3	-4	4	130	75	-46
4	-4	4	334	293	19
5	-4	4	522	513	15
6	-4	4	446	433	16
7	-4	4	328	329	24
8	-4	4	189	121	-45
-9	-3	4	176	184	16
-8	-3	4	97	109	-23
-7	-3	4	24	7	-64
-6	-3	4	342	332	11
-5	-3	4	401	420	13
-4	-3	4	949	963	14
-3	-3	4	919	898	14
-2	-3	4	410	388	12
-1	-3	4	366	379	13
0	-3	4	658	598	18
1	-3	4	664	592	23
2	-3	4	1136	937	25
3	-3	4	828	752	25
4	-3	4	360	389	20
5	-3	4	376	399	23
6	-3	4	187	66	-47
7	-3	4	81	106	-92
8	-3	4	191	193	41
-9	-2	4	126	153	19
-8	-2	4	381	385	13
-7	-2	4	361	358	12
-6	-2	4	398	420	13
-5	-2	4	282	288	12
-4	-2	4	39	41	-44
-3	-2	4	319	281	13
-2	-2	4	1116	1077	14
-1	-2	4	669	635	17
0	-2	4	1130	1052	20
1	-2	4	1121	847	23
2	-2	4	256	262	21
3	-2	4	48	25	-127
4	-2	4	444	488	27
5	-2	4	405	444	26
6	-2	4	517	531	23
7	-2	4	220	287	32
8	-2	4	127	122	-46
9	-2	4	45	54	-120
-10	-1	4	190	190	17
-9	-1	4	132	153	19
-8	-1	4	152	156	15
-7	-1	4	50	75	-36
-6	-1	4	390	385	11
-5	-1	4	619	615	18
-4	-1	4	848	870	15
-3	-1	4	753	739	16
-2	-1	4	787	688	17
-1	-1	4	188	126	22
0	-1	4	515	430	15
1	-1	4	894	809	24
2	-1	4	1013	1131	33

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
3	-1	4	625	672	27	-9	2	4	236	225	13
4	-1	4	577	608	22	-8	2	4	309	301	13
5	-1	4	227	221	25	-7	2	4	485	457	13
6	-1	4	41	79	-109	-6	2	4	373	338	14
7	-1	4	192	162	26	-5	2	4	110	101	-54
8	-1	4	242	268	24	-4	2	4	52	21	-138
9	-1	4	175	187	29	-3	2	4	473	539	20
-10	0	4	108	55	22	-2	2	4	996	899	19
-9	0	4	205	206	14	-1	2	4	1337	1423	15
-8	0	4	349	333	13	0	2	4	595	582	16
-7	0	4	405	400	12	1	2	4	292	299	13
-6	0	4	492	511	13	2	2	4	303	333	12
-5	0	4	107	81	21	3	2	4	410	449	15
-4	0	4	60	51	-39	4	2	4	493	483	15
-3	0	4	480	445	15	5	2	4	609	607	15
-2	0	4	1506	1190	21	6	2	4	502	477	14
-1	0	4	1092	871	21	7	2	4	252	231	17
0	0	4	1334	1455	24	8	2	4	136	141	27
1	0	4	868	800	25	-9	3	4	164	131	17
2	0	4	279	266	24	-8	3	4	31	29	-82
3	0	4	270	295	21	-7	3	4	194	162	22
4	0	4	530	558	20	-6	3	4	238	291	32
5	0	4	389	399	19	-5	3	4	569	670	20
6	0	4	557	586	17	-4	3	4	667	659	16
7	0	4	286	301	20	-3	3	4	666	674	18
8	0	4	129	143	-35	-2	3	4	420	426	12
9	0	4	39	2	-103	-1	3	4	265	260	11
-10	1	4	201	171	15	0	3	4	268	254	11
-9	1	4	128	137	18	1	3	4	869	905	13
-8	1	4	99	113	21	2	3	4	974	983	15
-7	1	4	203	195	13	3	3	4	803	781	16
-6	1	4	307	332	13	4	3	4	502	477	13
-5	1	4	663	628	22	5	3	4	70	82	-31
-4	1	4	865	830	22	6	3	4	30	48	-80
-3	1	4	794	758	30	7	3	4	283	273	15
-2	1	4	746	796	25	8	3	4	212	230	19
-1	1	4	333	322	19	-9	4	4	201	200	19
0	1	4	275	289	17	-8	4	4	286	262	25
1	1	4	712	755	19	-7	4	4	345	388	22
2	1	4	874	951	18	-6	4	4	286	259	16
3	1	4	616	644	24	-5	4	4	178	168	17
4	1	4	544	593	16	-4	4	4	191	169	15
5	1	4	134	115	21	-3	4	4	675	655	16
6	1	4	32	16	-86	-2	4	4	695	692	14
7	1	4	249	249	18	-1	4	4	1018	999	13
8	1	4	271	269	19	0	4	4	614	618	14
9	1	4	177	175	26	1	4	4	503	495	16

H	K	L	$10F_o$	$10F_c$	10σ
2	4	4	39	49	-47
3	4	4	392	386	14
4	4	4	349	365	13
5	4	4	487	503	16
6	4	4	314	328	15
7	4	4	269	255	15
8	4	4	96	91	-32
-9	5	4	132	123	-43
-8	5	4	34	19	-92
-7	5	4	173	146	17
-6	5	4	328	352	14
-5	5	4	429	422	14
-4	5	4	485	470	12
-3	5	4	683	657	15
-2	5	4	114	95	18
-1	5	4	109	99	15
0	5	4	443	455	16
1	5	4	728	695	15
2	5	4	661	645	16
3	5	4	699	675	17
4	5	4	202	209	13
5	5	4	52	62	-41
6	5	4	122	124	22
7	5	4	278	261	15
8	5	4	214	203	19
-9	6	4	146	141	20
-8	6	4	259	245	14
-7	6	4	272	274	15
-6	6	4	119	143	17
-5	6	4	90	87	19
-4	6	4	220	219	12
-3	6	4	531	492	17
-2	6	4	720	669	15
-1	6	4	713	687	15
0	6	4	489	481	18
1	6	4	363	348	13
2	6	4	124	125	16
3	6	4	294	272	11
4	6	4	370	366	13
5	6	4	432	449	14
6	6	4	321	318	16
7	6	4	192	207	19
-8	7	4	44	26	-46
-7	7	4	135	125	17
-6	7	4	307	298	12
-5	7	4	346	339	12
-4	7	4	501	465	13
-3	7	4	473	462	12
-2	7	4	106	79	17
-1	7	4	98	100	18
0	7	4	409	397	16
1	7	4	537	501	12
2	7	4	611	596	18
3	7	4	475	446	14
4	7	4	163	163	16
5	7	4	56	61	-42
6	7	4	166	153	19
7	7	4	181	180	19
-8	8	4	201	204	15
-7	8	4	187	177	15
-6	8	4	141	118	16
-5	8	4	25	16	-66
-4	8	4	164	165	14
-3	8	4	353	341	12
-2	8	4	576	552	18
-1	8	4	292	302	12
0	8	4	294	270	13
1	8	4	225	217	13
2	8	4	95	104	21
3	8	4	220	223	14
4	8	4	343	360	15
5	8	4	290	278	14
6	8	4	229	214	18
-7	9	4	140	111	17
-6	9	4	233	222	14
-5	9	4	253	232	12
-4	9	4	311	295	12
-3	9	4	214	208	12
-2	9	4	46	60	-38
-1	9	4	134	127	15
0	9	4	344	334	13
1	9	4	453	413	15
2	9	4	500	464	15
3	9	4	287	274	14
4	9	4	115	123	23
5	9	4	30	6	-79
-6	10	4	80	92	-28
-5	10	4	49	33	-40
-4	10	4	156	135	15
-3	10	4	302	276	13
-2	10	4	412	381	14
-1	10	4	307	298	13
0	10	4	240	252	14
1	10	4	52	68	-46

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
2	10	4	88	76	-27	-3	-9	5	93	48	-23
3	10	4	200	187	17	-2	-9	5	300	303	14
4	10	4	254	235	16	-1	-9	5	370	419	15
5	10	4	213	191	17	0	-9	5	464	487	14
-5	11	4	147	172	18	1	-9	5	368	381	14
-4	11	4	180	187	16	2	-9	5	101	115	-28
-3	11	4	95	104	-25	3	-9	5	83	63	-38
-2	11	4	28	28	-75	4	-9	5	162	140	26
-1	11	4	165	128	16	5	-9	5	189	188	25
0	11	4	193	190	17	6	-9	5	171	195	34
1	11	4	272	241	14	-7	-8	5	28	24	-75
2	11	4	296	267	14	-6	-8	5	140	153	19
3	11	4	162	156	19	-5	-8	5	215	230	14
-3	12	4	202	188	18	-4	-8	5	421	445	13
-2	12	4	247	222	16	-3	-8	5	401	407	13
-1	12	4	217	203	17	-2	-8	5	297	326	13
0	12	4	155	130	19	-1	-8	5	243	249	15
1	12	4	31	12	-83	0	-8	5	131	148	23
2	12	4	47	62	-57	1	-8	5	197	216	19
-2	-12	5	163	184	21	2	-8	5	334	336	15
-1	-12	5	102	121	-29	3	-8	5	316	361	17
0	-12	5	32	17	-86	4	-8	5	281	302	20
1	-12	5	35	109	-92	5	-8	5	182	193	31
2	-12	5	135	145	26	6	-8	5	45	9	-121
-4	-11	5	68	65	-35	-8	-7	5	212	212	14
-3	-11	5	30	42	-80	-7	-7	5	223	221	14
-2	-11	5	143	149	20	-6	-7	5	296	296	13
-1	-11	5	236	265	17	-5	-7	5	234	232	12
0	-11	5	210	229	19	-4	-7	5	64	54	-29
1	-11	5	238	261	19	-3	-7	5	136	139	18
2	-11	5	121	135	-29	-2	-7	5	400	421	13
3	-11	5	60	24	-57	-1	-7	5	455	477	15
4	-11	5	36	52	-97	0	-7	5	628	632	15
-5	-10	5	176	193	17	1	-7	5	340	348	14
-4	-10	5	229	241	15	2	-7	5	175	159	22
-3	-10	5	251	290	17	3	-7	5	51	63	-67
-2	-10	5	197	208	17	4	-7	5	276	286	21
-1	-10	5	171	167	17	5	-7	5	288	272	25
0	-10	5	31	45	-82	6	-7	5	327	283	24
1	-10	5	157	171	21	7	-7	5	228	180	22
2	-10	5	222	253	19	-8	-6	5	117	114	21
3	-10	5	273	304	18	-7	-6	5	27	48	-72
4	-10	5	178	192	25	-6	-6	5	187	192	14
5	-10	5	125	154	-35	-5	-6	5	423	434	12
-6	-9	5	261	255	15	-4	-6	5	609	649	18
-5	-9	5	205	206	16	-3	-6	5	377	372	12
-4	-9	5	27	22	-73	-2	-6	5	452	480	15

H	K	L	$10F_o$	$10F_c$	10σ
-1	-6	5	147	155	18
0	-6	5	239	215	16
1	-6	5	463	469	14
2	-6	5	607	595	18
3	-6	5	418	396	16
4	-6	5	577	523	19
5	-6	5	169	171	37
6	-6	5	69	12	-53
7	-6	5	61	59	-55
-9	-5	5	165	160	18
-8	-5	5	270	253	12
-7	-5	5	302	307	12
-6	-5	5	432	446	12
-5	-5	5	251	259	12
-4	-5	5	83	95	-21
-3	-5	5	335	327	13
-2	-5	5	498	480	14
-1	-5	5	675	663	18
0	-5	5	1032	1010	18
1	-5	5	523	488	17
2	-5	5	243	215	23
3	-5	5	113	49	-41
4	-5	5	362	290	22
5	-5	5	416	375	15
6	-5	5	321	345	16
7	-5	5	190	198	21
8	-5	5	168	141	26
-9	-4	5	160	167	19
-8	-4	5	122	120	18
-7	-4	5	97	109	-22
-6	-4	5	221	212	13
-5	-4	5	483	497	13
-4	-4	5	605	626	18
-3	-4	5	488	481	13
-2	-4	5	448	416	14
-1	-4	5	67	41	-39
0	-4	5	199	190	20
1	-4	5	762	681	24
2	-4	5	706	581	20
3	-4	5	535	435	17
4	-4	5	572	558	17
5	-4	5	102	143	-30
6	-4	5	36	8	-96
7	-4	5	160	142	31
8	-4	5	204	194	33
-9	-3	5	206	198	14
-8	-3	5	253	252	13

H	K	L	$10F_o$	$10F_c$	10σ
-7	-3	5	409	408	13
-6	-3	5	294	303	11
-5	-3	5	191	185	12
-4	-3	5	91	95	-23
-3	-3	5	576	550	19
-2	-3	5	569	557	18
-1	-3	5	1292	1287	17
0	-3	5	1191	1048	20
1	-3	5	492	379	19
2	-3	5	362	312	18
3	-3	5	294	263	18
4	-3	5	319	306	15
5	-3	5	575	601	18
6	-3	5	448	419	24
7	-3	5	158	199	-58
8	-3	5	172	158	-43
-9	-2	5	188	180	14
-8	-2	5	66	63	-29
-7	-2	5	88	102	-22
-6	-2	5	271	279	12
-5	-2	5	779	776	17
-4	-2	5	834	814	17
-3	-2	5	816	817	17
-2	-2	5	399	395	16
-1	-2	5	52	6	-61
0	-2	5	387	283	20
1	-2	5	816	746	19
2	-2	5	647	667	21
3	-2	5	746	791	19
4	-2	5	499	469	24
5	-2	5	168	180	-44
6	-2	5	49	18	-132
7	-2	5	168	210	-43
8	-2	5	147	178	-44
-9	-1	5	206	207	15
-8	-1	5	312	289	13
-7	-1	5	428	416	13
-6	-1	5	324	330	11
-5	-1	5	284	272	15
-4	-1	5	143	133	19
-3	-1	5	457	426	16
-2	-1	5	654	578	22
-1	-1	5	1321	1028	20
0	-1	5	738	711	18
1	-1	5	621	646	16
2	-1	5	259	140	34
3	-1	5	281	340	32

H	K	L	$10F_o$	$10F_c$	10σ
4	-1	5	337	397	26
5	-1	5	519	578	24
6	-1	5	294	353	25
7	-1	5	212	272	31
8	-1	5	72	121	-72
-9	0	5	142	166	19
-8	0	5	27	13	-72
-7	0	5	110	80	20
-6	0	5	402	416	13
-5	0	5	715	657	21
-4	0	5	542	542	16
-3	0	5	926	881	23
-2	0	5	296	282	17
-1	0	5	110	30	-36
0	0	5	669	725	22
1	0	5	859	978	19
2	0	5	587	669	22
3	0	5	957	989	28
4	0	5	305	352	22
5	0	5	126	157	-34
6	0	5	73	95	-54
7	0	5	207	250	24
8	0	5	211	205	27
-9	1	5	198	202	15
-8	1	5	344	347	14
-7	1	5	446	410	14
-6	1	5	388	368	15
-5	1	5	262	218	20
-4	1	5	474	415	20
-3	1	5	451	478	16
-2	1	5	1018	987	30
-1	1	5	1067	1208	24
0	1	5	799	869	25
1	1	5	513	548	18
2	1	5	108	81	-32
3	1	5	153	170	30
4	1	5	475	527	16
5	1	5	490	523	16
6	1	5	367	395	18
7	1	5	257	302	22
8	1	5	38	52	-101
-9	2	5	158	125	19
-8	2	5	46	15	-56
-7	2	5	124	112	-29
-6	2	5	403	364	17
-5	2	5	522	520	18
-4	2	5	618	737	26
-3	2	5	458	542	21
-2	2	5	299	328	18
-1	2	5	34	93	-90
0	2	5	593	651	20
1	2	5	556	613	15
2	2	5	735	801	19
3	2	5	665	684	22
4	2	5	301	319	15
5	2	5	166	152	19
6	2	5	157	190	22
7	2	5	200	206	21
8	2	5	250	232	19
-9	3	5	180	172	21
-8	3	5	361	319	17
-7	3	5	297	241	24
-6	3	5	245	269	32
-5	3	5	150	136	-33
-4	3	5	342	343	19
-3	3	5	436	467	16
-2	3	5	898	955	18
-1	3	5	735	731	20
0	3	5	570	611	18
1	3	5	428	437	14
2	3	5	90	80	-27
3	3	5	240	222	15
4	3	5	574	623	16
5	3	5	456	480	15
6	3	5	375	365	15
7	3	5	248	221	19
8	3	5	56	45	-62
-9	4	5	94	68	-47
-8	4	5	151	2	-41
-7	4	5	179	191	31
-6	4	5	366	406	18
-5	4	5	502	546	15
-4	4	5	759	771	21
-3	4	5	396	389	13
-2	4	5	272	240	14
-1	4	5	169	166	15
0	4	5	615	626	18
1	4	5	781	787	16
2	4	5	875	898	17
3	4	5	442	426	15
4	4	5	304	299	13
5	4	5	29	31	-77
6	4	5	154	177	21
7	4	5	182	186	21

H	K	L	$10F_o$	$10F_c$	10σ
8	4	5	236	244	20
-9	5	5	176	186	33
-8	5	5	218	263	24
-7	5	5	253	244	16
-6	5	5	229	226	16
-5	5	5	28	4	-75
-4	5	5	185	172	14
-3	5	5	515	496	13
-2	5	5	559	530	17
-1	5	5	474	470	12
0	5	5	633	677	17
1	5	5	232	227	13
2	5	5	26	30	-69
3	5	5	293	266	12
4	5	5	417	407	13
5	5	5	369	365	13
6	5	5	372	378	16
7	5	5	113	154	-33
-8	6	5	32	6	-85
-7	6	5	166	178	19
-6	6	5	260	251	14
-5	6	5	353	356	13
-4	6	5	511	511	13
-3	6	5	364	338	11
-2	6	5	163	139	13
-1	6	5	282	284	13
0	6	5	484	464	13
1	6	5	680	639	18
2	6	5	665	648	18
3	6	5	331	329	14
4	6	5	209	208	14
5	6	5	89	45	-29
6	6	5	185	149	19
7	6	5	189	204	21
-8	7	5	181	189	17
-7	7	5	199	206	16
-6	7	5	116	114	20
-5	7	5	39	75	-50
-4	7	5	211	195	12
-3	7	5	529	519	13
-2	7	5	537	507	13
-1	7	5	483	469	13
0	7	5	388	364	11
1	7	5	124	102	16
2	7	5	75	45	-25
3	7	5	330	310	12
4	7	5	344	319	13
5	7	5	388	353	14
6	7	5	282	264	16
-7	8	5	147	135	19
-6	8	5	218	218	15
-5	8	5	352	339	13
-4	8	5	307	289	12
-3	8	5	273	249	12
-2	8	5	26	63	-70
-1	8	5	174	173	14
0	8	5	278	268	12
1	8	5	516	502	15
2	8	5	456	414	13
3	8	5	301	284	14
4	8	5	137	133	21
5	8	5	31	52	-83
6	8	5	80	110	-40
-7	9	5	170	142	17
-6	9	5	94	69	-24
-5	9	5	27	26	-72
-4	9	5	144	156	16
-3	9	5	345	322	12
-2	9	5	359	336	13
-1	9	5	384	342	13
0	9	5	225	214	13
1	9	5	94	85	-25
2	9	5	106	109	23
3	9	5	301	268	15
4	9	5	268	240	15
5	9	5	264	242	17
-6	10	5	185	184	16
-5	10	5	238	232	14
-4	10	5	181	176	16
-3	10	5	102	135	-24
-2	10	5	28	30	-73
-1	10	5	188	156	16
0	10	5	305	279	14
1	10	5	364	345	14
2	10	5	272	258	14
3	10	5	213	197	19
4	10	5	32	48	-85
-5	11	5	49	25	-44
-4	11	5	136	139	21
-3	11	5	181	194	17
-2	11	5	262	245	15
-1	11	5	277	247	14
0	11	5	134	125	21
1	11	5	45	39	-57

H	K	L	$10F_o$	$10F_c$	10σ
2	11	5	134	99	22
3	11	5	173	158	20
-3	12	5	72	71	-36
-2	12	5	30	32	-81
-1	12	5	94	102	-31
0	12	5	199	186	18
1	12	5	218	202	17
-1	-12	6	188	200	20
0	-12	6	186	217	22
1	-12	6	146	149	26
-4	-11	6	226	244	16
-3	-11	6	189	213	19
-2	-11	6	232	230	16
-1	-11	6	32	70	-86
0	-11	6	34	31	-91
1	-11	6	122	102	-28
2	-11	6	239	226	19
3	-11	6	191	203	24
-5	-10	6	120	127	23
-4	-10	6	45	61	-51
-3	-10	6	58	88	-45
-2	-10	6	187	197	17
-1	-10	6	264	292	16
0	-10	6	291	318	16
1	-10	6	206	207	20
2	-10	6	161	173	25
3	-10	6	37	29	-98
4	-10	6	92	111	-48
-6	-9	6	114	104	24
-5	-9	6	250	253	15
-4	-9	6	229	256	16
-3	-9	6	304	307	13
-2	-9	6	292	304	16
-1	-9	6	32	55	-84
0	-9	6	32	62	-85
1	-9	6	222	257	20
2	-9	6	278	288	18
3	-9	6	274	316	20
4	-9	6	262	251	21
5	-9	6	119	82	-42
-7	-8	6	240	269	16
-6	-8	6	220	236	15
-5	-8	6	160	148	17
-4	-8	6	52	58	-40
-3	-8	6	208	207	15
-2	-8	6	281	315	16
-1	-8	6	553	562	17
0	-8	6	401	438	16
1	-8	6	262	232	16
2	-8	6	212	188	19
3	-8	6	94	67	-39
4	-8	6	108	150	-48
5	-8	6	276	244	24
6	-8	6	219	204	31
-7	-7	6	54	24	-42
-6	-7	6	134	142	20
-5	-7	6	336	354	13
-4	-7	6	348	372	14
-3	-7	6	444	453	13
-2	-7	6	284	278	15
-1	-7	6	95	99	-27
0	-7	6	117	95	25
1	-7	6	341	344	17
2	-7	6	303	318	17
3	-7	6	522	507	19
4	-7	6	345	302	21
5	-7	6	145	118	-41
6	-7	6	37	25	-98
-8	-6	6	199	197	15
-7	-6	6	279	289	14
-6	-6	6	219	231	14
-5	-6	6	275	267	12
-4	-6	6	27	29	-72
-3	-6	6	271	259	14
-2	-6	6	480	489	17
-1	-6	6	689	699	15
0	-6	6	508	467	14
1	-6	6	503	487	16
2	-6	6	121	108	-35
3	-6	6	148	129	-34
4	-6	6	330	267	22
5	-6	6	348	339	17
6	-6	6	222	210	19
7	-6	6	217	202	17
-8	-5	6	28	36	-75
-7	-5	6	28	51	-74
-6	-5	6	340	333	14
-5	-5	6	471	483	15
-4	-5	6	466	478	15
-3	-5	6	596	584	14
-2	-5	6	245	221	16
-1	-5	6	95	75	-35
0	-5	6	278	248	18
1	-5	6	541	501	21

H	K	L	$10F_o$	$10F_c$	10σ
2	−5	6	586	497	18
3	−5	6	740	574	21
4	−5	6	366	308	15
5	−5	6	177	164	18
6	−5	6	33	28	−87
7	−5	6	100	139	−34
−9	−4	6	155	141	20
−8	−4	6	273	282	14
−7	−4	6	339	353	13
−6	−4	6	312	313	12
−5	−4	6	203	222	13
−4	−4	6	91	82	−23
−3	−4	6	222	202	16
−2	−4	6	705	715	20
−1	−4	6	775	755	22
0	−4	6	729	642	17
1	−4	6	731	616	20
2	−4	6	43	34	−115
3	−4	6	105	107	−31
4	−4	6	411	391	14
5	−4	6	369	389	15
6	−4	6	290	283	16
7	−4	6	263	266	18
−9	−3	6	143	124	17
−8	−3	6	48	45	−45
−7	−3	6	27	72	−72
−6	−3	6	362	364	13
−5	−3	6	372	375	13
−4	−3	6	691	718	19
−3	−3	6	640	620	20
−2	−3	6	299	279	17
−1	−3	6	38	25	−101
0	−3	6	610	479	20
1	−3	6	535	430	19
2	−3	6	928	846	19
3	−3	6	581	573	15
4	−3	6	335	332	14
5	−3	6	191	209	23
6	−3	6	108	114	−46
7	−3	6	190	138	42
8	−3	6	198	213	41
−9	−2	6	191	172	16
−8	−2	6	323	333	15
−7	−2	6	320	323	13
−6	−2	6	341	341	14
−5	−2	6	137	108	19
−4	−2	6	193	181	18

H	K	L	$10F_o$	$10F_c$	10σ
−3	−2	6	488	434	17
−2	−2	6	1120	1001	21
−1	−2	6	1022	803	24
0	−2	6	730	612	20
1	−2	6	412	427	15
2	−2	6	128	78	25
3	−2	6	219	212	22
4	−2	6	508	503	22
5	−2	6	406	416	25
6	−2	6	338	359	28
7	−2	6	198	208	40
8	−2	6	51	74	−135
−9	−1	6	77	93	−31
−8	−1	6	29	54	−77
−7	−1	6	154	145	17
−6	−1	6	407	391	13
−5	−1	6	600	542	15
−4	−1	6	823	756	21
−3	−1	6	473	470	20
−2	−1	6	525	429	21
−1	−1	6	32	75	−86
0	−1	6	413	432	15
1	−1	6	517	557	17
2	−1	6	1068	1051	31
3	−1	6	568	547	25
4	−1	6	365	388	22
5	−1	6	47	99	−124
6	−1	6	134	138	−46
7	−1	6	143	152	−46
8	−1	6	240	260	32
−9	0	6	209	217	16
−8	0	6	319	285	15
−7	0	6	325	308	15
−6	0	6	450	421	15
−5	0	6	71	39	−44
−4	0	6	115	146	−37
−3	0	6	677	636	17
−2	0	6	772	762	19
−1	0	6	763	737	20
0	0	6	1103	1092	29
1	0	6	248	259	30
2	0	6	78	44	−76
3	0	6	363	361	23
4	0	6	421	475	21
5	0	6	348	403	24
6	0	6	405	439	22
7	0	6	192	176	28

Table 66. (continued)

H	K	L	$10F_o$	$10F_c$	10σ
8	0	6	44	92	-116
-9	1	6	108	93	-25
-8	1	6	78	1	-37
-7	1	6	319	252	15
-6	1	6	387	358	16
-5	1	6	684	605	21
-4	1	6	709	666	16
-3	1	6	455	469	15
-2	1	6	256	270	32
-1	1	6	282	273	25
0	1	6	484	558	19
1	1	6	792	852	18
2	1	6	647	675	20
3	1	6	441	503	20
4	1	6	418	375	16
5	1	6	36	18	-97
6	1	6	71	109	-56
7	1	6	175	227	31
8	1	6	260	230	23
-9	2	6	264	232	16
-8	2	6	303	270	17
-7	2	6	347	310	18
-6	2	6	294	249	22
-5	2	6	35	77	-92
-4	2	6	198	174	35
-3	2	6	567	689	20
-2	2	6	437	546	21
-1	2	6	762	799	26
0	2	6	778	843	25
1	2	6	228	231	21
2	2	6	88	39	-42
3	2	6	376	382	18
4	2	6	365	437	20
5	2	6	499	534	18
6	2	6	380	387	18
7	2	6	137	139	-32
8	2	6	118	74	-35
-9	3	6	191	102	21
-8	3	6	40	27	-108
-7	3	6	239	198	21
-6	3	6	257	282	27
-5	3	6	463	670	-22
-4	3	6	503	591	19
-3	3	6	404	412	20
-2	3	6	127	97	-30
-1	3	6	229	240	18
0	3	6	459	486	18
1	3	6	978	1022	20
2	3	6	522	560	16
3	3	6	438	458	15
4	3	6	297	294	16
5	3	6	47	39	-61
6	3	6	120	121	-30
7	3	6	224	242	22
-9	4	6	253	190	26
-8	4	6	273	236	25
-7	4	6	200	252	30
-6	4	6	104	106	-39
-5	4	6	75	69	-47
-4	4	6	284	290	17
-3	4	6	566	588	17
-2	4	6	511	506	16
-1	4	6	610	638	14
0	4	6	453	516	18
1	4	6	342	340	15
2	4	6	122	129	23
3	4	6	325	339	14
4	4	6	377	390	16
5	4	6	445	477	17
6	4	6	250	250	19
7	4	6	166	156	23
-9	5	6	44	70	-117
-8	5	6	77	54	-62
-7	5	6	144	171	31
-6	5	6	341	335	16
-5	5	6	448	474	15
-4	5	6	414	447	15
-3	5	6	346	338	14
-2	5	6	30	27	-80
-1	5	6	145	137	18
0	5	6	550	536	14
1	5	6	863	764	23
2	5	6	465	453	15
3	5	6	379	383	15
4	5	6	124	135	23
5	5	6	31	13	-83
6	5	6	172	162	22
7	5	6	237	225	19
-8	6	6	192	203	23
-7	6	6	186	208	21
-6	6	6	50	82	-50
-5	6	6	29	10	-77
-4	6	6	297	286	13
-3	6	6	418	389	12

Table 66. (continued)

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
-2	6	6	532	498	14	4	9	6	34	61	-90
-1	6	6	602	605	13	-6	10	6	60	51	-40
0	6	6	401	370	12	-5	10	6	29	66	-78
1	6	6	163	155	16	-4	10	6	162	163	17
2	6	6	218	205	14	-3	10	6	259	236	14
3	6	6	255	253	16	-2	10	6	296	278	15
4	6	6	376	361	14	-1	10	6	245	234	15
5	6	6	412	393	15	0	10	6	184	179	18
6	6	6	225	224	18	1	10	6	31	12	-82
-8	7	6	33	62	-87	2	10	6	141	112	21
-7	7	6	143	133	22	3	10	6	183	180	20
-6	7	6	274	281	16	-4	11	6	138	141	21
-5	7	6	322	320	13	-3	11	6	30	51	-80
-4	7	6	389	359	13	-2	11	6	79	20	-31
-3	7	6	205	200	13	-1	11	6	187	154	18
-2	7	6	65	48	-30	0	11	6	233	217	18
-1	7	6	178	170	15	1	11	6	243	226	18
0	7	6	476	449	15	2	11	6	193	193	19
1	7	6	433	428	13	-3	-11	7	34	84	-90
2	7	6	419	407	14	-2	-11	7	132	174	28
3	7	6	290	284	15	-1	-11	7	228	243	19
4	7	6	109	87	24	0	-11	7	166	173	25
5	7	6	83	18	-33	1	-11	7	209	189	23
6	7	6	206	172	20	2	-11	7	39	84	-104
-7	8	6	135	125	22	-5	-10	7	182	188	20
-6	8	6	88	84	-28	-4	-10	7	206	225	17
-5	8	6	84	52	-25	-3	-10	7	253	245	18
-4	8	6	237	228	13	-2	-10	7	160	157	23
-3	8	6	315	288	13	-1	-10	7	81	94	-39
-2	8	6	453	412	13	0	-10	7	36	96	-96
-1	8	6	368	349	14	1	-10	7	185	175	24
0	8	6	245	246	15	2	-10	7	234	247	22
1	8	6	87	54	-26	3	-10	7	267	263	21
2	8	6	162	161	17	4	-10	7	166	141	31
3	8	6	231	224	16	-6	-9	7	192	196	18
4	8	6	345	333	16	-5	-9	7	105	131	-27
5	8	6	261	252	18	-4	-9	7	64	38	-40
-6	9	6	199	211	18	-3	-9	7	87	103	-33
-5	9	6	224	234	15	-2	-9	7	300	313	16
-4	9	6	248	224	13	-1	-9	7	332	360	17
-3	9	6	69	91	-33	0	-9	7	324	337	18
-2	9	6	48	12	-48	1	-9	7	247	256	22
-1	9	6	193	173	16	2	-9	7	85	55	-48
0	9	6	378	354	15	3	-9	7	40	16	-105
1	9	6	378	337	13	4	-9	7	157	159	-38
2	9	6	343	316	14	5	-9	7	208	167	30
3	9	6	199	172	17	-7	-8	7	31	30	-83

H	K	L	$10F_o$	$10F_c$	10σ
-6	-8	7	181	181	18
-5	-8	7	212	212	17
-4	-8	7	325	362	15
-3	-8	7	283	322	15
-2	-8	7	192	222	21
-1	-8	7	124	101	25
0	-8	7	191	194	20
1	-8	7	228	205	19
2	-8	7	372	361	17
3	-8	7	288	315	23
4	-8	7	220	199	29
5	-8	7	173	118	28
-7	-7	7	223	212	16
-6	-7	7	218	233	16
-5	-7	7	83	111	-33
-4	-7	7	31	17	-82
-3	-7	7	229	208	15
-2	-7	7	459	461	15
-1	-7	7	421	419	14
0	-7	7	470	447	17
1	-7	7	224	212	23
2	-7	7	73	96	-61
3	-7	7	76	75	-63
4	-7	7	316	264	23
5	-7	7	196	209	22
6	-7	7	231	237	19
-8	-6	7	79	67	-32
-7	-6	7	94	87	-29
-6	-6	7	209	219	17
-5	-6	7	346	362	13
-4	-6	7	487	501	14
-3	-6	7	330	343	15
-2	-6	7	317	320	15
-1	-6	7	53	32	-59
0	-6	7	246	220	19
1	-6	7	419	356	17
2	-6	7	667	574	19
3	-6	7	510	400	18
4	-6	7	349	287	17
5	-6	7	115	83	-28
6	-6	7	74	41	-39
-8	-5	7	225	227	15
-7	-5	7	285	280	14
-6	-5	7	310	324	14
-5	-5	7	61	68	-39
-4	-5	7	91	32	-26
-3	-5	7	347	351	14
-2	-5	7	584	558	17
-1	-5	7	555	510	19
0	-5	7	656	601	20
1	-5	7	351	279	21
2	-5	7	106	129	-45
3	-5	7	255	207	16
4	-5	7	295	296	15
5	-5	7	227	231	16
6	-5	7	300	303	16
7	-5	7	155	147	21
-8	-4	7	63	53	-38
-7	-4	7	165	147	18
-6	-4	7	251	264	14
-5	-4	7	450	448	13
-4	-4	7	398	409	14
-3	-4	7	484	460	14
-2	-4	7	420	390	16
-1	-4	7	174	180	26
0	-4	7	289	232	24
1	-4	7	777	595	19
2	-4	7	646	561	16
3	-4	7	471	453	16
4	-4	7	341	331	15
5	-4	7	86	17	-31
6	-4	7	33	19	-88
7	-4	7	118	189	-33
-9	-3	7	185	194	18
-8	-3	7	235	224	16
-7	-3	7	362	368	14
-6	-3	7	282	259	14
-5	-3	7	90	34	-27
-4	-3	7	72	114	-35
-3	-3	7	532	499	17
-2	-3	7	727	654	17
-1	-3	7	1098	898	25
0	-3	7	623	498	19
1	-3	7	282	252	18
2	-3	7	198	123	15
3	-3	7	329	315	14
4	-3	7	333	342	13
5	-3	7	391	400	14
6	-3	7	300	305	19
7	-3	7	165	178	35
-9	-2	7	74	105	-38
-8	-2	7	31	8	-81
-7	-2	7	146	150	20
-6	-2	7	335	312	14

H	K	L	$10F_o$	$10F_c$	10σ
-5	-2	7	676	615	16
-4	-2	7	528	489	18
-3	-2	7	583	543	19
-2	-2	7	399	353	20
-1	-2	7	245	184	19
0	-2	7	397	345	16
1	-2	7	713	669	18
2	-2	7	581	604	14
3	-2	7	562	579	18
4	-2	7	290	300	18
5	-2	7	43	17	-115
6	-2	7	50	52	-133
7	-2	7	170	219	-44
-9	-1	7	208	194	17
-8	-1	7	252	246	16
-7	-1	7	373	354	15
-6	-1	7	256	239	15
-5	-1	7	147	132	21
-4	-1	7	290	276	19
-3	-1	7	539	441	22
-2	-1	7	657	607	21
-1	-1	7	1012	970	17
0	-1	7	377	350	13
1	-1	7	372	369	15
2	-1	7	64	7	-75
3	-1	7	374	343	23
4	-1	7	372	400	24
5	-1	7	460	495	23
6	-1	7	222	227	32
7	-1	7	196	205	38
-9	0	7	112	98	-26
-8	0	7	88	58	-33
-7	0	7	177	146	21
-6	0	7	504	452	16
-5	0	7	668	570	19
-4	0	7	507	426	18
-3	0	7	459	458	16
-2	0	7	128	101	25
-1	0	7	159	123	23
0	0	7	708	707	19
1	0	7	735	714	24
2	0	7	548	594	22
3	0	7	554	603	21
4	0	7	163	177	35
5	0	7	77	47	-65
6	0	7	139	137	-40
7	0	7	155	212	-44
-9	1	7	179	184	23
-8	1	7	318	276	17
-7	1	7	342	303	17
-6	1	7	276	222	20
-5	1	7	117	82	-31
-4	1	7	342	333	15
-3	1	7	419	440	15
-2	1	7	685	718	21
-1	1	7	1069	973	29
0	1	7	576	647	20
1	1	7	244	264	28
2	1	7	123	158	-45
3	1	7	219	257	26
4	1	7	395	470	21
5	1	7	443	462	21
6	1	7	257	277	27
7	1	7	186	191	33
-9	2	7	113	71	-36
-8	2	7	76	53	-55
-7	2	7	173	169	32
-6	2	7	470	436	16
-5	2	7	416	453	15
-4	2	7	437	541	22
-3	2	7	307	360	25
-2	2	7	46	19	-122
-1	2	7	171	168	32
0	2	7	691	723	20
1	2	7	430	458	20
2	2	7	488	534	18
3	2	7	490	491	18
4	2	7	153	164	27
5	2	7	38	36	-101
6	2	7	189	208	28
7	2	7	165	182	33
-9	3	7	209	159	26
-8	3	7	328	260	22
-7	3	7	181	192	22
-6	3	7	132	159	-38
-5	3	7	41	37	-110
-4	3	7	251	265	22
-3	3	7	356	415	24
-2	3	7	744	792	20
-1	3	7	550	595	20
0	3	7	485	518	21
1	3	7	160	156	24
2	3	7	169	177	22
3	3	7	302	318	18

H	K	L	$10F_o$	$10F_c$	10σ
4	3	7	553	556	16
5	3	7	323	369	21
6	3	7	227	262	23
7	3	7	105	122	-42
-9	4	7	76	24	-54
-8	4	7	43	34	-114
-7	4	7	182	203	32
-6	4	7	346	403	19
-5	4	7	378	459	19
-4	4	7	378	463	17
-3	4	7	216	232	20
-2	4	7	139	66	26
-1	4	7	289	306	17
0	4	7	532	563	18
1	4	7	586	535	17
2	4	7	546	561	18
3	4	7	302	333	17
4	4	7	167	192	24
5	4	7	51	41	-68
6	4	7	194	176	23
7	4	7	194	173	26
-8	5	7	182	209	32
-7	5	7	155	190	30
-6	5	7	154	139	25
-5	5	7	146	106	23
-4	5	7	155	186	23
-3	5	7	409	393	15
-2	5	7	605	614	16
-1	5	7	479	469	13
0	5	7	416	404	14
1	5	7	93	44	-28
2	5	7	119	127	24
3	5	7	356	334	15
4	5	7	405	418	15
5	5	7	269	276	18
6	5	7	261	236	19
-8	6	7	39	39	-104
-7	6	7	193	190	22
-6	6	7	260	265	17
-5	6	7	304	323	16
-4	6	7	280	288	15
-3	6	7	140	150	22
-2	6	7	29	33	-78
-1	6	7	364	351	15
0	6	7	411	401	14
1	6	7	473	445	14
2	6	7	465	416	14
3	6	7	225	236	17
4	6	7	107	131	-31
5	6	7	99	92	-33
6	6	7	160	147	26
-8	7	7	148	139	26
-7	7	7	120	154	-30
-6	7	7	32	65	-84
-5	7	7	97	111	-28
-4	7	7	209	207	16
-3	7	7	399	388	15
-2	7	7	472	461	13
-1	7	7	448	447	14
0	7	7	214	208	16
1	7	7	65	23	-38
2	7	7	130	109	21
3	7	7	332	311	16
4	7	7	312	313	17
5	7	7	288	274	18
-7	8	7	146	146	22
-6	8	7	192	209	18
-5	8	7	262	281	15
-4	8	7	209	201	17
-3	8	7	152	118	18
-2	8	7	69	37	-32
-1	8	7	240	241	15
0	8	7	283	272	15
1	8	7	400	360	13
2	8	7	332	289	15
3	8	7	208	195	17
4	8	7	33	56	-88
5	8	7	79	89	-41
-6	9	7	57	23	-45
-5	9	7	89	60	-27
-4	9	7	189	172	16
-3	9	7	289	268	14
-2	9	7	253	263	15
-1	9	7	282	272	16
0	9	7	135	121	22
1	9	7	62	4	-42
2	9	7	133	136	24
3	9	7	230	240	19
4	9	7	207	219	20
-5	10	7	171	184	19
-4	10	7	113	132	-26
-3	10	7	117	69	22
-2	10	7	100	79	-28
-1	10	7	184	180	18

H	K	L	$10F_o$	$10F_c$	10σ
0	10	7	305	264	16
1	10	7	315	274	15
2	10	7	218	183	17
3	10	7	106	124	-31
-3	11	7	186	183	18
-2	11	7	179	186	20
-1	11	7	183	164	19
0	11	7	97	74	-30
1	11	7	33	10	-88
-2	-11	8	122	142	-31
-1	-11	8	71	17	-54
0	-11	8	38	52	-102
1	-11	8	141	136	-34
-4	-10	8	32	12	-86
-3	-10	8	155	140	24
-2	-10	8	194	187	22
-1	-10	8	209	217	22
0	-10	8	256	252	20
1	-10	8	184	159	26
2	-10	8	111	76	-42
3	-10	8	132	66	-38
-5	-9	8	210	225	19
-4	-9	8	191	241	20
-3	-9	8	245	243	19
-2	-9	8	163	165	24
-1	-9	8	89	19	-39
0	-9	8	66	79	-58
1	-9	8	283	293	22
2	-9	8	304	281	21
3	-9	8	253	201	23
4	-9	8	185	168	36
-6	-8	8	153	149	20
-5	-8	8	74	81	-39
-4	-8	8	32	13	-84
-3	-8	8	236	260	20
-2	-8	8	288	289	17
-1	-8	8	400	390	17
0	-8	8	330	319	18
1	-8	8	259	208	20
2	-8	8	74	59	-66
3	-8	8	144	118	-41
4	-8	8	141	110	-36
5	-8	8	231	222	19
-7	-7	8	56	68	-51
-6	-7	8	148	154	22
-5	-7	8	265	286	17
-4	-7	8	314	334	17
-3	-7	8	397	385	16
-2	-7	8	152	131	23
-1	-7	8	35	3	-93
0	-7	8	146	129	29
1	-7	8	423	375	19
2	-7	8	415	349	22
3	-7	8	368	319	18
4	-7	8	161	166	25
5	-7	8	108	75	-27
-7	-6	8	231	241	17
-6	-6	8	105	136	-28
-5	-6	8	114	127	-26
-4	-6	8	134	113	22
-3	-6	8	347	325	16
-2	-6	8	418	408	15
-1	-6	8	494	465	18
0	-6	8	322	301	22
1	-6	8	394	315	21
2	-6	8	87	6	-52
3	-6	8	184	180	19
4	-6	8	215	182	17
5	-6	8	315	295	15
6	-6	8	181	191	19
-8	-5	8	31	11	-83
-7	-5	8	90	93	-32
-6	-5	8	313	305	16
-5	-5	8	387	382	14
-4	-5	8	420	402	16
-3	-5	8	457	450	17
-2	-5	8	36	99	-96
-1	-5	8	38	14	-101
0	-5	8	411	317	19
1	-5	8	609	491	17
2	-5	8	541	479	14
3	-5	8	443	426	14
4	-5	8	150	127	18
5	-5	8	52	101	-49
6	-5	8	96	88	-27
-8	-4	8	270	257	16
-7	-4	8	293	274	15
-6	-4	8	220	218	17
-5	-4	8	111	92	-26
-4	-4	8	171	195	21
-3	-4	8	293	297	18
-2	-4	8	661	590	19
-1	-4	8	638	517	21
0	-4	8	578	462	17

H	K	L	$10F_o$	$10F_c$	10σ
1	-4	8	351	306	16
2	-4	8	145	98	18
3	-4	8	147	144	17
4	-4	8	317	319	13
5	-4	8	280	286	15
6	-4	8	250	255	16
-8	-3	8	34	15	-91
-7	-3	8	124	121	-27
-6	-3	8	336	330	15
-5	-3	8	345	329	15
-4	-3	8	499	489	16
-3	-3	8	448	388	17
-2	-3	8	217	153	24
-1	-3	8	80	62	-51
0	-3	8	586	514	15
1	-3	8	507	467	14
2	-3	8	544	537	14
3	-3	8	439	436	13
4	-3	8	207	190	16
5	-3	8	54	64	-53
6	-3	8	109	141	-33
7	-3	8	136	156	30
-9	-2	8	160	168	23
-8	-2	8	287	284	16
-7	-2	8	249	234	18
-6	-2	8	243	237	17
-5	-2	8	35	20	-92
-4	-2	8	298	282	18
-3	-2	8	548	440	18
-2	-2	8	926	792	22
-1	-2	8	665	598	20
0	-2	8	543	497	13
1	-2	8	197	166	16
2	-2	8	67	84	-33
3	-2	8	201	200	17
4	-2	8	493	490	16
5	-2	8	303	303	19
6	-2	8	248	274	25
7	-2	8	122	143	-52
-9	-1	8	105	47	-30
-8	-1	8	33	15	-88
-7	-1	8	242	202	19
-6	-1	8	395	350	16
-5	-1	8	531	482	17
-4	-1	8	710	550	20
-3	-1	8	240	203	18
-2	-1	8	259	239	14
-1	-1	8	219	189	15
0	-1	8	462	452	14
1	-1	8	492	520	16
2	-1	8	632	652	17
3	-1	8	361	359	20
4	-1	8	362	280	23
5	-1	8	50	29	-134
6	-1	8	138	138	-49
7	-1	8	185	164	38
-9	0	8	210	189	21
-8	0	8	292	244	18
-7	0	8	257	225	20
-6	0	8	263	235	19
-5	0	8	39	14	-104
-4	0	8	208	194	15
-3	0	8	471	513	15
-2	0	8	623	658	19
-1	0	8	694	663	21
0	0	8	538	572	19
1	0	8	104	66	-58
2	0	8	103	87	-56
3	0	8	316	351	25
4	0	8	413	450	24
5	0	8	300	319	26
6	0	8	265	269	30
7	0	8	100	112	-64
-9	1	8	39	42	-104
-8	1	8	38	42	-101
-7	1	8	307	269	21
-6	1	8	400	347	17
-5	1	8	463	480	14
-4	1	8	437	463	13
-3	1	8	217	209	18
-2	1	8	96	94	-44
-1	1	8	405	372	23
0	1	8	449	469	25
1	1	8	530	574	21
2	1	8	522	558	21
3	1	8	342	350	21
4	1	8	216	234	27
5	1	8	77	81	-76
6	1	8	99	129	-58
7	1	8	202	214	33
-9	2	8	247	200	22
-8	2	8	290	220	21
-7	2	8	279	257	18
-6	2	8	124	116	23

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
-5	2	8	32	61	-84	-5	5	8	322	341	17
-4	2	8	142	193	29	-4	5	8	193	217	20
-3	2	8	514	589	22	-3	5	8	227	234	19
-2	2	8	566	577	20	-2	5	8	78	66	-41
-1	2	8	680	723	23	-1	5	8	247	239	17
0	2	8	409	390	24	0	5	8	422	418	17
1	2	8	40	21	-108	1	5	8	469	481	17
2	2	8	137	78	-32	2	5	8	440	372	14
3	2	8	406	432	21	3	5	8	313	322	19
4	2	8	313	367	22	4	5	8	54	34	-62
5	2	8	335	373	22	5	5	8	56	63	-67
6	2	8	235	237	28	6	5	8	145	153	31
7	2	8	116	80	-48	-8	6	8	165	153	30
-9	3	8	153	42	33	-7	6	8	140	152	30
-8	3	8	36	60	-95	-6	6	8	36	61	-95
-7	3	8	186	197	20	-5	6	8	89	66	-33
-6	3	8	280	296	19	-4	6	8	258	270	16
-5	3	8	360	442	20	-3	6	8	314	340	17
-4	3	8	239	348	25	-2	6	8	522	485	15
-3	3	8	272	301	21	-1	6	8	410	404	17
-2	3	8	145	20	-35	0	6	8	157	149	21
-1	3	8	284	327	23	1	6	8	33	33	-88
0	3	8	356	377	19	2	6	8	213	210	17
1	3	8	584	544	17	3	6	8	290	282	17
2	3	8	478	474	19	4	6	8	307	311	18
3	3	8	416	408	18	5	6	8	273	247	19
4	3	8	112	122	-39	-7	7	8	107	143	-39
5	3	8	67	90	-62	-6	7	8	214	246	22
6	3	8	73	136	-74	-5	7	8	250	245	15
-8	4	8	98	180	-50	-4	7	8	207	199	16
-7	4	8	203	211	30	-3	7	8	106	88	-25
-6	4	8	39	55	-105	-2	7	8	121	98	24
-5	4	8	124	92	-32	-1	7	8	253	227	15
-4	4	8	237	286	22	0	7	8	397	366	15
-3	4	8	452	509	19	1	7	8	334	319	16
-2	4	8	535	553	18	2	7	8	293	303	19
-1	4	8	527	514	16	3	7	8	185	191	22
0	4	8	174	194	24	4	7	8	36	9	-95
1	4	8	35	74	-93	5	7	8	105	68	-36
2	4	8	182	188	21	-6	8	8	33	30	-88
3	4	8	369	410	18	-5	8	8	136	86	21
4	4	8	321	337	18	-4	8	8	229	223	17
5	4	8	283	306	21	-3	8	8	276	255	15
6	4	8	91	156	-56	-2	8	8	340	340	16
-8	5	8	43	92	-114	-1	8	8	258	243	16
-7	5	8	167	173	32	0	8	8	149	120	22
-6	5	8	228	320	26	1	8	8	34	18	-91

H	K	L	$10F_o$	$10F_c$	10σ
2	8	8	157	168	22
3	8	8	227	221	21
4	8	8	287	272	20
-6	9	8	181	178	21
-5	9	8	190	185	18
-4	9	8	150	160	22
-3	9	8	73	27	-37
-2	9	8	79	67	-34
-1	9	8	215	188	19
0	9	8	295	284	17
1	9	8	300	257	16
2	9	8	236	228	18
3	9	8	107	97	-32
-4	10	8	135	154	26
-3	10	8	202	198	18
-2	10	8	212	203	18
-1	10	8	147	152	25
0	10	8	106	91	-31
1	10	8	35	53	-93
2	10	8	131	124	26
-3	-10	9	167	179	24
-2	-10	9	100	75	-38
-1	-10	9	72	35	-58
0	-10	9	78	120	-60
1	-10	9	146	189	-42
-5	-9	9	96	71	-34
-4	-9	9	85	69	-37
-3	-9	9	67	124	-59
-2	-9	9	269	254	20
-1	-9	9	232	251	23
0	-9	9	254	256	24
1	-9	9	198	176	30
2	-9	9	111	23	-52
3	-9	9	60	39	-75
-6	-8	9	165	176	22
-5	-8	9	169	193	24
-4	-8	9	234	294	21
-3	-8	9	242	227	19
-2	-8	9	109	110	-39
-1	-8	9	39	14	-103
0	-8	9	221	211	26
1	-8	9	277	239	28
2	-8	9	341	295	24
3	-8	9	244	186	20
4	-8	9	129	135	-29
-6	-7	9	132	150	26
-5	-7	9	70	30	-45
-4	-7	9	35	73	-94
-3	-7	9	208	225	21
-2	-7	9	419	387	18
-1	-7	9	327	301	18
0	-7	9	360	312	21
1	-7	9	231	153	28
2	-7	9	39	6	-103
3	-7	9	134	95	24
4	-7	9	243	219	17
5	-7	9	197	196	16
-7	-6	9	77	106	-41
-6	-6	9	197	203	20
-5	-6	9	284	297	17
-4	-6	9	376	394	17
-3	-6	9	216	243	23
-2	-6	9	213	172	22
-1	-6	9	141	126	-33
0	-6	9	314	242	22
1	-6	9	402	317	18
2	-6	9	507	455	15
3	-6	9	220	228	17
4	-6	9	167	176	18
5	-6	9	29	17	-77
-7	-5	9	194	202	21
-6	-5	9	207	184	18
-5	-5	9	33	25	-89
-4	-5	9	108	101	-31
-3	-5	9	386	350	17
-2	-5	9	450	431	20
-1	-5	9	472	392	18
0	-5	9	470	369	18
1	-5	9	188	135	17
2	-5	9	50	42	-51
3	-5	9	246	235	13
4	-5	9	241	236	16
5	-5	9	234	230	14
6	-5	9	216	218	16
-8	-4	9	33	6	-89
-7	-4	9	202	168	20
-6	-4	9	273	247	18
-5	-4	9	370	377	16
-4	-4	9	353	334	16
-3	-4	9	308	300	20
-2	-4	9	179	165	31
-1	-4	9	257	216	18
0	-4	9	313	286	15
1	-4	9	498	470	15

H	K	L	10F$_o$	10F$_c$	10σ	H	K	L	10F$_o$	10F$_c$	10σ
2	-4	9	453	444	12	4	-1	9	318	324	18
3	-4	9	304	306	13	5	-1	9	297	321	26
4	-4	9	145	166	20	6	-1	9	165	178	-38
5	-4	9	71	22	-34	-9	0	9	37	57	-99
6	-4	9	58	75	-43	-8	0	9	73	80	-54
-8	-3	9	203	200	22	-7	0	9	207	188	26
-7	-3	9	257	258	19	-6	0	9	438	350	18
-6	-3	9	137	143	26	-5	0	9	430	405	15
-5	-3	9	34	16	-89	-4	0	9	375	376	13
-4	-3	9	167	144	24	-3	0	9	328	333	13
-3	-3	9	600	486	18	-2	0	9	82	105	-27
-2	-3	9	609	502	18	-1	0	9	189	196	15
-1	-3	9	642	583	15	0	0	9	387	403	15
0	-3	9	400	357	13	1	0	9	596	632	19
1	-3	9	75	98	-31	2	0	9	474	497	21
2	-3	9	28	13	-74	3	0	9	399	361	22
3	-3	9	336	328	12	4	0	9	45	68	-121
4	-3	9	248	266	14	5	0	9	50	15	-132
5	-3	9	294	302	15	6	0	9	123	152	-52
6	-3	9	232	235	18	-8	1	9	315	242	21
-8	-2	9	35	57	-94	-7	1	9	246	209	21
-7	-2	9	227	181	20	-6	1	9	30	53	-80
-6	-2	9	286	267	17	-5	1	9	28	22	-74
-5	-2	9	497	443	18	-4	1	9	301	312	13
-4	-2	9	473	367	19	-3	1	9	436	472	13
-3	-2	9	376	361	17	-2	1	9	582	631	16
-2	-2	9	57	17	-40	-1	1	9	425	446	17
-1	-2	9	232	227	14	0	1	9	331	257	25
0	-2	9	326	300	13	1	1	9	134	183	-41
1	-2	9	557	551	13	2	1	9	313	282	22
2	-2	9	419	413	12	3	1	9	249	280	25
3	-2	9	423	417	14	4	1	9	335	335	21
4	-2	9	122	130	26	5	1	9	243	299	31
5	-2	9	35	33	-92	6	1	9	53	186	-142
6	-2	9	55	101	-69	-7	2	9	210	196	19
-8	-1	9	244	223	19	-6	2	9	325	329	13
-7	-1	9	247	236	21	-5	2	9	236	275	15
-6	-1	9	62	81	-55	-4	2	9	349	419	16
-5	-1	9	39	35	-103	-3	2	9	197	251	26
-4	-1	9	286	261	16	-2	2	9	88	98	-55
-3	-1	9	505	495	15	-1	2	9	183	219	33
-2	-1	9	536	557	13	0	2	9	384	436	21
-1	-1	9	530	521	13	1	2	9	511	468	18
0	-1	9	240	256	13	2	2	9	521	548	18
1	-1	9	219	220	15	3	2	9	274	260	22
2	-1	9	157	171	21	4	2	9	132	45	-38
3	-1	9	331	349	17	5	2	9	44	31	-118

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
6	2	9	212	203	32	-5	6	9	192	245	24
-8	3	9	225	214	17	-4	6	9	150	189	25
-7	3	9	152	160	22	-3	6	9	76	54	-42
-6	3	9	73	58	-41	-2	6	9	98	67	-34
-5	3	9	64	112	-70	-1	6	9	322	285	16
-4	3	9	274	302	22	0	6	9	349	347	18
-3	3	9	388	473	20	1	6	9	397	379	17
-2	3	9	516	593	21	2	6	9	271	293	19
-1	3	9	312	317	20	3	6	9	165	126	27
0	3	9	209	220	24	4	6	9	91	32	-44
1	3	9	42	36	-111	5	6	9	103	108	-41
2	3	9	230	249	25	-7	7	9	116	81	-34
3	3	9	270	302	24	-6	7	9	76	15	-48
4	3	9	355	353	21	-5	7	9	110	109	-32
5	3	9	243	250	26	-4	7	9	199	207	19
6	3	9	163	184	35	-3	7	9	348	331	15
-8	4	9	124	71	-31	-2	7	9	299	302	17
-7	4	9	195	196	30	-1	7	9	265	257	18
-6	4	9	240	297	24	0	7	9	115	123	-33
-5	4	9	214	275	23	1	7	9	78	68	-43
-4	4	9	243	325	23	2	7	9	140	147	28
-3	4	9	121	126	-37	3	7	9	284	260	20
-2	4	9	40	55	-107	4	7	9	249	227	21
-1	4	9	248	257	22	-6	8	9	156	165	25
0	4	9	404	395	18	-5	8	9	209	209	20
1	4	9	432	436	18	-4	8	9	36	127	-95
2	4	9	563	488	18	-3	8	9	74	31	-42
3	4	9	219	183	23	-2	8	9	88	89	-36
4	4	9	97	46	-44	-1	8	9	213	213	22
5	4	9	114	81	-40	0	8	9	245	248	20
6	4	9	194	172	28	1	8	9	298	289	18
-8	5	9	113	153	-46	2	8	9	192	188	23
-7	5	9	97	123	-50	3	8	9	105	102	-37
-6	5	9	113	67	-37	-5	9	9	67	80	-47
-5	5	9	82	133	-54	-4	9	9	193	167	20
-4	5	9	228	233	20	-3	9	9	238	221	18
-3	5	9	342	408	20	-2	9	9	180	198	22
-2	5	9	411	417	17	-1	9	9	183	174	23
-1	5	9	288	268	18	0	9	9	35	46	-93
0	5	9	216	227	23	1	9	9	36	54	-96
1	5	9	89	54	-43	2	9	9	155	146	25
2	5	9	167	190	26	-3	10	9	85	13	-38
3	5	9	278	301	23	-2	10	9	88	91	-38
4	5	9	269	281	22	-1	10	9	175	160	23
5	5	9	197	191	28	0	10	9	257	206	19
-7	6	9	171	181	28	-4	-9	10	152	183	26
-6	6	9	149	220	32	-3	-9	10	118	146	-39

H	K	L	$10F_o$	$10F_c$	10σ
-2	-9	10	87	83	-50
-1	-9	10	107	56	-47
0	-9	10	113	122	-48
1	-9	10	291	243	25
2	-9	10	203	184	25
-5	-8	10	121	27	-30
-4	-8	10	134	65	28
-3	-8	10	201	211	25
-2	-8	10	244	227	23
-1	-8	10	334	312	22
0	-8	10	248	225	27
1	-8	10	154	102	31
2	-8	10	36	3	-97
3	-8	10	113	112	-27
-6	-7	10	135	155	-32
-5	-7	10	258	261	19
-4	-7	10	217	235	22
-3	-7	10	255	228	20
-2	-7	10	41	55	-108
-1	-7	10	144	76	-35
0	-7	10	201	187	28
1	-7	10	358	303	18
2	-7	10	234	215	19
3	-7	10	252	228	16
4	-7	10	135	107	21
-6	-6	10	53	86	-68
-5	-6	10	39	43	-104
-4	-6	10	149	172	28
-3	-6	10	246	257	23
-2	-6	10	385	310	18
-1	-6	10	492	381	19
0	-6	10	218	193	22
1	-6	10	212	159	19
2	-6	10	60	61	-46
3	-6	10	148	156	19
4	-6	10	225	204	15
-7	-5	10	140	98	27
-6	-5	10	249	254	21
-5	-5	10	367	333	16
-4	-5	10	282	296	19
-3	-5	10	257	220	22
-2	-5	10	39	24	-104
-1	-5	10	114	68	-31
0	-5	10	344	330	15
1	-5	10	386	366	15
2	-5	10	336	330	13
3	-5	10	278	262	14

H	K	L	$10F_o$	$10F_c$	10σ
4	-5	10	108	81	23
5	-5	10	28	14	-75
-7	-4	10	177	168	25
-6	-4	10	138	127	30
-5	-4	10	60	19	-57
-4	-4	10	267	240	20
-3	-4	10	341	262	18
-2	-4	10	456	407	17
-1	-4	10	454	418	14
0	-4	10	307	286	13
1	-4	10	162	132	17
2	-4	10	139	138	17
3	-4	10	167	161	16
4	-4	10	253	260	15
5	-4	10	252	245	14
-8	-3	10	121	57	-31
-7	-3	10	140	134	29
-6	-3	10	289	277	20
-5	-3	10	349	294	17
-4	-3	10	437	370	18
-3	-3	10	163	172	23
-2	-3	10	30	7	-80
-1	-3	10	120	114	20
0	-3	10	474	463	14
1	-3	10	377	368	13
2	-3	10	422	400	12
3	-3	10	246	240	13
4	-3	10	81	86	-31
5	-3	10	30	10	-79
-8	-2	10	236	213	21
-7	-2	10	117	140	-36
-6	-2	10	145	120	29
-5	-2	10	37	60	-100
-4	-2	10	310	273	16
-3	-2	10	414	395	14
-2	-2	10	522	494	14
-1	-2	10	379	365	12
0	-2	10	362	354	12
1	-2	10	68	27	-30
2	-2	10	154	139	15
3	-2	10	199	214	16
4	-2	10	302	328	15
5	-2	10	239	239	17
6	-2	10	189	200	20
-8	-1	10	126	50	-32
-7	-1	10	227	188	24
-6	-1	10	339	279	19

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
-5	-1	10	396	364	18	-3	2	10	424	457	14
-4	-1	10	443	414	13	-2	2	10	385	407	19
-3	-1	10	144	140	17	-1	2	10	386	378	20
-2	-1	10	37	24	-50	0	2	10	219	184	27
-1	-1	10	186	206	13	1	2	10	133	30	-39
0	-1	10	409	412	12	2	2	10	81	149	-67
1	-1	10	461	475	15	3	2	10	259	299	25
2	-1	10	463	456	13	4	2	10	249	263	27
3	-1	10	204	201	19	5	2	10	292	272	25
4	-1	10	130	107	27	-8	3	10	100	83	-30
5	-1	10	55	62	-68	-7	3	10	212	178	16
6	-1	10	177	160	28	-6	3	10	211	233	17
-8	0	10	249	190	22	-5	3	10	261	314	18
-7	0	10	202	144	25	-4	3	10	176	215	28
-6	0	10	85	95	-34	-3	3	10	154	144	33
-5	0	10	133	127	19	-2	3	10	43	68	-115
-4	0	10	237	238	13	-1	3	10	300	302	22
-3	0	10	424	443	15	0	3	10	312	350	22
-2	0	10	404	435	12	1	3	10	478	476	19
-1	0	10	294	299	13	2	3	10	372	311	20
0	0	10	398	343	14	3	3	10	122	179	-46
1	0	10	33	23	-88	4	3	10	64	22	-78
2	0	10	138	155	26	5	3	10	45	116	-120
3	0	10	271	284	22	-7	4	10	118	128	-35
4	0	10	330	302	23	-6	4	10	41	4	-109
5	0	10	227	228	32	-5	4	10	124	120	-38
6	0	10	210	204	38	-4	4	10	241	291	21
-8	1	10	64	65	-60	-3	4	10	315	376	21
-7	1	10	224	222	18	-2	4	10	285	347	22
-6	1	10	236	265	14	-1	4	10	294	340	23
-5	1	10	337	354	15	0	4	10	42	84	-113
-4	1	10	257	302	14	1	4	10	93	23	-47
-3	1	10	149	156	16	2	4	10	178	203	30
-2	1	10	30	10	-80	3	4	10	277	290	27
-1	1	10	308	330	16	4	4	10	222	244	29
0	1	10	375	399	18	5	4	10	212	237	32
1	1	10	620	573	21	-7	5	10	172	160	33
2	1	10	389	380	21	-6	5	10	225	249	23
3	1	10	122	161	-54	-5	5	10	213	249	24
4	1	10	46	92	-122	-4	5	10	105	153	-42
5	1	10	105	111	-58	-3	5	10	86	83	-46
6	1	10	109	143	-59	-2	5	10	59	121	-73
-8	2	10	147	166	23	-1	5	10	227	238	23
-7	2	10	160	170	19	0	5	10	379	373	18
-6	2	10	30	34	-79	1	5	10	354	364	22
-5	2	10	141	139	18	2	5	10	256	242	22
-4	2	10	243	261	15	3	5	10	155	151	-36

H	K	L	10F$_o$	10F$_c$	10σ	H	K	L	10F$_o$	10F$_c$	10σ
4	5	10	42	28	-113	-2	-7	11	369	307	22
-7	6	10	100	76	-46	-1	-7	11	288	234	20
-6	6	10	98	4	-41	0	-7	11	230	210	20
-5	6	10	38	90	-102	1	-7	11	49	50	-64
-4	6	10	192	235	24	2	-7	11	65	37	-42
-3	6	10	257	272	19	3	-7	11	111	112	23
-2	6	10	301	302	20	-6	-6	11	204	176	24
-1	6	10	230	247	22	-5	-6	11	253	241	21
0	6	10	102	74	-40	-4	-6	11	241	257	25
1	6	10	74	45	-53	-3	-6	11	44	112	-118
2	6	10	192	204	26	-2	-6	11	106	63	-40
3	6	10	227	220	25	-1	-6	11	150	141	24
4	6	10	213	219	27	0	-6	11	219	218	18
-6	7	10	136	188	-34	1	-6	11	257	255	15
-5	7	10	137	164	29	2	-6	11	291	273	14
-4	7	10	37	127	-98	3	-6	11	171	151	15
-3	7	10	52	22	-67	-6	-5	11	82	101	-52
-2	7	10	133	130	-32	-5	-5	11	75	54	-58
-1	7	10	216	213	23	-4	-5	11	146	143	-34
0	7	10	315	303	21	-3	-5	11	339	284	18
1	7	10	241	237	21	-2	-5	11	335	299	17
2	7	10	178	189	26	-1	-5	11	317	292	15
3	7	10	97	92	-44	0	-5	11	267	250	14
-5	8	10	112	101	-33	1	-5	11	29	25	-79
-4	8	10	168	185	25	2	-5	11	87	59	-26
-3	8	10	189	223	24	3	-5	11	167	184	17
-2	8	10	238	244	20	4	-5	11	216	215	15
-1	8	10	107	132	-37	-7	-4	11	177	162	25
0	8	10	98	43	-42	-6	-4	11	209	206	25
1	8	10	38	62	-103	-5	-4	11	363	312	19
2	8	10	152	165	31	-4	-4	11	280	244	20
-4	9	10	36	90	-96	-3	-4	11	111	118	-29
-3	9	10	75	3	-46	-2	-4	11	31	36	-82
-2	9	10	156	91	24	-1	-4	11	226	200	14
-1	9	10	181	166	25	0	-4	11	290	273	13
0	9	10	220	203	23	1	-4	11	400	398	13
-1	-9	11	197	193	34	2	-4	11	267	269	13
-4	-8	11	183	191	26	3	-4	11	150	148	16
-3	-8	11	145	126	-34	4	-4	11	131	114	19
-2	-8	11	43	42	-114	-7	-3	11	163	154	28
-1	-8	11	107	69	-45	-6	-3	11	39	59	-104
0	-8	11	239	195	21	-5	-3	11	64	43	-58
1	-8	11	190	175	23	-4	-3	11	178	181	18
2	-8	11	201	208	19	-3	-3	11	369	371	15
-5	-7	11	38	20	-102	-2	-3	11	309	296	13
-4	-7	11	131	100	-33	-1	-3	11	409	399	12
-3	-7	11	220	192	25	0	-3	11	223	228	13

H	K	L	$10F_o$	$10F_c$	10σ
1	-3	11	27	9	-73
2	-3	11	73	95	-31
3	-3	11	220	225	14
4	-3	11	225	206	15
5	-3	11	242	258	15
-7	-2	11	210	165	26
-6	-2	11	249	221	21
-5	-2	11	344	329	16
-4	-2	11	283	263	12
-3	-2	11	166	158	16
-2	-2	11	98	79	20
-1	-2	11	208	208	13
0	-2	11	348	342	12
1	-2	11	428	432	12
2	-2	11	241	248	14
3	-2	11	213	200	15
4	-2	11	31	58	-83
5	-2	11	78	72	-34
-7	-1	11	143	138	-33
-6	-1	11	31	11	-84
-5	-1	11	74	56	-32
-4	-1	11	264	270	13
-3	-1	11	371	379	12
-2	-1	11	310	313	13
-1	-1	11	358	364	12
0	-1	11	203	173	14
1	-1	11	80	34	-28
2	-1	11	166	166	18
3	-1	11	247	247	16
4	-1	11	231	243	18
5	-1	11	243	268	19
-8	0	11	83	90	-45
-7	0	11	165	156	21
-6	0	11	288	278	15
-5	0	11	290	308	13
-4	0	11	210	247	15
-3	0	11	161	155	15
-2	0	11	127	129	16
-1	0	11	191	192	14
0	0	11	432	437	13
1	0	11	440	435	15
2	0	11	241	257	17
3	0	11	212	201	19
4	0	11	36	8	-97
5	0	11	38	62	-102
-8	1	11	172	159	24
-7	1	11	105	111	-26
-6	1	11	70	14	-28
-5	1	11	116	98	19
-4	1	11	263	296	13
-3	1	11	300	317	12
-2	1	11	359	382	15
-1	1	11	275	302	16
0	1	11	159	163	21
1	1	11	83	7	-46
2	1	11	240	215	22
3	1	11	193	209	31
4	1	11	319	283	24
5	1	11	231	220	32
-7	2	11	178	160	16
-6	2	11	228	260	14
-5	2	11	211	241	15
-4	2	11	203	218	15
-3	2	11	66	70	-41
-2	2	11	109	113	-29
-1	2	11	205	242	26
0	2	11	453	436	21
1	2	11	339	333	24
2	2	11	304	253	25
3	2	11	151	143	-42
4	2	11	113	3	-51
5	2	11	47	81	-124
-7	3	11	67	73	-37
-6	3	11	73	27	-33
-5	3	11	100	127	-31
-4	3	11	257	281	17
-3	3	11	277	303	22
-2	3	11	337	384	22
-1	3	11	195	241	31
0	3	11	143	125	-36
1	3	11	72	66	-75
2	3	11	157	195	-37
3	3	11	203	221	34
4	3	11	299	295	24
-7	4	11	170	160	23
-6	4	11	189	217	24
-5	4	11	191	230	28
-4	4	11	139	180	-35
-3	4	11	40	18	-107
-2	4	11	79	91	-57
-1	4	11	243	257	25
0	4	11	332	339	22
1	4	11	317	290	23
2	4	11	261	252	24

H	K	L	10F$_o$	10F$_c$	10σ	H	K	L	10F$_o$	10F$_c$	10σ
3	4	11	135	82	-44	1	-6	12	49	46	-52
4	4	11	46	3	-123	2	-6	12	99	70	-25
-6	5	11	40	4	-107	-5	-5	12	271	225	22
-5	5	11	95	129	-46	-4	-5	12	141	171	28
-4	5	11	173	218	28	-3	-5	12	84	118	-37
-3	5	11	206	278	26	-2	-5	12	30	36	-81
-2	5	11	246	267	23	-1	-5	12	124	117	21
-1	5	11	156	190	-36	0	-5	12	267	263	15
0	5	11	138	95	-35	1	-5	12	240	248	14
1	5	11	70	106	-78	2	-5	12	213	198	14
2	5	11	169	173	35	3	-5	12	168	179	17
3	5	11	215	226	30	-6	-4	12	39	49	-104
-6	6	11	133	162	-33	-5	-4	12	87	44	-38
-5	6	11	137	181	-32	-4	-4	12	207	193	17
-4	6	11	146	122	30	-3	-4	12	210	203	16
-3	6	11	39	18	-104	-2	-4	12	332	326	13
-2	6	11	58	103	-75	-1	-4	12	260	267	15
-1	6	11	257	245	26	0	-4	12	156	140	17
0	6	11	299	267	22	1	-4	12	68	34	-31
1	6	11	243	257	26	2	-4	12	131	135	18
2	6	11	202	177	29	3	-4	12	145	142	17
3	6	11	43	53	-115	-6	-3	12	219	238	22
-5	7	11	39	110	-104	-5	-3	12	198	204	18
-4	7	11	162	180	27	-4	-3	12	192	210	17
-3	7	11	258	250	21	-3	-3	12	92	84	-24
-2	7	11	172	189	29	-2	-3	12	87	51	-25
-1	7	11	132	138	-41	-1	-3	12	229	198	12
0	7	11	41	34	-110	0	-3	12	344	335	13
1	7	11	129	93	-37	1	-3	12	250	243	14
2	7	11	47	145	-126	2	-3	12	255	247	14
-4	8	11	38	72	-100	3	-3	12	148	135	17
-3	8	11	72	7	-53	4	-3	12	29	31	-77
-2	8	11	39	108	-105	-7	-2	12	113	91	-32
-1	8	11	198	175	24	-6	-2	12	56	37	-46
0	8	11	232	187	25	-5	-2	12	105	103	-25
-4	-7	12	157	132	32	-4	-2	12	185	201	15
-3	-7	12	132	130	-32	-3	-2	12	286	275	12
-2	-7	12	35	3	-93	-2	-2	12	371	381	13
-1	-7	12	100	107	-31	-1	-2	12	255	246	12
0	-7	12	186	175	18	0	-2	12	161	146	16
1	-7	12	208	202	17	1	-2	12	28	16	-74
-5	-6	12	118	18	-39	2	-2	12	125	130	19
-4	-6	12	175	156	27	3	-2	12	192	194	16
-3	-6	12	202	203	21	4	-2	12	270	267	14
-2	-6	12	255	254	18	-7	-1	12	162	165	23
-1	-6	12	293	265	14	-6	-1	12	230	237	14
0	-6	12	118	99	24	-5	-1	12	219	231	14

H	K	L	10F$_O$	10F$_C$	10σ
-4	-1	12	213	220	13
-3	-1	12	46	52	-42
-2	-1	12	93	49	20
-1	-1	12	246	270	13
0	-1	12	299	309	12
1	-1	12	261	252	14
2	-1	12	290	292	14
3	-1	12	142	107	20
4	-1	12	30	27	-80
-7	0	12	105	92	-25
-6	0	12	27	21	-73
-5	0	12	136	152	17
-4	0	12	163	186	15
-3	0	12	291	312	12
-2	0	12	330	332	12
-1	0	12	234	237	14
0	0	12	137	131	19
1	0	12	88	70	-30
2	0	12	128	129	23
3	0	12	256	269	17
4	0	12	242	236	18
-7	1	12	196	178	15
-6	1	12	202	224	15
-5	1	12	202	236	14
-4	1	12	98	141	-22
-3	1	12	28	43	-75
-2	1	12	28	83	-76
-1	1	12	290	306	14
0	1	12	293	300	16
1	1	12	280	297	16
2	1	12	248	226	19
3	1	12	129	104	-33
4	1	12	38	7	-101
-7	2	12	79	88	-29
-6	2	12	40	5	-50
-5	2	12	112	135	22
-4	2	12	190	198	15
-3	2	12	314	319	14
-2	2	12	247	293	16
-1	2	12	241	248	18
0	2	12	38	74	-102
1	2	12	40	82	-108
2	2	12	168	140	32
3	2	12	274	266	27
4	2	12	185	206	32
-6	3	12	185	188	17
-5	3	12	198	219	16
-4	3	12	64	101	-42
-3	3	12	36	27	-96
-2	3	12	164	136	26
-1	3	12	264	258	23
0	3	12	277	263	28
1	3	12	277	286	28
2	3	12	124	163	-51
3	3	12	159	103	-38
-6	4	12	33	37	-88
-5	4	12	87	112	-41
-4	4	12	191	225	26
-3	4	12	230	266	26
-2	4	12	189	231	31
-1	4	12	138	185	-43
0	4	12	103	24	-51
1	4	12	100	66	-55
2	4	12	170	182	37
3	4	12	218	224	33
-5	5	12	158	171	28
-4	5	12	80	93	-54
-3	5	12	40	2	-107
-2	5	12	104	144	-46
-1	5	12	139	194	-44

Table 67. F_o F_c Tables for $K_2[Pt(NO_2)_2(NO)Cl_3]$, 2, F(obs), F(calc), and σ_F ($-\sigma_F$ indicates omitted data).

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
1	0	0	2470	2196	22	1	5	0	1665	1638	22
2	0	0	297	233	-70	2	5	0	1807	1818	27
3	0	0	1638	1534	29	3	5	0	846	807	53
4	0	0	2313	2190	10	4	5	0	405	403	44
5	0	0	1481	1317	30	5	5	0	712	687	46
6	0	0	546	477	72	6	5	0	1234	1240	37
7	0	0	779	722	47	7	5	0	610	612	52
8	0	0	448	582	67	8	5	0	256	381	-140
1	1	0	2389	2079	329	0	6	0	2320	2370	9
2	1	0	1335	1201	139	1	6	0	1177	1244	44
3	1	0	1451	1313	109	2	6	0	100	63	-64
4	1	0	942	831	71	3	6	0	699	690	28
5	1	0	888	803	60	4	6	0	977	915	32
6	1	0	1482	1345	43	5	6	0	1355	1277	81
7	1	0	1317	1397	43	6	6	0	186	129	-86
8	1	0	304	364	-84	7	6	0	457	358	-158
0	2	0	2796	2749	26	8	6	0	317	333	-131
1	2	0	2189	2118	25	1	7	0	396	402	29
2	2	0	523	506	103	2	7	0	1275	1270	26
3	2	0	1168	1040	75	3	7	0	477	477	52
4	2	0	2060	1956	167	4	7	0	709	681	34
5	2	0	1493	1442	33	5	7	0	514	519	76
6	2	0	808	736	51	6	7	0	641	665	48
7	2	0	276	283	-83	7	7	0	461	500	64
8	2	0	707	849	86	0	8	0	348	345	42
1	3	0	809	760	44	1	8	0	516	497	27
2	3	0	1958	1817	160	2	8	0	499	486	35
3	3	0	2135	1968	170	3	8	0	530	527	35
4	3	0	152	147	-71	4	8	0	780	766	35
5	3	0	312	382	-88	5	8	0	619	614	50
6	3	0	1355	1304	99	6	8	0	308	363	-77
7	3	0	1124	1123	46	7	8	0	146	154	-119
8	3	0	494	567	-114	1	9	0	420	408	34
0	4	0	1848	1840	37	2	9	0	819	832	27
1	4	0	2541	2633	117	3	9	0	620	608	45
2	4	0	82	104	-77	4	9	0	177	218	-89
3	4	0	1178	1115	65	5	9	0	212	183	-112
4	4	0	1404	1391	119	6	9	0	187	218	-129
5	4	0	1346	1269	88	7	9	0	236	294	-106
6	4	0	165	232	-95	0	10	0	551	538	40
7	4	0	93	133	-167	1	10	0	450	455	36
8	4	0	528	620	-167	2	10	0	193	208	-57

Table 67. (continued)

H	K	L	$10F_o$	$10F_c$	10σ
3	10	0	179	193	-69
4	10	0	433	427	48
5	10	0	86	89	-155
6	10	0	102	24	-182
1	11	0	776	754	28
2	11	0	63	36	-113
3	11	0	262	366	-70
4	11	0	181	85	-76
5	11	0	93	119	-236
6	11	0	211	258	-111
0	12	0	124	55	-85
1	12	0	414	388	40
2	12	0	70	14	-125
3	12	0	433	378	60
4	12	0	176	14	-84
5	12	0	97	162	-174
1	13	0	102	17	-99
2	13	0	174	119	-82
3	13	0	81	56	-146
4	13	0	118	24	-118
5	13	0	171	7	-122
0	14	0	334	233	69
1	14	0	246	301	-74
2	14	0	147	72	-99
3	14	0	123	91	-112
4	14	0	232	170	-100
1	15	0	167	195	-87
2	15	0	127	56	-110
3	15	0	227	304	-86
0	16	0	452	431	88
1	16	0	129	179	-107
2	16	0	77	149	-139
-8	1	1	108	101	-275
-7	1	1	173	190	-136
-6	1	1	201	269	-120
-5	1	1	128	140	-121
-4	1	1	634	670	39
-3	1	1	962	953	28
-2	1	1	833	813	26
-1	1	1	216	225	28
0	1	1	244	239	17
1	1	1	765	694	29
2	1	1	636	542	36
3	1	1	612	554	43
4	1	1	494	433	54
5	1	1	81	14	-204
6	1	1	89	175	-226
7	1	1	70	173	-179

H	K	L	$10F_o$	$10F_c$	10σ
8	1	1	155	193	-132
-8	2	1	317	365	-136
-7	2	1	233	195	-129
-6	2	1	83	67	-211
-5	2	1	331	437	-77
-4	2	1	817	814	36
-3	2	1	324	359	48
-2	2	1	376	404	33
-1	2	1	392	433	23
0	2	1	405	397	18
1	2	1	759	782	26
2	2	1	629	559	36
3	2	1	77	173	-197
4	2	1	406	344	68
5	2	1	214	117	-99
6	2	1	187	263	-107
7	2	1	282	424	-111
8	2	1	93	179	-236
-8	3	1	108	260	-273
-7	3	1	178	299	-143
-6	3	1	604	589	50
-5	3	1	590	589	47
-4	3	1	266	423	-63
-3	3	1	760	765	33
-2	3	1	51	91	-128
-1	3	1	1082	1039	28
0	3	1	913	973	26
1	3	1	740	772	27
2	3	1	278	287	-60
3	3	1	1340	1174	44
4	3	1	225	261	-108
5	3	1	125	272	-148
6	3	1	77	37	-195
7	3	1	494	549	91
8	3	1	81	204	-206
-8	4	1	372	305	-117
-7	4	1	202	372	-152
-6	4	1	85	79	-216
-5	4	1	338	384	66
-4	4	1	656	649	41
-3	4	1	467	468	39
-2	4	1	974	981	28
-1	4	1	1930	1931	39
0	4	1	1160	1200	28
1	4	1	1416	1500	30
2	4	1	1529	1483	33
3	4	1	400	354	50
4	4	1	819	746	50

Table 67. (continued)

H	K	L	$10F_O$	$10F_C$	10σ	H	K	L	$10F_O$	$10F_C$	10σ
5	4	1	903	905	50	4	7	1	875	838	51
6	4	1	995	971	53	5	7	1	484	350	73
7	4	1	75	116	-190	6	7	1	88	193	-223
8	4	1	286	320	-94	7	7	1	336	464	-111
-8	5	1	274	293	-158	-7	8	1	528	494	87
-7	5	1	245	269	-113	-6	8	1	266	201	-106
-6	5	1	549	664	66	-5	8	1	142	294	-146
-5	5	1	1196	1217	40	-4	8	1	746	798	46
-4	5	1	65	92	-165	-3	8	1	1240	1262	40
-3	5	1	319	326	54	-2	8	1	1245	1272	38
-2	5	1	585	563	30	-1	8	1	236	252	-55
-1	5	1	1456	1436	31	0	8	1	282	316	53
0	5	1	661	612	24	1	8	1	2098	2098	40
1	5	1	151	23	-48	2	8	1	1514	1517	37
2	5	1	967	980	35	3	8	1	230	264	-95
3	5	1	417	430	59	4	8	1	710	682	57
4	5	1	1116	971	45	5	8	1	1466	1360	52
5	5	1	551	541	66	6	8	1	684	620	73
6	5	1	90	76	-227	7	8	1	370	397	-102
7	5	1	473	651	89	-7	9	1	156	173	-189
8	5	1	464	493	71	-6	9	1	1057	1058	55
-8	6	1	552	520	98	-5	9	1	847	871	49
-7	6	1	694	683	70	-4	9	1	584	537	53
-6	6	1	453	430	73	-3	9	1	289	178	58
-5	6	1	341	327	62	-2	9	1	1250	1228	39
-4	6	1	1125	1101	36	-1	9	1	1251	1245	37
-3	6	1	1824	1779	42	0	9	1	1173	1168	37
-2	6	1	532	555	32	1	9	1	66	30	-169
-1	6	1	265	241	37	2	9	1	853	930	38
0	6	1	1734	1754	33	3	9	1	1308	1361	39
1	6	1	1527	1656	35	4	9	1	1064	1088	49
2	6	1	904	983	31	5	9	1	483	491	98
3	6	1	76	42	-191	6	9	1	416	490	-118
4	6	1	653	642	59	7	9	1	577	601	77
5	6	1	868	763	54	-6	10	1	468	492	82
6	6	1	743	797	66	-5	10	1	534	542	75
7	6	1	89	239	-227	-4	10	1	868	941	46
-7	7	1	256	373	-127	-3	10	1	1068	1088	40
-6	7	1	928	910	51	-2	10	1	1212	1122	35
-5	7	1	1000	998	43	-1	10	1	88	51	-107
-4	7	1	579	627	49	0	10	1	858	851	35
-3	7	1	450	477	48	1	10	1	1667	1614	37
-2	7	1	1734	1742	40	2	10	1	930	977	37
-1	7	1	1040	1030	33	3	10	1	184	218	-105
0	7	1	741	728	29	4	10	1	189	304	-110
1	7	1	288	278	37	5	10	1	1274	1207	57
2	7	1	817	843	34	6	10	1	800	805	83
3	7	1	937	990	43	-6	11	1	652	789	78

H	K	L	$10F_o$	$10F_c$	10σ
-5	11	1	1202	1143	49
-4	11	1	351	427	-84
-3	11	1	366	345	75
-2	11	1	1154	1169	40
-1	11	1	1430	1409	42
0	11	1	682	730	41
1	11	1	57	59	-145
2	11	1	828	883	44
3	11	1	748	790	50
4	11	1	911	942	55
5	11	1	345	345	-103
6	11	1	348	265	-138
-5	12	1	89	265	-226
-4	12	1	871	917	51
-3	12	1	1248	1274	44
-2	12	1	457	433	59
-1	12	1	64	45	-163
0	12	1	1100	1086	41
1	12	1	1093	1066	40
2	12	1	903	934	46
3	12	1	84	157	-212
4	12	1	683	605	64
5	12	1	634	652	79
-5	13	1	670	702	76
-4	13	1	512	497	68
-3	13	1	314	214	-78
-2	13	1	778	730	47
-1	13	1	999	1017	43
0	13	1	728	782	52
1	13	1	315	291	62
2	13	1	656	636	54
3	13	1	1153	1139	47
4	13	1	721	782	63
5	13	1	87	129	-221
-4	14	1	760	744	60
-3	14	1	818	775	55
-2	14	1	538	531	70
-1	14	1	138	154	-124
0	14	1	643	667	51
1	14	1	910	928	47
2	14	1	772	825	58
3	14	1	227	224	-110
4	14	1	512	585	85
-3	15	1	186	218	-127
-2	15	1	513	420	75
-1	15	1	860	872	55
0	15	1	757	727	55
1	15	1	83	153	-209
2	15	1	294	360	-94
3	15	1	823	824	61
-2	16	1	368	425	-112
-1	16	1	172	95	-109
0	16	1	586	596	60
1	16	1	662	652	59
-8	0	2	615	602	84
-7	0	2	1277	1182	52
-6	0	2	1331	1299	42
-5	0	2	282	393	-83
-4	0	2	1219	1216	32
-3	0	2	2074	2060	35
-2	0	2	287	326	36
-1	0	2	1986	1918	28
0	0	2	185	174	29
1	0	2	1969	1605	45
2	0	2	2974	2374	53
3	0	2	2635	2243	44
4	0	2	517	510	53
5	0	2	261	258	-93
6	0	2	2195	2026	50
7	0	2	1277	1245	52
8	0	2	289	397	-116
-8	1	2	1101	1001	65
-7	1	2	349	320	-88
-6	1	2	135	272	-162
-5	1	2	1944	1872	40
-4	1	2	2545	2469	41
-3	1	2	904	895	28
-2	1	2	61	158	-155
-1	1	2	2273	2167	29
0	1	2	2621	2767	27
1	1	2	2422	2428	41
2	1	2	247	215	-80
3	1	2	1209	1053	35
4	1	2	1389	1286	42
5	1	2	1312	1208	42
6	1	2	772	636	54
7	1	2	392	473	-84
8	1	2	618	746	85
-8	2	2	555	533	90
-7	2	2	998	944	57
-6	2	2	827	808	48
-5	2	2	860	903	42
-4	2	2	306	354	62
-3	2	2	1623	1631	35
-2	2	2	2552	2527	39
-1	2	2	1762	1745	33

Table 67. (continued)

H	K	L	$10F_o$	$10F_c$	10σ
0	2	2	49	76	-123
1	2	2	1915	1865	41
2	2	2	3943	3572	53
3	2	2	2488	2136	47
4	2	2	81	73	-205
5	2	2	832	767	48
6	2	2	1264	1193	48
7	2	2	1093	1173	56
8	2	2	283	430	-129
-8	3	2	782	776	74
-7	3	2	518	397	73
-6	3	2	633	596	50
-5	3	2	1277	1276	38
-4	3	2	2335	2390	42
-3	3	2	1802	1867	36
-2	3	2	985	942	26
-1	3	2	1945	1919	37
0	3	2	2217	2218	35
1	3	2	981	960	26
2	3	2	506	477	37
3	3	2	2133	1904	49
4	3	2	1443	1286	45
5	3	2	712	693	54
6	3	2	348	436	-105
7	3	2	89	168	-226
8	3	2	702	728	77
-8	4	2	532	461	94
-7	4	2	902	905	58
-6	4	2	919	887	48
-5	4	2	486	548	53
-4	4	2	433	450	51
-3	4	2	1194	1149	32
-2	4	2	2142	2142	45
-1	4	2	471	456	26
0	4	2	637	669	24
1	4	2	1074	1094	27
2	4	2	2434	2410	39
3	4	2	1708	1615	40
4	4	2	878	785	48
5	4	2	981	907	49
6	4	2	991	982	53
7	4	2	1118	1144	57
8	4	2	377	468	-93
-8	5	2	463	525	-105
-7	5	2	350	453	-111
-6	5	2	596	600	58
-5	5	2	1160	1221	39
-4	5	2	1206	1185	34
-3	5	2	736	758	34
-2	5	2	709	742	29
-1	5	2	866	902	28
0	5	2	1811	1899	43
1	5	2	1559	1643	34
2	5	2	48	44	-122
3	5	2	194	226	-94
4	5	2	1323	1182	43
5	5	2	1232	1169	48
6	5	2	296	210	-100
7	5	2	175	285	-180
8	5	2	478	629	95
-8	6	2	258	253	-155
-7	6	2	562	602	78
-6	6	2	1064	1100	48
-5	6	2	72	105	-182
-4	6	2	108	117	-119
-3	6	2	1280	1281	36
-2	6	2	983	1022	32
-1	6	2	838	847	26
0	6	2	253	273	43
1	6	2	1431	1510	30
2	6	2	1014	1063	32
3	6	2	829	866	43
4	6	2	684	670	56
5	6	2	519	569	78
6	6	2	1034	1006	56
7	6	2	506	594	72
-6	7	2	86	128	-218
-5	7	2	783	755	47
-4	7	2	910	841	40
-3	7	2	1035	1041	33
-2	7	2	55	21	-139
-1	7	2	1094	1095	33
0	7	2	1100	1092	31
1	7	2	1368	1423	32
2	7	2	479	501	40
3	7	2	304	303	-73
4	7	2	1095	1080	46
5	7	2	712	722	68
7	7	2	208	69	-122
-7	8	2	365	440	-111
-6	8	2	559	501	68
-5	8	2	217	314	-99
-4	8	2	76	193	-192
-3	8	2	1045	1074	36
-2	8	2	1301	1270	36
-1	8	2	480	534	42

Table 67. (continued)

H	K	L	$10F_o$	$10F_c$	10σ
0	8	2	325	305	49
1	8	2	718	758	34
2	8	2	927	965	36
3	8	2	671	689	47
4	8	2	90	300	-228
5	8	2	328	335	-108
6	8	2	311	293	-120
7	8	2	207	310	-140
-7	9	2	101	31	-257
-6	9	2	85	135	-216
-5	9	2	259	248	-81
-4	9	2	493	484	58
-3	9	2	447	401	47
-2	9	2	169	151	-68
-1	9	2	399	398	39
0	9	2	426	377	42
1	9	2	526	546	42
2	9	2	591	627	43
3	9	2	602	651	52
4	9	2	697	675	57
5	9	2	441	403	82
6	9	2	104	197	-265
7	9	2	102	167	-260
-6	10	2	218	220	-112
-5	10	2	217	388	-126
-4	10	2	425	456	58
-3	10	2	200	200	-92
-2	10	2	339	363	61
-1	10	2	141	69	-79
0	10	2	55	20	-139
1	10	2	170	130	-74
2	10	2	305	294	54
3	10	2	78	220	-197
4	10	2	87	122	-222
5	10	2	93	38	-235
6	10	2	98	206	-247
-6	11	2	83	45	-211
-5	11	2	150	67	-153
-4	11	2	84	123	-214
-3	11	2	431	338	62
-2	11	2	68	151	-172
0	11	2	570	556	47
1	11	2	65	44	-163
2	11	2	183	199	-91
3	11	2	162	252	-121
4	11	2	85	46	-217
5	11	2	106	246	-270
6	11	2	212	160	-150
-5	12	2	417	328	-94
-4	12	2	186	41	-96
-3	12	2	207	3	-65
-2	12	2	169	89	-81
-1	12	2	428	479	65
0	12	2	66	108	-169
1	12	2	214	256	-98
2	12	2	70	83	-178
3	12	2	237	221	-77
4	12	2	90	134	-228
5	12	2	95	79	-240
-5	13	2	94	102	-240
-4	13	2	74	13	-188
-3	13	2	144	108	-128
-2	13	2	256	180	-87
-1	13	2	60	25	-152
0	13	2	184	126	-98
1	13	2	128	16	-124
2	13	2	78	123	-199
3	13	2	175	108	-106
4	13	2	93	39	-237
5	13	2	236	113	-151
-4	14	2	83	161	-210
-3	14	2	79	65	-199
-2	14	2	89	254	-225
-1	14	2	131	177	-114
0	14	2	126	47	-107
1	14	2	245	338	-101
2	14	2	298	216	-74
3	14	2	258	72	-87
4	14	2	256	266	-119
-3	15	2	142	153	-146
-2	15	2	115	26	-117
-1	15	2	245	294	-100
0	15	2	560	541	65
1	15	2	209	76	-104
2	15	2	86	86	-219
3	15	2	89	155	-226
-1	16	2	226	275	-107
0	16	2	89	106	-227
1	16	2	190	175	-106
-8	1	3	110	204	-279
-7	1	3	97	23	-246
-6	1	3	83	75	-210
-5	1	3	308	326	-80
-4	1	3	148	145	-93
-3	1	3	570	605	33
-2	1	3	79	181	-95

H	K	L	10F$_o$	10F$_c$	10σ	H	K	L	10F$_o$	10F$_c$	10σ
-1	1	3	49	87	-124	-4	4	3	72	107	-183
0	1	3	277	290	31	-3	4	3	809	846	30
1	1	3	274	244	44	-2	4	3	582	560	29
2	1	3	1488	1351	34	-1	4	3	1425	1406	30
3	1	3	505	477	51	0	4	3	213	115	32
4	1	3	507	493	59	1	4	3	512	531	30
5	1	3	81	63	-204	2	4	3	373	407	50
6	1	3	110	111	-136	3	4	3	902	836	39
7	1	3	80	35	-204	4	4	3	566	532	55
8	1	3	80	101	-203	5	4	3	901	840	50
-8	2	3	97	10	-246	6	4	3	191	233	-114
-7	2	3	507	472	76	7	4	3	480	463	70
-6	2	3	75	180	-190	8	4	3	313	383	-140
-5	2	3	538	562	52	-8	5	3	479	565	99
-4	2	3	58	50	-148	-7	5	3	574	544	72
-3	2	3	201	246	-53	-6	5	3	591	652	59
-2	2	3	790	818	27	-5	5	3	220	247	-84
-1	2	3	556	589	22	-4	5	3	1261	1287	38
0	2	3	360	340	24	-3	5	3	887	874	31
1	2	3	1825	1848	43	-2	5	3	1559	1654	35
2	2	3	841	833	33	-1	5	3	197	200	-54
3	2	3	1061	980	40	0	5	3	892	929	29
4	2	3	528	507	56	1	5	3	1704	1772	35
5	2	3	147	45	-92	2	5	3	788	731	34
6	2	3	196	113	-86	3	5	3	153	62	-87
7	2	3	184	398	-144	4	5	3	583	571	61
8	2	3	169	299	-163	5	5	3	886	869	54
-8	3	3	243	407	-185	6	5	3	531	539	75
-7	3	3	298	324	-100	7	5	3	212	164	-109
-6	3	3	390	396	71	-8	6	3	97	74	-245
-5	3	3	154	155	-111	-7	6	3	437	522	85
-4	3	3	1048	1055	33	-6	6	3	784	799	52
-3	3	3	752	734	30	-5	6	3	284	323	-71
-2	3	3	536	584	29	-4	6	3	456	423	46
-1	3	3	170	196	-45	-3	6	3	562	537	39
0	3	3	860	825	23	-2	6	3	815	777	30
1	3	3	140	157	-79	-1	6	3	1077	1047	29
2	3	3	875	843	31	0	6	3	1268	1332	30
3	3	3	391	368	65	1	6	3	507	554	35
4	3	3	278	243	-103	2	6	3	389	428	44
5	3	3	225	233	-95	3	6	3	1596	1620	43
6	3	3	487	557	72	4	6	3	1054	1012	46
7	3	3	77	46	-196	5	6	3	233	379	-151
8	3	3	79	80	-201	6	6	3	376	372	-93
-8	4	3	110	34	-280	7	6	3	659	676	82
-7	4	3	203	162	-136	-7	7	3	744	726	61
-6	4	3	755	739	48	-6	7	3	172	288	-163
-5	4	3	1064	1023	38	-5	7	3	73	98	-186

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
-4	7	3	618	647	45	1	10	3	190	166	-60
-3	7	3	2017	2022	43	2	10	3	794	826	44
-2	7	3	829	869	32	3	10	3	983	1027	47
-1	7	3	134	212	-70	4	10	3	1305	1278	49
0	7	3	888	940	30	5	10	3	194	321	-158
1	7	3	1739	1816	39	6	10	3	119	386	-303
2	7	3	1266	1316	39	-6	11	3	173	316	-177
3	7	3	161	94	-108	-5	11	3	243	274	-82
4	7	3	1003	946	49	-4	11	3	851	842	50
5	7	3	954	932	62	-3	11	3	1064	980	43
6	7	3	428	519	76	-2	11	3	1036	990	40
7	7	3	362	446	-94	-1	11	3	110	33	-79
-7	8	3	535	562	83	0	11	3	937	941	40
-6	8	3	879	927	54	1	11	3	1457	1513	42
-5	8	3	818	847	48	2	11	3	769	883	46
-4	8	3	596	582	45	3	11	3	201	273	-96
-3	8	3	456	408	50	4	11	3	658	653	64
-2	8	3	1863	1847	43	5	11	3	950	967	65
-1	8	3	1025	1018	31	6	11	3	667	696	99
0	8	3	862	853	31	-5	12	3	692	652	64
1	8	3	143	148	-88	-4	12	3	577	619	61
2	8	3	787	832	37	-3	12	3	271	307	-92
3	8	3	1005	1020	41	-2	12	3	933	924	44
4	8	3	1344	1383	46	-1	12	3	1265	1221	38
5	8	3	172	171	-126	0	12	3	904	846	44
6	8	3	88	75	-224	1	12	3	209	215	-91
7	8	3	584	696	92	2	12	3	465	553	67
-7	9	3	895	948	63	3	12	3	1298	1333	47
-6	9	3	318	281	-102	4	12	3	678	688	73
-5	9	3	448	478	69	5	12	3	177	307	-167
-4	9	3	964	955	43	-5	13	3	104	160	-263
-3	9	3	1754	1695	40	-4	13	3	822	827	55
-2	9	3	524	514	45	-3	13	3	1018	1032	50
-1	9	3	58	53	-147	-2	13	3	689	688	52
0	9	3	1332	1366	37	-1	13	3	473	470	57
1	9	3	1122	1128	34	0	13	3	605	552	50
2	9	3	523	576	47	1	13	3	891	907	46
3	9	3	300	306	-77	2	13	3	965	959	46
4	9	3	591	546	62	4	13	3	428	429	-106
5	9	3	883	871	65	-4	14	3	456	362	78
6	9	3	717	722	84	-2	14	3	931	865	47
-6	10	3	889	971	60	-1	14	3	1017	949	48
-5	10	3	905	916	49	0	14	3	244	342	-104
-4	10	3	338	306	65	1	14	3	137	62	-109
-3	10	3	388	227	59	2	14	3	559	558	66
-2	10	3	1006	1001	38	3	14	3	880	810	62
-1	10	3	1436	1444	39	4	14	3	561	474	85
0	10	3	1186	1183	40	-3	15	3	552	578	66

H	K	L	$10F_O$	$10F_C$	10σ
-2	15	3	460	457	66
-1	15	3	180	82	-104
0	15	3	732	670	61
1	15	3	618	666	65
2	15	3	740	709	59
3	15	3	78	27	-199
-1	16	3	835	788	61
0	16	3	665	574	67
1	16	3	164	118	-113
-8	0	4	786	686	73
-7	0	4	631	614	67
-6	0	4	383	479	72
-5	0	4	1568	1602	40
-4	0	4	1673	1662	34
-3	0	4	1018	1016	30
-2	0	4	332	355	29
-1	0	4	2456	2486	36
0	0	4	2457	2521	38
1	0	4	1357	1258	36
2	0	4	275	255	-77
3	0	4	1626	1471	40
4	0	4	1051	1015	42
5	0	4	1750	1661	47
6	0	4	167	301	-126
7	0	4	330	439	-109
8	0	4	438	599	88
-8	1	4	629	582	79
-7	1	4	927	897	54
-6	1	4	1311	1374	42
-5	1	4	916	940	39
-4	1	4	747	747	33
-3	1	4	1491	1442	28
-2	1	4	3801	3859	40
-1	1	4	1848	1813	36
0	1	4	77	25	-93
1	1	4	2133	2001	46
2	1	4	3531	3107	57
3	1	4	1722	1532	41
4	1	4	488	506	64
5	1	4	883	892	47
6	1	4	1247	1260	48
7	1	4	627	754	74
8	1	4	214	394	-131
-8	2	4	1032	1019	61
-7	2	4	88	162	-222
-6	2	4	661	675	52
-5	2	4	1582	1659	41
-4	2	4	1584	1563	34

H	K	L	$10F_O$	$10F_C$	10σ
-3	2	4	823	821	28
-2	2	4	633	622	26
-1	2	4	1674	1652	38
0	2	4	589	595	23
1	2	4	1195	1201	28
2	2	4	673	611	37
3	2	4	1122	992	39
4	2	4	1928	1784	44
5	2	4	1464	1399	42
6	2	4	478	562	81
7	2	4	257	284	-88
8	2	4	771	899	69
-8	3	4	712	547	69
-7	3	4	991	1028	52
-6	3	4	736	788	50
-5	3	4	250	341	-79
-4	3	4	100	88	-110
-3	3	4	1958	1920	36
-2	3	4	1849	1830	31
-1	3	4	1989	1999	40
0	3	4	50	14	-126
1	3	4	644	656	27
2	3	4	2393	2326	41
3	3	4	2567	2395	49
4	3	4	354	222	65
5	3	4	549	611	58
6	3	4	972	991	55
7	3	4	760	857	65
8	3	4	253	449	-139
-8	4	4	812	919	71
-7	4	4	97	242	-246
-6	4	4	488	448	61
-5	4	4	1171	1205	37
-4	4	4	1558	1562	35
-3	4	4	1263	1225	32
-2	4	4	490	506	29
-1	4	4	1888	1948	44
0	4	4	1833	1847	31
1	4	4	1231	1235	30
2	4	4	259	225	-70
3	4	4	837	754	41
4	4	4	1846	1746	49
5	4	4	758	795	55
6	4	4	330	399	-107
7	4	4	140	259	-169
-8	5	4	221	132	-122
-7	5	4	834	932	58
-6	5	4	1008	977	45

H	K	L	10F$_o$	10F$_c$	10σ	H	K	L	10F$_o$	10F$_c$	10σ
-5	5	4	496	491	52	-3	8	4	542	471	44
-4	5	4	131	92	-95	-2	8	4	134	56	-87
-3	5	4	1535	1554	33	-1	8	4	391	334	44
-2	5	4	1700	1739	35	0	8	4	687	715	34
-1	5	4	1630	1652	34	1	8	4	289	365	-64
0	5	4	306	331	39	2	8	4	532	533	46
1	5	4	1714	1891	37	3	8	4	385	442	57
2	5	4	1016	1136	33	4	8	4	829	813	56
3	5	4	1155	1143	39	5	8	4	469	511	89
4	5	4	246	249	-107	6	8	4	198	257	-168
5	5	4	578	520	60	7	8	4	91	154	-230
6	5	4	924	779	58	-7	9	4	333	352	-119
7	5	4	663	771	75	-6	9	4	283	359	-91
-8	6	4	492	489	98	-5	9	4	234	210	-96
-7	6	4	549	562	72	-4	9	4	70	25	-177
-6	6	4	567	609	61	-3	9	4	618	642	47
-5	6	4	717	725	46	-2	9	4	719	728	37
-4	6	4	1090	1105	35	-1	9	4	156	273	-114
-3	6	4	681	647	34	0	9	4	331	314	51
-2	6	4	172	182	-57	1	9	4	157	187	-88
-1	6	4	915	900	28	2	9	4	536	631	48
0	6	4	2305	2351	51	3	9	4	380	441	70
1	6	4	498	524	35	4	9	4	213	70	-94
2	6	4	60	20	-153	5	9	4	249	154	-103
3	6	4	480	503	59	6	9	4	183	257	-154
4	6	4	1065	1016	47	-6	10	4	96	242	-244
5	6	4	934	868	56	-5	10	4	90	324	-228
6	6	4	203	207	-121	-4	10	4	322	318	-86
7	6	4	233	356	-141	-3	10	4	550	541	51
-7	7	4	776	753	64	-2	10	4	117	102	-91
-6	7	4	704	651	56	-1	10	4	903	850	35
-5	7	4	175	225	-98	0	10	4	431	482	50
-4	7	4	461	441	54	1	10	4	612	682	44
-3	7	4	629	631	39	2	10	4	201	230	-76
-2	7	4	1202	1148	35	3	10	4	349	380	67
-1	7	4	557	594	33	4	10	4	207	322	-127
0	7	4	320	307	46	5	10	4	103	93	-260
1	7	4	931	967	32	6	10	4	94	71	-238
2	7	4	845	831	37	-6	11	4	223	330	-132
3	7	4	1127	1065	40	-5	11	4	90	91	-227
4	7	4	397	520	68	-4	11	4	225	140	-104
5	7	4	691	601	67	-3	11	4	131	85	-130
6	7	4	571	606	85	-2	11	4	129	61	-80
7	7	4	606	672	88	-1	11	4	189	151	-75
-7	8	4	92	124	-232	0	11	4	176	174	-85
-6	8	4	432	408	80	1	11	4	185	42	-92
-5	8	4	180	303	-131	2	11	4	115	188	-119
-4	8	4	768	694	43	3	11	4	128	70	-126

Table 67. (continued)

H	K	L	10F$_o$	10F$_c$	10σ
4	11	4	77	63	-196
5	11	4	98	73	-250
-5	12	4	249	241	-122
-4	12	4	229	123	-93
-3	12	4	76	35	-191
-2	12	4	210	175	-77
-1	12	4	72	52	-182
0	12	4	67	48	-169
1	12	4	287	284	-68
2	12	4	70	9	-178
3	12	4	187	62	-92
4	12	4	80	27	-204
5	12	4	101	259	-258
-5	13	4	95	15	-241
-4	13	4	173	132	-118
-3	13	4	302	317	-100
-2	13	4	79	99	-201
-1	13	4	347	338	68
0	13	4	155	135	-102
1	13	4	323	287	63
2	13	4	87	110	-219
3	13	4	79	86	-201
4	13	4	94	90	-238
-4	14	4	150	36	-142
-3	14	4	205	72	-91
-2	14	4	75	35	-189
-1	14	4	174	137	-116
0	14	4	71	165	-181
1	14	4	215	170	-95
2	14	4	86	151	-218
3	14	4	90	114	-227
-3	15	4	95	115	-241
-2	15	4	178	132	-122
-1	15	4	377	273	71
0	15	4	79	70	-202
1	15	4	74	151	-188
2	15	4	182	274	-112
-1	16	4	286	305	-87
0	16	4	184	222	-122
-8	1	5	98	81	-248
-7	1	5	94	106	-238
-6	1	5	199	307	-101
-5	1	5	76	85	-193
-4	1	5	316	372	46
-3	1	5	336	330	43
-2	1	5	714	759	25
-1	1	5	119	109	-55
0	1	5	472	528	27
1	1	5	1129	1076	31
2	1	5	444	420	44
3	1	5	439	348	65
4	1	5	149	32	-100
5	1	5	111	250	-139
6	1	5	148	68	-125
7	1	5	74	41	-189
8	1	5	244	339	-106
-8	2	5	397	497	-112
-7	2	5	93	146	-235
-6	2	5	322	369	-79
-5	2	5	418	377	54
-4	2	5	290	370	56
-3	2	5	794	769	29
-2	2	5	247	261	33
-1	2	5	2331	2365	41
0	2	5	410	441	29
1	2	5	710	730	29
2	2	5	125	137	-106
3	2	5	222	202	-114
4	2	5	198	159	-119
5	2	5	247	265	-102
6	2	5	81	75	-206
7	2	5	212	323	-110
-8	3	5	102	204	-260
-7	3	5	164	85	-120
-6	3	5	482	436	60
-5	3	5	363	426	64
-4	3	5	318	368	61
-3	3	5	394	432	39
-2	3	5	525	597	32
-1	3	5	1107	1152	27
0	3	5	1019	1073	27
1	3	5	722	731	30
2	3	5	779	810	35
3	3	5	1013	945	40
4	3	5	768	705	54
5	3	5	74	214	-188
6	3	5	417	526	88
7	3	5	97	173	-246
-8	4	5	318	302	-115
-7	4	5	500	455	74
-6	4	5	427	428	71
-5	4	5	396	498	57
-4	4	5	679	651	38
-3	4	5	655	643	33
-2	4	5	753	780	28
-1	4	5	275	287	39

Table 67. (continued)

H	K	L	$10F_o$	$10F_c$	10σ
0	4	5	1067	1082	28
1	4	5	1143	1178	32
2	4	5	503	526	46
3	4	5	63	113	-160
4	4	5	214	182	-101
5	4	5	1075	1005	50
6	4	5	495	501	64
7	4	5	152	67	-137
-8	5	5	103	65	-262
-7	5	5	382	373	-85
-6	5	5	635	659	53
-5	5	5	1110	1099	38
-4	5	5	69	65	-176
-3	5	5	258	164	-63
-2	5	5	1089	1046	32
-1	5	5	1383	1372	29
0	5	5	1235	1336	30
1	5	5	126	135	-73
2	5	5	841	870	37
3	5	5	741	709	45
4	5	5	1232	1225	45
5	5	5	82	166	-207
6	5	5	331	446	-109
7	5	5	424	565	85
-8	6	5	542	538	90
-7	6	5	932	871	57
-6	6	5	87	301	-220
-5	6	5	216	239	-93
-4	6	5	1088	1114	36
-3	6	5	1292	1297	37
-2	6	5	140	153	-89
-1	6	5	583	604	33
0	6	5	1473	1502	31
1	6	5	648	661	34
2	6	5	736	761	37
3	6	5	77	139	-196
4	6	5	434	384	67
5	6	5	645	621	71
6	6	5	723	800	72
7	6	5	378	449	-95
-7	7	5	676	674	69
-6	7	5	909	904	49
-5	7	5	767	749	46
-4	7	5	730	708	41
-3	7	5	401	444	50
-2	7	5	1352	1295	35
-1	7	5	1409	1457	33
0	7	5	959	953	30
1	7	5	459	448	44
2	7	5	387	440	66
3	7	5	1426	1410	45
4	7	5	817	820	54
5	7	5	173	141	-157
6	7	5	98	199	-250
7	7	5	597	699	84
-7	8	5	513	686	93
-6	8	5	78	164	-199
-5	8	5	183	229	-89
-4	8	5	955	968	40
-3	8	5	1156	1148	35
-2	8	5	811	777	34
-1	8	5	342	373	46
0	8	5	1124	1119	37
1	8	5	1423	1484	38
2	8	5	825	863	39
3	8	5	217	237	-91
4	8	5	941	931	53
5	8	5	757	723	65
6	8	5	773	777	78
-7	9	5	234	397	-132
-6	9	5	863	881	55
-5	9	5	768	743	48
-4	9	5	789	830	44
-3	9	5	287	296	-66
-2	9	5	297	414	-70
-1	9	5	1905	1899	46
0	9	5	1572	1573	38
1	9	5	156	148	-63
2	9	5	725	665	44
3	9	5	1597	1540	48
4	9	5	872	934	55
5	9	5	333	346	-125
6	9	5	330	420	-156
-6	10	5	260	418	-118
-5	10	5	467	490	73
-4	10	5	1226	1205	42
-3	10	5	1031	954	42
-2	10	5	665	675	44
-1	10	5	62	45	-158
0	10	5	1397	1425	40
1	10	5	1294	1338	43
2	10	5	525	509	54
3	10	5	238	247	-106
4	10	5	437	460	84
5	10	5	1009	967	61
6	10	5	850	817	79

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
-6	11	5	876	879	61	-7	0	6	1004	1048	52
-5	11	5	1034	1027	50	-6	0	6	1722	1774	45
-4	11	5	252	283	-99	-5	0	6	413	404	56
-3	11	5	276	356	-88	-4	0	6	452	419	42
-2	11	5	941	914	42	-3	0	6	1741	1710	36
-1	11	5	1270	1241	43	-2	0	6	2076	2073	45
0	11	5	983	934	38	-1	0	6	1991	2060	44
1	11	5	67	94	-169	0	0	6	248	197	45
2	11	5	532	519	56	1	0	6	1637	1584	40
3	11	5	815	791	49	2	0	6	2163	1980	46
4	11	5	987	956	58	3	0	6	1226	1172	41
5	11	5	327	359	-145	4	0	6	804	779	50
-5	12	5	271	290	-121	5	0	6	860	842	50
-4	12	5	704	771	59	6	0	6	1284	1392	50
-3	12	5	1164	1092	45	7	0	6	555	711	84
-2	12	5	402	466	63	-8	1	6	561	686	85
-1	12	5	261	225	-93	-7	1	6	236	254	-100
0	12	5	1024	959	41	-6	1	6	668	659	49
1	12	5	866	907	45	-5	1	6	1682	1740	39
2	12	5	918	926	48	-4	1	6	848	874	33
3	12	5	82	53	-207	-3	1	6	987	992	27
4	12	5	268	408	-134	-2	1	6	405	421	34
5	12	5	778	745	74	-1	1	6	1398	1501	33
-5	13	5	781	715	65	0	1	6	2070	2122	46
-4	13	5	408	359	77	1	1	6	2381	2283	54
-3	13	5	173	78	-126	2	1	6	122	40	-108
-2	13	5	1076	1098	48	3	1	6	658	512	46
-1	13	5	1042	971	42	4	1	6	1996	1902	46
0	13	5	621	628	59	5	1	6	1609	1668	50
1	13	5	347	304	70	6	1	6	173	338	-157
2	13	5	775	822	55	7	1	6	337	379	-111
3	13	5	933	920	58	-8	2	6	524	448	81
4	13	5	635	678	74	-7	2	6	985	935	50
-4	14	5	355	480	-103	-6	2	6	1287	1284	41
-3	14	5	806	796	60	-5	2	6	882	887	39
-2	14	5	783	736	48	-4	2	6	343	304	50
-1	14	5	77	127	-196	-3	2	6	2097	2047	37
0	14	5	376	474	76	-2	2	6	2866	2897	45
1	14	5	991	1051	49	-1	2	6	1184	1229	27
2	14	5	813	810	59	0	2	6	183	225	-60
3	14	5	83	99	-211	1	2	6	2036	2123	38
-3	15	5	193	167	-112	2	2	6	1923	1946	45
-2	15	5	492	582	87	3	2	6	1129	1028	41
-1	15	5	767	814	60	4	2	6	227	143	-101
0	15	5	304	463	-126	5	2	6	697	717	58
1	15	5	122	20	-122	6	2	6	683	776	69
2	15	5	403	486	-87	7	2	6	610	757	71
-8	0	6	303	300	-113	-8	3	6	707	770	70

Table 67. (continued)

H	K	L	$10F_O$	$10F_C$	10σ
-7	3	6	237	321	-90
-6	3	6	664	655	50
-5	3	6	962	991	39
-4	3	6	2173	2140	42
-3	3	6	950	984	30
-2	3	6	418	438	38
-1	3	6	1522	1530	33
0	3	6	2130	2202	48
1	3	6	1072	1129	34
2	3	6	312	356	-68
3	3	6	1443	1430	46
4	3	6	1475	1415	51
5	3	6	1163	1187	49
6	3	6	436	485	76
7	3	6	128	217	-152
-8	4	6	575	512	75
-7	4	6	925	956	52
-6	4	6	897	941	46
-5	4	6	701	652	43
-4	4	6	774	779	38
-3	4	6	1298	1279	33
-2	4	6	1727	1799	36
-1	4	6	934	949	32
0	4	6	95	49	-69
1	4	6	1322	1407	33
2	4	6	1436	1453	38
3	4	6	1166	1158	42
4	4	6	80	103	-202
5	4	6	534	504	73
6	4	6	756	781	65
7	4	6	765	838	67
-8	5	6	724	651	70
-7	5	6	104	228	-263
-6	5	6	359	446	-79
-5	5	6	1019	1025	40
-4	5	6	1066	1002	34
-3	5	6	253	119	-55
-2	5	6	401	459	43
-1	5	6	899	897	29
0	5	6	2060	2140	37
1	5	6	1195	1266	35
2	5	6	694	701	41
3	5	6	738	778	50
4	5	6	1198	1242	47
5	5	6	1170	1154	53
6	5	6	492	476	70
7	5	6	490	616	92
-8	6	6	171	162	-165
-7	6	6	739	723	59
-6	6	6	897	875	49
-5	6	6	421	471	56
-4	6	6	589	581	44
-3	6	6	821	841	36
-2	6	6	703	720	33
-1	6	6	1776	1803	39
0	6	6	393	430	39
1	6	6	838	878	32
2	6	6	1134	1155	37
3	6	6	896	859	43
4	6	6	208	230	-105
5	6	6	165	172	-134
6	6	6	869	992	66
7	6	6	387	613	-101
-6	7	6	79	49	-201
-5	7	6	1068	1051	42
-4	7	6	956	948	38
-3	7	6	445	442	48
-2	7	6	121	97	-84
-1	7	6	1091	1124	36
0	7	6	1252	1231	35
1	7	6	422	481	44
2	7	6	174	442	-122
3	7	6	393	481	75
4	7	6	636	664	59
5	7	6	431	424	87
6	7	6	435	373	77
-7	8	6	316	483	-133
-6	8	6	334	377	-99
-5	8	6	409	436	71
-4	8	6	111	52	-123
-3	8	6	907	894	38
-2	8	6	748	750	39
-1	8	6	832	837	35
0	8	6	117	132	-98
1	8	6	572	599	44
2	8	6	958	983	40
3	8	6	591	658	53
4	8	6	222	71	-84
5	8	6	225	181	-136
6	8	6	451	445	-96
-7	9	6	96	149	-243
-6	9	6	147	208	-160
-5	9	6	144	290	-163
-4	9	6	608	637	52
-3	9	6	403	393	59
-2	9	6	301	264	52

Table 67. (continued) 254

H	K	L	$10F_o$	$10F_c$	10σ
-1	9	6	297	371	62
0	9	6	435	443	49
1	9	6	472	478	46
2	9	6	62	86	-158
3	9	6	357	429	63
4	9	6	407	438	-86
5	9	6	112	285	-284
-6	10	6	149	230	-159
-5	10	6	76	95	-192
-4	10	6	186	134	-102
-3	10	6	122	57	-123
-2	10	6	281	363	-72
-1	10	6	176	127	-100
0	10	6	516	531	47
1	10	6	178	194	-77
2	10	6	280	315	-95
3	10	6	365	407	-86
4	10	6	381	325	77
5	10	6	106	313	-268
-6	11	6	166	49	-155
-5	11	6	137	124	-152
-4	11	6	84	119	-213
-3	11	6	165	213	-104
-2	11	6	155	45	-89
-1	11	6	124	167	-119
0	11	6	424	399	50
1	11	6	68	146	-174
2	11	6	124	98	-143
3	11	6	211	21	-111
4	11	6	152	37	-160
5	11	6	196	256	-145
-5	12	6	96	66	-243
-4	12	6	87	35	-220
-3	12	6	138	99	-134
-2	12	6	143	161	-104
-1	12	6	61	33	-154
0	12	6	78	26	-199
1	12	6	168	196	-105
2	12	6	73	14	-185
3	12	6	90	174	-227
4	12	6	259	231	-134
-5	13	6	88	47	-223
-4	13	6	95	13	-241
-3	13	6	259	257	-124
-2	13	6	77	83	-196
-1	13	6	186	76	-89
1	13	6	60	63	-153
2	13	6	415	299	71
3	13	6	149	99	-124
4	13	6	101	57	-257
-4	14	6	85	193	-215
-3	14	6	122	63	-131
-2	14	6	291	312	-98
-1	14	6	166	150	-117
0	14	6	69	20	-176
1	14	6	364	366	68
2	14	6	80	90	-204
3	14	6	81	47	-206
-2	15	6	83	58	-211
-1	15	6	165	273	-145
0	15	6	497	400	70
1	15	6	159	130	-144
2	15	6	75	117	-189
-8	1	7	176	41	-145
-7	1	7	158	202	-135
-6	1	7	72	166	-183
-5	1	7	360	309	59
-4	1	7	57	115	-145
-3	1	7	765	759	31
-2	1	7	287	298	40
-1	1	7	143	132	-60
0	1	7	699	734	29
1	1	7	523	510	39
2	1	7	897	845	39
3	1	7	178	182	-79
4	1	7	332	436	-87
5	1	7	123	201	-139
7	1	7	172	150	-145
-8	2	7	101	46	-257
-7	2	7	86	141	-218
-6	2	7	130	178	-156
-5	2	7	165	182	-88
-4	2	7	221	314	-68
-3	2	7	631	646	33
-2	2	7	1121	1139	30
-1	2	7	58	71	-147
0	2	7	682	717	29
1	2	7	127	202	-96
2	2	7	420	399	58
3	2	7	492	403	59
4	2	7	423	480	81
5	2	7	500	469	71
6	2	7	88	22	-223
7	2	7	217	172	-124
-8	3	7	178	270	-193
-7	3	7	480	558	78

Table 67. (continued)

H	K	L	$10F_o$	$10F_c$	10σ
-6	3	7	141	101	-102
-5	3	7	526	538	49
-4	3	7	542	629	43
-3	3	7	917	916	31
-2	3	7	121	210	-75
-1	3	7	274	224	49
0	3	7	519	499	30
1	3	7	659	638	34
2	3	7	325	327	-69
3	3	7	536	547	53
4	3	7	84	48	-213
5	3	7	660	673	58
6	3	7	335	416	-118
7	3	7	283	326	-124
-8	4	7	156	139	-156
-7	4	7	193	60	-117
-6	4	7	940	906	46
-5	4	7	695	663	42
-4	4	7	649	620	39
-3	4	7	244	334	-71
-2	4	7	552	578	33
-1	4	7	800	799	29
0	4	7	740	789	31
1	4	7	537	617	40
2	4	7	859	752	38
3	4	7	437	345	71
4	4	7	766	780	58
5	4	7	192	196	-128
6	4	7	252	396	-107
7	4	7	296	322	-115
-8	5	7	605	526	76
-7	5	7	461	392	80
-6	5	7	85	197	-217
-5	5	7	792	826	44
-4	5	7	830	809	37
-3	5	7	766	800	35
-2	5	7	371	388	49
-1	5	7	265	224	55
0	5	7	535	570	34
1	5	7	1450	1526	36
2	5	7	302	296	53
3	5	7	642	660	50
4	5	7	186	181	-112
5	5	7	895	802	59
6	5	7	623	672	77
7	5	7	216	285	-121
-7	6	7	150	272	-161
-6	6	7	725	640	51
-5	6	7	734	811	46
-4	6	7	998	978	38
-3	6	7	72	79	-182
-2	6	7	746	765	34
-1	6	7	1763	1823	40
0	6	7	1110	1101	36
1	6	7	62	50	-158
2	6	7	1025	1026	39
3	6	7	1465	1401	47
4	6	7	512	446	62
5	6	7	86	57	-218
6	6	7	311	525	-132
7	6	7	309	531	-152
-7	7	7	477	450	79
-6	7	7	189	117	-106
-5	7	7	210	330	-124
-4	7	7	1060	1043	38
-3	7	7	991	1049	36
-2	7	7	625	657	40
-1	7	7	395	479	48
0	7	7	975	994	35
1	7	7	1125	1167	34
2	7	7	1550	1538	43
3	7	7	173	141	-95
4	7	7	548	582	59
5	7	7	698	665	75
6	7	7	739	792	70
-7	8	7	500	434	72
-6	8	7	620	593	60
-5	8	7	1320	1312	42
-4	8	7	519	466	53
-3	8	7	65	136	-166
-2	8	7	1133	1148	35
-1	8	7	1183	1234	39
0	8	7	667	637	38
1	8	7	199	165	-77
2	8	7	868	823	43
3	8	7	1349	1293	43
4	8	7	589	561	59
5	8	7	317	172	-95
6	8	7	198	233	-131
-7	9	7	684	723	70
-6	9	7	173	169	-137
-5	9	7	510	540	56
-4	9	7	1603	1560	45
-3	9	7	858	841	43
-2	9	7	395	418	59
-1	9	7	55	76	-140

H	K	L	$10F_O$	$10F_C$	10σ
0	9	7	1114	1143	37
1	9	7	858	884	39
2	9	7	1254	1188	40
3	9	7	146	91	-121
4	9	7	177	222	-136
5	9	7	709	767	80
6	9	7	982	1009	74
-6	10	7	731	719	61
-5	10	7	1044	1074	49
-4	10	7	388	329	69
-3	10	7	219	232	-95
-2	10	7	668	622	43
-1	10	7	1306	1274	43
0	10	7	918	983	41
1	10	7	170	99	-96
2	10	7	901	951	46
3	10	7	881	881	54
4	10	7	799	708	63
5	10	7	275	323	-156
-6	11	7	234	348	-138
-5	11	7	258	343	-106
-4	11	7	1005	955	44
-3	11	7	966	999	47
-2	11	7	780	771	48
-1	11	7	130	25	-100
0	11	7	1004	1006	42
1	11	7	1611	1569	47
2	11	7	818	804	51
3	11	7	81	107	-207
4	11	7	699	562	69
5	11	7	893	784	73
-5	12	7	653	671	67
-4	12	7	669	671	59
-3	12	7	285	315	-88
-2	12	7	901	810	46
-1	12	7	1237	1144	43
0	12	7	732	772	51
1	12	7	74	140	-188
2	12	7	624	684	56
3	12	7	1040	1052	52
4	12	7	688	653	81
-4	13	7	765	668	58
-3	13	7	1050	1037	50
-2	13	7	392	383	75
-1	13	7	314	367	-70
0	13	7	504	472	54
1	13	7	991	965	46
2	13	7	579	661	64

H	K	L	$10F_O$	$10F_C$	10σ
3	13	7	172	255	-135
-3	14	7	155	220	-154
-2	14	7	807	807	58
-1	14	7	566	608	60
0	14	7	480	537	68
1	14	7	68	26	-171
2	14	7	400	442	-90
-2	15	7	231	374	-106
-1	15	7	153	78	-113
0	15	7	610	629	58
1	15	7	770	793	66
-8	0	8	677	662	70
-7	0	8	724	683	56
-6	0	8	811	734	48
-5	0	8	1040	1050	38
-4	0	8	1956	1994	43
-3	0	8	778	772	33
-2	0	8	61	138	-154
-1	0	8	1872	1993	37
0	0	8	3224	3343	12
1	0	8	1185	1109	38
2	0	8	98	71	-125
3	0	8	1102	966	48
4	0	8	1509	1510	51
5	0	8	1118	1166	48
6	0	8	200	168	-115
7	0	8	272	400	-131
-8	1	8	326	461	-134
-7	1	8	1174	1154	49
-6	1	8	1361	1375	41
-5	1	8	544	476	49
-4	1	8	673	664	37
-3	1	8	1889	1922	40
-2	1	8	1909	1973	37
-1	1	8	846	921	28
0	1	8	125	66	-66
1	1	8	1861	1873	43
2	1	8	1213	1157	39
3	1	8	1470	1287	50
4	1	8	437	473	76
5	1	8	537	602	69
6	1	8	855	879	58
7	1	8	887	1058	58
-8	2	8	835	757	63
-7	2	8	194	131	-107
-6	2	8	490	554	63
-5	2	8	947	935	38
-4	2	8	1530	1499	37

H	K	L	$10F_o$	$10F_c$	10σ
-3	2	8	1336	1304	34
-2	2	8	335	383	43
-1	2	8	901	958	28
0	2	8	1837	1903	39
1	2	8	1863	1886	43
2	2	8	364	320	54
3	2	8	1302	1191	44
4	2	8	1956	1844	51
5	2	8	1013	1019	48
6	2	8	334	348	-115
7	2	8	334	355	-128
-8	3	8	513	571	90
-7	3	8	1216	1194	48
-6	3	8	740	765	48
-5	3	8	468	449	52
-4	3	8	281	341	-66
-3	3	8	2022	1992	41
-2	3	8	1456	1489	31
-1	3	8	856	903	30
0	3	8	51	54	-128
1	3	8	613	589	34
2	3	8	2315	2200	49
3	3	8	1368	1332	43
4	3	8	190	140	-112
5	3	8	517	510	73
6	3	8	980	911	56
7	3	8	688	835	73
-8	4	8	615	634	81
-7	4	8	88	79	-222
-6	4	8	87	93	-222
-5	4	8	1184	1160	38
-4	4	8	1165	1130	34
-3	4	8	1170	1173	36
-2	4	8	387	381	43
-1	4	8	1251	1282	33
0	4	8	1318	1387	33
1	4	8	1565	1675	36
2	4	8	150	136	-101
3	4	8	987	953	46
4	4	8	1238	1226	48
5	4	8	838	854	60
6	4	8	275	391	-112
7	4	8	147	313	-179
-8	5	8	311	362	-115
-7	5	8	684	700	62
-6	5	8	1126	1152	45
-5	5	8	765	756	46
-4	5	8	855	841	40
-3	5	8	1342	1280	37
-2	5	8	1663	1658	34
-1	5	8	842	877	31
0	5	8	705	717	35
1	5	8	1054	1053	35
2	5	8	1289	1313	44
3	5	8	492	469	66
4	5	8	78	93	-199
5	5	8	215	210	-136
6	5	8	772	867	72
-7	6	8	160	295	-190
-6	6	8	217	187	-104
-5	6	8	1074	1077	42
-4	6	8	1058	1018	38
-3	6	8	73	119	-185
-2	6	8	67	181	-170
-1	6	8	1216	1292	36
0	6	8	1304	1316	37
1	6	8	880	907	38
2	6	8	120	132	-117
3	6	8	890	846	48
4	6	8	544	580	63
5	6	8	906	925	64
6	6	8	100	149	-255
-7	7	8	417	320	-94
-6	7	8	475	588	77
-5	7	8	90	386	-229
-4	7	8	329	394	-70
-3	7	8	262	300	-76
-2	7	8	1048	1029	34
-1	7	8	546	536	44
0	7	8	481	512	45
1	7	8	501	559	48
2	7	8	1198	1165	39
3	7	8	773	843	51
4	7	8	180	165	-120
5	7	8	425	344	89
6	7	8	611	666	86
-7	8	8	99	37	-252
-6	8	8	206	278	-117
-5	8	8	408	399	58
-4	8	8	918	847	43
-3	8	8	323	307	-73
-2	8	8	187	237	-80
-1	8	8	497	470	42
0	8	8	435	404	54
1	8	8	632	660	42
2	8	8	301	299	-80

Table 67. (continued)

H	K	L	$10F_o$	$10F_c$	10σ
3	8	8	734	700	56
4	8	8	388	551	-95
5	8	8	555	455	71
6	8	8	166	196	-163
-6	9	8	204	190	-127
-5	9	8	410	280	72
-4	9	8	270	228	-81
-3	9	8	776	690	44
-2	9	8	599	627	47
-1	9	8	256	258	-56
0	9	8	57	65	-143
1	9	8	251	255	-75
2	9	8	627	718	59
3	9	8	258	395	-108
4	9	8	78	48	-199
5	9	8	117	237	-296
-6	10	8	226	35	-112
-5	10	8	236	341	-122
-4	10	8	374	332	77
-3	10	8	349	369	-82
-2	10	8	354	464	72
-1	10	8	247	298	-89
0	10	8	426	424	48
1	10	8	123	128	-122
2	10	8	114	201	-129
3	10	8	60	100	-153
4	10	8	106	290	-269
5	10	8	220	42	-128
-6	11	8	148	185	-157
-5	11	8	88	81	-224
-4	11	8	95	71	-241
-3	11	8	193	209	-100
-2	11	8	66	38	-166
-1	11	8	522	496	57
0	11	8	135	87	-101
1	11	8	267	366	-68
2	11	8	72	62	-183
3	11	8	86	121	-219
4	11	8	261	33	-93
-5	12	8	89	41	-226
-4	12	8	85	66	-214
-3	12	8	160	94	-109
-2	12	8	76	91	-194
-1	12	8	231	229	-82
0	12	8	69	171	-174
1	12	8	73	42	-184
2	12	8	81	34	-205
3	12	8	264	243	-115

H	K	L	$10F_o$	$10F_c$	10σ
4	12	8	167	137	-174
-4	13	8	187	204	-127
-3	13	8	157	215	-109
-2	13	8	153	105	-134
-1	13	8	68	10	-173
0	13	8	245	274	-113
1	13	8	80	40	-204
2	13	8	147	110	-139
3	13	8	98	144	-249
-3	14	8	84	14	-214
-2	14	8	71	41	-181
-1	14	8	76	73	-193
0	14	8	295	293	-99
1	14	8	201	242	-104
2	14	8	89	64	-226
-1	15	8	231	259	-115
0	15	8	134	13	-159
-8	1	9	96	140	-243
-7	1	9	241	342	-122
-6	1	9	84	226	-212
-5	1	9	62	55	-158
-4	1	9	191	217	-89
-3	1	9	838	865	34
-2	1	9	82	54	-100
-1	1	9	62	114	-156
0	1	9	435	468	41
1	1	9	63	122	-160
2	1	9	304	378	-76
3	1	9	84	230	-213
4	1	9	77	52	-196
5	1	9	190	30	-102
6	1	9	205	125	-117
7	1	9	94	161	-239
-8	2	9	460	408	88
-7	2	9	96	151	-244
-6	2	9	85	17	-215
-5	2	9	129	62	-96
-4	2	9	227	166	-76
-3	2	9	645	620	38
-2	2	9	90	62	-86
-1	2	9	177	149	-66
0	2	9	136	135	-76
1	2	9	499	505	42
2	2	9	409	390	59
3	2	9	660	668	55
4	2	9	641	550	62
5	2	9	126	129	-153
6	2	9	293	300	-117

Table 67. (continued)

H	K	L	$10F_o$	$10F_c$	10σ
7	2	9	261	259	-108
-8	3	9	120	266	-305
-7	3	9	95	260	-241
-6	3	9	454	435	69
-5	3	9	181	331	-113
-4	3	9	622	593	41
-3	3	9	508	492	44
-2	3	9	386	457	44
-1	3	9	1058	1101	36
0	3	9	425	440	43
1	3	9	769	766	38
2	3	9	511	534	59
3	3	9	739	693	54
4	3	9	230	298	-118
5	3	9	72	29	-183
6	3	9	86	32	-218
-8	4	9	185	252	-160
-7	4	9	445	557	86
-6	4	9	78	95	-197
-5	4	9	253	195	-84
-4	4	9	622	676	43
-3	4	9	751	780	38
-2	4	9	800	837	34
-1	4	9	727	721	35
0	4	9	965	975	33
1	4	9	941	994	37
2	4	9	549	571	55
3	4	9	137	192	-132
4	4	9	398	375	73
5	4	9	662	683	64
6	4	9	352	449	-112
-7	5	9	87	147	-221
-6	5	9	718	724	52
-5	5	9	836	844	46
-4	5	9	164	181	-103
-3	5	9	239	130	-59
-2	5	9	1144	1149	36
-1	5	9	826	904	36
0	5	9	815	823	36
1	5	9	612	651	42
2	5	9	667	714	48
3	5	9	733	690	52
4	5	9	640	754	70
5	5	9	182	196	-141
6	5	9	196	174	-135
-7	6	9	549	616	66
-6	6	9	162	55	-120
-5	6	9	375	407	71
-4	6	9	974	976	40
-3	6	9	873	844	37
-2	6	9	448	486	51
-1	6	9	58	93	-148
0	6	9	541	616	42
1	6	9	757	743	41
2	6	9	1150	1140	42
3	6	9	89	282	-225
4	6	9	308	297	-108
5	6	9	852	801	66
6	6	9	619	606	88
-7	7	9	205	343	-155
-6	7	9	660	705	58
-5	7	9	866	845	47
-4	7	9	426	412	61
-3	7	9	379	428	66
-2	7	9	1305	1375	40
-1	7	9	1082	1047	35
0	7	9	332	275	51
1	7	9	156	201	-94
2	7	9	790	792	45
3	7	9	1072	1036	49
4	7	9	573	658	64
5	7	9	290	205	-115
6	7	9	342	222	-87
-7	8	9	278	343	-126
-6	8	9	293	351	-111
-5	8	9	298	438	-98
-4	8	9	731	709	49
-3	8	9	1332	1260	37
-2	8	9	936	962	39
-1	8	9	208	299	-105
0	8	9	542	476	46
1	8	9	1352	1371	44
2	8	9	1118	1119	42
3	8	9	184	138	-98
4	8	9	595	613	70
5	8	9	843	750	69
-6	9	9	712	712	59
-5	9	9	881	912	50
-4	9	9	559	553	59
-3	9	9	214	287	-94
-2	9	9	1083	1057	40
-1	9	9	1499	1488	43
0	9	9	595	507	44
1	9	9	153	50	-108
2	9	9	1238	1225	45
3	9	9	1057	1113	52

H	K	L	$10F_o$	$10F_c$	10σ
4	9	9	488	598	96
5	9	9	177	257	-168
-6	10	9	496	406	77
-5	10	9	539	553	74
-4	10	9	875	905	49
-3	10	9	1062	1036	44
-2	10	9	828	829	46
-1	10	9	61	102	-156
0	10	9	594	634	54
1	10	9	1329	1275	42
2	10	9	844	843	53
3	10	9	73	192	-184
4	10	9	254	338	-116
5	10	9	952	917	72
-5	11	9	896	870	56
-4	11	9	161	184	-133
-3	11	9	366	344	68
-2	11	9	1069	1020	46
-1	11	9	862	839	47
0	11	9	631	619	50
1	11	9	77	49	-194
2	11	9	538	558	64
3	11	9	904	838	58
4	11	9	799	775	68
-5	12	9	192	193	-130
-4	12	9	882	862	54
-3	12	9	842	902	53
-2	12	9	411	431	76
-1	12	9	112	145	-117
0	12	9	724	752	50
1	12	9	802	759	52
2	12	9	844	852	60
3	12	9	106	141	-269
-4	13	9	565	543	73
-3	13	9	81	115	-207
-2	13	9	911	861	50
-1	13	9	869	897	53
0	13	9	648	686	59
1	13	9	84	24	-214
2	13	9	446	541	87
3	13	9	971	972	62
-3	14	9	828	866	62
-2	14	9	414	439	-92
-1	14	9	78	40	-197
0	14	9	823	746	56
1	14	9	592	767	65
-8	0	10	537	419	82
-7	0	10	1351	1387	48

H	K	L	$10F_o$	$10F_c$	10σ
-6	0	10	921	859	45
-5	0	10	542	491	50
-4	0	10	827	788	37
-3	0	10	916	990	34
-2	0	10	755	827	35
-1	0	10	2130	2221	43
0	0	10	354	315	57
1	0	10	948	926	39
2	0	10	1591	1421	46
3	0	10	1565	1419	53
4	0	10	465	481	75
5	0	10	568	584	58
6	0	10	1192	1264	56
-8	1	10	803	789	67
-7	1	10	285	296	-104
-6	1	10	346	402	-83
-5	1	10	1340	1310	38
-4	1	10	1422	1443	39
-3	1	10	813	851	36
-2	1	10	219	226	-56
-1	1	10	1678	1734	35
0	1	10	2544	2680	44
1	1	10	988	1047	39
2	1	10	234	20	-81
3	1	10	1001	979	53
4	1	10	1504	1507	48
5	1	10	863	847	55
6	1	10	270	369	-109
-8	2	10	590	575	75
-7	2	10	1205	1182	50
-6	2	10	1000	1014	46
-5	2	10	508	479	54
-4	2	10	500	437	44
-3	2	10	1523	1526	37
-2	2	10	1697	1765	43
-1	2	10	816	853	36
0	2	10	135	220	-87
1	2	10	829	866	41
2	2	10	1465	1338	46
3	2	10	1430	1344	46
4	2	10	220	212	-99
5	2	10	237	409	-118
6	2	10	709	883	69
-8	3	10	764	678	68
-6	3	10	660	616	55
-5	3	10	923	894	42
-4	3	10	1745	1754	39
-3	3	10	879	910	37

H	K	L	$10F_o$	$10F_c$	10σ
-2	3	10	598	619	39
-1	3	10	1922	2015	43
0	3	10	1186	1209	38
1	3	10	877	866	40
2	3	10	70	23	-177
3	3	10	1175	1191	47
4	3	10	1035	1008	56
5	3	10	675	732	71
6	3	10	276	260	-115
-7	4	10	752	771	63
-6	4	10	1098	1089	46
-5	4	10	204	238	-99
-4	4	10	212	221	-78
-3	4	10	1101	1049	35
-2	4	10	1731	1825	44
-1	4	10	496	513	43
0	4	10	360	367	57
1	4	10	972	982	37
2	4	10	1347	1376	40
3	4	10	1193	1146	48
4	4	10	304	271	-106
5	4	10	674	645	71
6	4	10	747	810	72
-7	5	10	97	211	-247
-6	5	10	496	383	66
-5	5	10	911	899	44
-4	5	10	636	629	42
-3	5	10	630	621	42
-2	5	10	64	52	-162
-1	5	10	999	996	35
0	5	10	1505	1493	39
1	5	10	1319	1299	36
2	5	10	61	88	-154
3	5	10	440	550	79
4	5	10	966	1061	56
5	5	10	1002	980	63
6	5	10	181	67	-143
-7	6	10	480	572	87
-6	6	10	826	848	55
-5	6	10	208	313	-107
-4	6	10	344	302	64
-3	6	10	698	685	43
-2	6	10	1054	1061	36
-1	6	10	833	815	37
0	6	10	134	88	-81
1	6	10	703	759	42
2	6	10	998	1003	45
3	6	10	421	513	72
4	6	10	534	513	69
5	6	10	535	565	99
6	6	10	639	724	89
-7	7	10	243	213	-111
-6	7	10	133	142	-145
-5	7	10	940	938	47
-4	7	10	618	606	54
-3	7	10	883	857	40
-2	7	10	586	544	41
-1	7	10	821	830	40
0	7	10	831	845	43
1	7	10	532	578	57
2	7	10	79	191	-200
3	7	10	88	266	-222
4	7	10	701	739	68
5	7	10	449	539	93
-6	8	10	517	371	69
-5	8	10	231	291	-108
-4	8	10	73	54	-184
-3	8	10	851	806	41
-2	8	10	835	885	41
-1	8	10	128	148	-95
0	8	10	152	318	-122
1	8	10	68	247	-173
2	8	10	708	709	54
3	8	10	350	401	-82
4	8	10	91	36	-230
5	8	10	105	196	-267
-6	9	10	293	258	-79
-5	9	10	86	158	-218
-4	9	10	513	456	61
-3	9	10	261	351	-83
-2	9	10	123	31	-109
-1	9	10	289	377	-85
0	9	10	192	246	-96
1	9	10	498	509	63
2	9	10	370	329	-81
3	9	10	307	416	-95
4	9	10	381	506	-96
5	9	10	211	232	-138
-6	10	10	299	194	-104
-5	10	10	189	144	-119
-4	10	10	147	18	-117
-3	10	10	129	154	-105
-2	10	10	330	385	-79
-1	10	10	353	343	63
0	10	10	68	115	-173
1	10	10	263	367	-100

H	K	L	$10F_o$	$10F_c$	10σ
2	10	10	355	284	70
3	10	10	399	438	77
4	10	10	279	150	-124
-5	11	10	91	26	-231
-4	11	10	123	209	-140
-3	11	10	326	300	61
-2	11	10	269	358	-118
-1	11	10	63	25	-159
0	11	10	251	365	-87
1	11	10	77	53	-194
2	11	10	178	204	-105
3	11	10	91	19	-231
4	11	10	89	87	-225
-4	12	10	131	61	-132
-3	12	10	85	86	-215
-2	12	10	80	9	-201
-1	12	10	300	291	-98
0	12	10	327	228	-72
1	12	10	244	267	-92
2	12	10	93	130	-237
3	12	10	85	63	-217
-3	13	10	74	17	-188
-2	13	10	79	22	-201
-1	13	10	85	174	-216
0	13	10	63	101	-160
1	13	10	338	236	-75
2	13	10	210	21	-121
-2	14	10	222	152	-129
-1	14	10	78	51	-198
0	14	10	147	42	-132
-8	1	11	102	100	-260
-7	1	11	158	59	-136
-6	1	11	71	88	-179
-5	1	11	570	576	51
-4	1	11	139	296	-122
-3	1	11	223	223	-67
-2	1	11	332	356	65
-1	1	11	67	37	-170
0	1	11	405	479	56
1	1	11	257	274	-65
2	1	11	539	526	62
3	1	11	311	378	-111
4	1	11	366	287	72
5	1	11	87	42	-221
6	1	11	171	29	-147
-7	2	11	214	265	-142
-6	2	11	167	171	-113
-5	2	11	545	494	53
-4	2	11	68	151	-171
-3	2	11	119	255	-128
-2	2	11	742	733	37
-1	2	11	394	437	49
0	2	11	299	374	58
1	2	11	93	111	-115
2	2	11	140	149	-97
3	2	11	558	609	66
4	2	11	187	51	-110
5	2	11	81	39	-204
6	2	11	88	99	-225
-7	3	11	339	309	-104
-6	3	11	77	61	-196
-5	3	11	135	57	-118
-4	3	11	579	705	49
-3	3	11	165	113	-81
-2	3	11	459	472	48
-1	3	11	236	192	-86
0	3	11	527	582	45
1	3	11	299	292	61
2	3	11	662	636	55
3	3	11	194	92	-118
4	3	11	308	304	-99
5	3	11	311	330	-119
6	3	11	532	497	84
-7	4	11	274	370	-109
-6	4	11	687	692	57
-5	4	11	743	688	46
-4	4	11	255	240	-71
-3	4	11	543	550	48
-2	4	11	140	131	-77
-1	4	11	963	969	38
0	4	11	196	206	-92
1	4	11	71	28	-180
2	4	11	252	226	-72
3	4	11	495	533	73
4	4	11	535	606	79
5	4	11	581	576	77
6	4	11	164	151	-113
-7	5	11	165	380	-160
-6	5	11	432	475	76
-5	5	11	545	491	56
-4	5	11	558	575	51
-3	5	11	763	784	43
-2	5	11	721	763	36
-1	5	11	127	110	-96
0	5	11	932	947	38
1	5	11	1166	1133	39

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
2	5	11	389	371	76	0	9	11	626	652	54
3	5	11	158	19	-111	1	9	11	894	948	48
4	5	11	505	565	85	2	9	11	656	672	62
5	5	11	711	599	72	3	9	11	130	180	-132
6	5	11	507	525	91	4	9	11	393	342	-113
-7	6	11	308	396	-113	-5	10	11	706	761	63
-6	6	11	693	653	58	-4	10	11	156	213	-143
-5	6	11	658	671	53	-3	10	11	81	202	-205
-4	6	11	455	393	56	-2	10	11	1008	996	46
-3	6	11	442	502	56	-1	10	11	1076	1069	43
-2	6	11	808	889	41	0	10	11	786	773	52
-1	6	11	1225	1248	42	1	10	11	230	231	-100
0	6	11	580	566	45	2	10	11	712	694	63
1	6	11	63	50	-158	3	10	11	717	681	59
2	6	11	680	628	58	4	10	11	794	858	82
3	6	11	728	710	57	-5	11	11	355	347	-94
4	6	11	704	592	67	-4	11	11	699	639	63
5	6	11	266	268	-136	-3	11	11	1018	979	46
-7	7	11	599	564	77	-2	11	11	769	712	51
-6	7	11	95	234	-241	-1	11	11	70	66	-177
-5	7	11	88	85	-222	0	11	11	945	922	52
-4	7	11	630	629	49	1	11	11	1126	1112	49
-3	7	11	1297	1325	40	2	11	11	579	551	69
-2	7	11	584	638	49	3	11	11	199	62	-140
-1	7	11	189	277	-85	-4	12	11	400	459	-85
0	7	11	823	816	44	-3	12	11	217	352	-116
1	7	11	1351	1361	41	-2	12	11	814	762	53
2	7	11	709	728	51	-1	12	11	1159	1158	47
4	7	11	748	732	58	0	12	11	547	479	75
5	7	11	731	787	84	1	12	11	79	72	-200
-6	8	11	994	949	53	2	12	11	610	602	74
-5	8	11	662	672	60	-3	13	11	799	750	65
-4	8	11	262	302	-96	-2	13	11	290	355	-112
-3	8	11	395	348	54	-1	13	11	211	196	-108
-2	8	11	1386	1368	46	0	13	11	517	533	76
-1	8	11	588	609	49	1	13	11	744	681	65
0	8	11	739	797	47	-7	0	12	364	352	-93
1	8	11	64	7	-163	-6	0	12	407	483	82
2	8	11	579	490	64	-5	0	12	1578	1669	45
3	8	11	882	862	59	-4	0	12	1614	1714	42
4	8	11	1007	960	61	-3	0	12	143	116	-88
5	8	11	97	210	-247	-2	0	12	199	102	-60
-6	9	11	213	96	-113	-1	0	12	1820	1847	40
-5	9	11	242	384	-119	0	0	12	1574	1663	42
-4	9	11	770	756	51	1	0	12	969	955	46
-3	9	11	926	868	47	2	0	12	128	20	-109
-2	9	11	566	575	56	3	0	12	647	601	68
-1	9	11	191	66	-79	4	0	12	508	552	91

Table 67. (continued)

H	K	L	$10F_o$	$10F_c$	10σ
5	0	12	1023	1118	56
6	0	12	95	387	-242
-7	1	12	760	711	57
-6	1	12	1132	1105	45
-5	1	12	518	489	54
-4	1	12	602	637	46
-3	1	12	982	957	38
-2	1	12	1438	1378	40
-1	1	12	1064	1060	37
0	1	12	151	113	-88
1	1	12	1320	1326	40
2	1	12	1632	1569	50
3	1	12	1072	1004	51
4	1	12	159	137	-137
5	1	12	462	488	93
6	1	12	1027	1132	62
-7	2	12	156	105	-125
-6	2	12	541	485	64
-5	2	12	1349	1361	40
-4	2	12	1418	1363	37
-3	2	12	763	793	42
-2	2	12	258	283	-64
-1	2	12	1319	1331	42
0	2	12	1562	1546	41
1	2	12	1168	1139	41
2	2	12	141	141	-111
3	2	12	1078	1002	51
4	2	12	1044	1023	57
5	2	12	772	762	71
6	2	12	162	344	-180
-7	3	12	878	844	55
-6	3	12	563	519	62
-5	3	12	440	534	69
-4	3	12	165	189	-111
-3	3	12	835	872	42
-2	3	12	1181	1302	40
-1	3	12	1031	1106	38
0	3	12	63	64	-160
1	3	12	733	705	49
2	3	12	1891	1874	49
3	3	12	1144	1176	51
4	3	12	86	115	-219
5	3	12	713	673	74
-7	4	12	160	245	-188
-6	4	12	459	524	78
-5	4	12	1227	1192	41
-4	4	12	1070	1110	40
-3	4	12	809	836	43
-2	4	12	755	791	42
-1	4	12	959	980	39
0	4	12	1436	1439	43
1	4	12	713	724	49
2	4	12	76	72	-194
3	4	12	498	438	65
4	4	12	953	969	62
5	4	12	425	578	-111
-7	5	12	727	728	66
-6	5	12	909	859	53
-5	5	12	268	312	-107
-4	5	12	227	309	-93
-3	5	12	1088	1102	39
-2	5	12	920	918	40
-1	5	12	633	700	48
0	5	12	63	144	-160
1	5	12	1091	1149	43
2	5	12	745	695	51
3	5	12	623	623	66
4	5	12	322	386	-129
5	5	12	302	483	-115
-7	6	12	335	377	-118
-6	6	12	559	490	66
-5	6	12	659	680	57
-4	6	12	969	922	45
-3	6	12	284	313	-71
-2	6	12	76	149	-193
-1	6	12	754	746	44
0	6	12	1318	1324	41
1	6	12	572	617	51
2	6	12	259	229	-110
3	6	12	140	147	-139
4	6	12	639	760	80
5	6	12	568	677	87
-6	7	12	577	629	71
-5	7	12	208	65	-86
-4	7	12	129	37	-120
-3	7	12	622	625	50
-2	7	12	785	711	45
-1	7	12	600	500	49
0	7	12	244	249	-98
1	7	12	951	911	46
2	7	12	557	547	59
3	7	12	658	704	72
4	7	12	98	156	-249
5	7	12	403	430	-124
-6	8	12	228	178	-120
-5	8	12	99	201	-251

Table 67. (continued)

H	K	L	$10F_o$	$10F_c$	10σ
-4	8	12	552	578	60
-3	8	12	513	523	60
-2	8	12	184	155	-84
-1	8	12	456	460	55
0	8	12	577	609	58
1	8	12	595	590	54
2	8	12	271	192	-97
3	8	12	485	514	78
4	8	12	569	645	88
-5	9	12	294	227	-92
-4	9	12	187	196	-106
-3	9	12	512	506	66
-2	9	12	503	603	63
-1	9	12	126	116	-119
0	9	12	291	219	-92
1	9	12	72	94	-184
2	9	12	452	443	76
3	9	12	318	256	-91
4	9	12	91	21	-230
-5	10	12	253	354	-106
-4	10	12	87	141	-221
-3	10	12	97	187	-245
-2	10	12	195	109	-104
-1	10	12	300	251	-79
1	10	12	73	142	-184
2	10	12	75	68	-190
3	10	12	94	198	-239
-4	11	12	233	317	-136
-3	11	12	84	36	-213
-2	11	12	74	93	-186
-1	11	12	224	291	-112
0	11	12	189	176	-110
1	11	12	77	17	-196
2	11	12	89	164	-225
3	11	12	91	125	-232
-3	12	12	167	78	-141
-2	12	12	288	322	-108
-1	12	12	185	67	-88
0	12	12	166	143	-125
1	12	12	83	184	-210
2	12	12	98	57	-247
-2	13	12	86	27	-218
-1	13	12	79	23	-201
0	13	12	72	109	-183
-7	1	13	251	268	-120
-6	1	13	78	27	-199
-5	1	13	77	93	-195
-4	1	13	69	40	-176
-3	1	13	162	175	-82
-2	1	13	148	124	-93
-1	1	13	53	40	-136
0	1	13	68	136	-172
1	1	13	830	747	50
2	1	13	81	114	-206
3	1	13	99	258	-252
4	1	13	86	114	-218
5	1	13	166	103	-145
-7	2	13	94	51	-237
-6	2	13	223	219	-101
-5	2	13	86	306	-219
-4	2	13	72	105	-184
-3	2	13	507	526	52
-2	2	13	147	112	-81
-1	2	13	370	415	66
0	2	13	70	82	-177
1	2	13	421	399	55
2	2	13	443	452	75
3	2	13	253	116	-110
4	2	13	181	193	-150
5	2	13	94	109	-238
-7	3	13	91	142	-230
-6	3	13	89	258	-226
-5	3	13	504	591	66
-4	3	13	186	92	-87
-3	3	13	157	38	-88
-2	3	13	463	387	56
-1	3	13	677	723	47
0	3	13	198	259	-88
1	3	13	168	319	-112
2	3	13	625	599	61
3	3	13	565	498	71
4	3	13	187	245	-136
5	3	13	191	233	-149
-7	4	13	311	360	-127
-6	4	13	406	441	-89
-5	4	13	133	299	-138
-4	4	13	915	917	45
-3	4	13	417	545	67
-2	4	13	750	763	46
-1	4	13	393	368	55
0	4	13	930	914	44
1	4	13	861	790	46
2	4	13	81	235	-206
3	4	13	198	375	-157
4	4	13	96	142	-244
5	4	13	459	437	91

H	K	L	$10F_o$	$10F_c$	10σ
-7	5	13	91	187	-231
-6	5	13	559	658	64
-5	5	13	626	615	57
-4	5	13	79	80	-201
-3	5	13	69	127	-175
-2	5	13	544	529	55
-1	5	13	611	592	49
0	5	13	738	745	51
1	5	13	74	26	-189
2	5	13	340	359	-100
3	5	13	739	672	57
4	5	13	531	566	86
5	5	13	107	235	-271
-6	6	13	244	99	-104
-5	6	13	92	147	-232
-4	6	13	941	931	45
-3	6	13	653	763	52
-2	6	13	405	369	57
-1	6	13	130	261	-94
0	6	13	655	709	51
1	6	13	867	884	50
2	6	13	735	746	51
3	6	13	212	24	-104
4	6	13	237	419	-123
-6	7	13	634	620	68
-5	7	13	367	431	-82
-4	7	13	453	443	73
-3	7	13	400	427	71
-2	7	13	845	782	47
-1	7	13	497	596	62
0	7	13	673	686	48
1	7	13	196	301	-108
2	7	13	430	357	76
3	7	13	809	870	68
4	7	13	641	698	85
-6	8	13	99	199	-250
-5	8	13	196	231	-140
-4	8	13	676	683	61
-3	8	13	1348	1332	43
-2	8	13	275	277	-83
-1	8	13	243	208	-81
0	8	13	977	1014	50
1	8	13	1068	1062	48
2	8	13	360	438	-78
3	8	13	160	56	-148
4	8	13	455	661	-116
-5	9	13	701	728	60
-4	9	13	498	516	73
-3	9	13	277	350	-126
-2	9	13	677	639	53
-1	9	13	1210	1208	47
0	9	13	741	720	51
1	9	13	243	185	-93
2	9	13	591	645	67
3	9	13	749	780	74
-5	10	13	428	456	89
-4	10	13	856	831	56
-3	10	13	865	812	48
-2	10	13	411	455	84
-1	10	13	72	32	-184
0	10	13	977	944	52
1	10	13	997	998	54
2	10	13	327	384	-93
3	10	13	88	168	-224
-4	11	13	314	171	-87
-3	11	13	206	312	-122
-2	11	13	570	626	60
-1	11	13	763	782	60
0	11	13	639	696	74
1	11	13	76	18	-193
2	11	13	378	383	-114
-3	12	13	629	663	63
-2	12	13	450	470	81
-1	12	13	81	217	-206
0	12	13	519	534	68
1	12	13	857	789	64
-7	0	14	750	706	62
-6	0	14	866	861	53
-5	0	14	564	547	62
-4	0	14	431	497	62
-3	0	14	1005	1020	44
-2	0	14	1923	1864	43
-1	0	14	1059	1041	42
0	0	14	144	111	-108
1	0	14	1466	1348	44
2	0	14	2091	1956	53
3	0	14	677	663	75
4	0	14	204	240	-142
5	0	14	652	730	71
-7	1	14	105	241	-265
-6	1	14	475	460	76
-5	1	14	1134	1212	46
-4	1	14	798	879	44
-3	1	14	763	791	47
-2	1	14	326	432	63
-1	1	14	748	809	46

H	K	L	$10F_o$	$10F_c$	10σ
0	1	14	1109	1105	44
1	1	14	1110	1083	47
2	1	14	81	80	-206
3	1	14	674	596	72
4	1	14	976	936	64
5	1	14	868	937	62
-7	2	14	675	674	66
-6	2	14	819	850	56
-5	2	14	495	404	63
-4	2	14	298	426	-100
-3	2	14	1445	1452	45
-2	2	14	1534	1526	44
-1	2	14	347	496	-81
0	2	14	156	193	-99
1	2	14	933	962	49
2	2	14	1468	1423	49
3	2	14	948	892	58
4	2	14	160	96	-176
5	2	14	481	415	83
-6	3	14	498	477	70
-5	3	14	910	950	48
-4	3	14	1473	1439	41
-3	3	14	465	404	60
-2	3	14	299	363	-80
-1	3	14	1107	1082	41
0	3	14	642	668	50
1	3	14	730	742	51
2	3	14	181	166	-143
3	3	14	744	696	69
4	3	14	902	877	70
5	3	14	574	638	83
-6	4	14	614	615	67
-5	4	14	208	261	-113
-4	4	14	81	164	-205
-3	4	14	1151	1151	41
-2	4	14	1092	1086	42
-1	4	14	776	801	47
0	4	14	156	40	-103
1	4	14	1045	1003	48
2	4	14	1078	1089	54
3	4	14	1014	997	61
4	4	14	95	95	-240
-6	5	14	326	345	-104
-5	5	14	611	622	61
-4	5	14	912	923	48
-3	5	14	296	357	-80
-2	5	14	166	75	-96
-1	5	14	677	709	48
0	5	14	1407	1354	42
1	5	14	632	662	56
2	5	14	136	116	-135
3	5	14	446	551	94
4	5	14	776	825	76
-6	6	14	513	449	84
-5	6	14	411	371	77
-4	6	14	396	351	70
-3	6	14	639	651	50
-2	6	14	676	719	57
-1	6	14	924	883	46
0	6	14	160	164	-120
1	6	14	701	779	60
2	6	14	680	755	65
3	6	14	600	605	75
4	6	14	201	169	-177
-6	7	14	301	250	-96
-5	7	14	617	603	57
-4	7	14	747	653	55
-3	7	14	299	358	-97
-2	7	14	343	343	68
-1	7	14	431	413	63
0	7	14	875	843	53
1	7	14	142	171	-128
2	7	14	83	35	-210
3	7	14	314	266	-113
4	7	14	573	529	93
-5	8	14	199	269	-113
-4	8	14	335	250	-74
-3	8	14	537	581	64
-2	8	14	442	482	62
-1	8	14	165	234	-109
0	8	14	69	141	-174
1	8	14	199	186	-106
2	8	14	570	502	75
3	8	14	392	400	-84
-5	9	14	228	187	-109
-4	9	14	491	421	75
-3	9	14	379	317	71
-2	9	14	78	47	-197
-1	9	14	414	404	62
0	9	14	224	318	-130
1	9	14	411	445	85
2	9	14	232	8	-98
3	9	14	328	353	-120
-4	10	14	87	104	-220
-3	10	14	245	129	-93
-2	10	14	294	291	-99

H	K	L	$10F_o$	$10F_c$	10σ
-1	10	14	84	160	-214
0	10	14	141	232	-131
1	10	14	82	167	-206
2	10	14	375	316	-88
-3	11	14	87	101	-222
-2	11	14	84	82	-212
-1	11	14	372	285	67
1	11	14	196	320	-138
-6	1	15	87	14	-220
-5	1	15	117	119	-139
-4	1	15	168	208	-115
-3	1	15	403	405	69
-2	1	15	87	128	-220
-1	1	15	550	576	54
0	1	15	73	35	-185
1	1	15	248	228	-99
2	1	15	87	143	-221
3	1	15	205	175	-122
4	1	15	100	56	-255
-6	2	15	303	300	-88
-5	2	15	72	48	-182
-4	2	15	344	384	72
-3	2	15	78	125	-198
-2	2	15	787	811	49
-1	2	15	65	82	-166
0	2	15	343	342	66
1	2	15	155	63	-134
2	2	15	286	299	-95
3	2	15	339	346	-108
4	2	15	217	154	-124
-6	3	15	84	50	-212
-5	3	15	332	359	-101
-4	3	15	334	386	-93
-3	3	15	395	428	73
-2	3	15	193	106	-100
-1	3	15	351	293	-78
0	3	15	135	95	-115
1	3	15	398	450	-90
2	3	15	312	241	-97
3	3	15	186	106	-138
4	3	15	108	56	-275
-6	4	15	431	439	78
-5	4	15	416	374	82
-4	4	15	123	56	-145
-3	4	15	82	41	-208
-2	4	15	200	302	-87
-1	4	15	593	582	57
0	4	15	609	591	54

H	K	L	$10F_o$	$10F_c$	10σ
1	4	15	191	70	-101
2	4	15	615	538	76
3	4	15	589	463	82
4	4	15	664	683	75
-6	5	15	305	249	-96
-5	5	15	490	503	75
-4	5	15	434	499	75
-3	5	15	839	774	47
-2	5	15	83	166	-209
-1	5	15	64	64	-162
0	5	15	621	617	63
1	5	15	729	597	56
2	5	15	141	257	-153
3	5	15	174	222	-167
4	5	15	209	183	-132
-5	6	15	613	630	71
-4	6	15	393	421	79
-3	6	15	82	237	-208
-2	6	15	854	830	50
-1	6	15	1099	1082	47
0	6	15	299	377	-113
1	6	15	186	39	-102
2	6	15	670	659	72
3	6	15	728	736	67
-5	7	15	212	184	-122
-4	7	15	729	780	60
-3	7	15	869	880	50
-2	7	15	310	344	-88
-1	7	15	530	470	65
0	7	15	630	679	64
1	7	15	607	635	69
2	7	15	562	656	87
3	7	15	87	34	-220
-5	8	15	562	521	76
-4	8	15	372	359	76
-3	8	15	131	214	-131
-2	8	15	693	647	60
-1	8	15	834	854	56
0	8	15	574	620	71
1	8	15	79	60	-200
2	8	15	451	413	75
3	8	15	1061	1065	61
-4	9	15	1017	968	55
-3	9	15	453	458	88
-2	9	15	438	486	82
-1	9	15	73	117	-185
0	9	15	673	731	69
1	9	15	644	672	63

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
2	9	15	663	611	73	1	3	16	641	683	65
-3	10	15	86	225	-219	2	3	16	1198	1148	55
-2	10	15	561	490	62	3	3	16	688	657	79
-1	10	15	1024	963	54	4	3	16	89	27	-227
0	10	15	669	670	69	-6	4	16	338	333	-116
1	10	15	180	190	-123	-5	4	16	702	725	60
-2	11	15	452	397	77	-4	4	16	750	750	55
-1	11	15	142	137	-125	-3	4	16	486	473	71
-6	0	16	587	593	77	-2	4	16	243	265	-117
-5	0	16	851	906	55	-1	4	16	766	740	54
-4	0	16	655	695	60	0	4	16	1008	991	52
-3	0	16	136	316	-134	1	4	16	578	572	70
-2	0	16	346	272	60	2	4	16	164	228	-184
-1	0	16	1090	1044	48	3	4	16	646	662	83
0	0	16	1033	1058	47	-5	5	16	304	296	-118
1	0	16	842	779	58	-4	5	16	615	616	63
2	0	16	188	70	-97	-3	5	16	680	663	59
3	0	16	310	296	-122	-2	5	16	907	880	50
4	0	16	1054	1113	66	-1	5	16	680	599	55
-6	1	16	1013	1079	57	0	5	16	316	368	-71
-5	1	16	241	156	-111	1	5	16	492	468	86
-4	1	16	300	270	-79	2	5	16	714	693	64
-3	1	16	1386	1321	43	3	5	16	458	486	-109
-2	1	16	1371	1359	43	-5	6	16	832	756	57
-1	1	16	659	676	60	-4	6	16	547	514	71
0	1	16	77	160	-195	-3	6	16	83	80	-211
1	1	16	1058	1032	54	-2	6	16	236	151	-94
2	1	16	739	781	61	-1	6	16	878	848	54
3	1	16	785	724	64	0	6	16	694	719	59
4	1	16	108	274	-275	1	6	16	598	438	69
-6	2	16	506	424	75	2	6	16	225	25	-118
-5	2	16	490	605	69	3	6	16	319	398	-141
-4	2	16	789	867	57	-5	7	16	204	199	-118
-3	2	16	792	757	52	-4	7	16	232	61	-101
-2	2	16	290	264	-71	-3	7	16	424	420	72
-1	2	16	805	833	53	-2	7	16	663	639	65
0	2	16	1251	1232	49	-1	7	16	625	653	69
1	2	16	888	879	53	0	7	16	78	41	-197
2	2	16	263	32	-100	1	7	16	555	509	62
3	2	16	791	811	78	2	7	16	686	672	65
4	2	16	1204	1162	59	-4	8	16	629	569	67
-6	3	16	482	514	88	-3	8	16	272	273	-111
-5	3	16	493	530	77	-2	8	16	77	34	-196
-4	3	16	326	373	-105	-1	8	16	481	493	77
-3	3	16	1079	1042	46	0	8	16	483	409	87
-2	3	16	1409	1366	43	1	8	16	325	375	-111
-1	3	16	729	629	54	2	8	16	94	7	-238
0	3	16	185	164	-114	-3	9	16	298	346	-102

H	K	L	$10F_o$	$10F_c$	10σ
-2	9	16	423	385	-95
-1	9	16	157	116	-123
0	9	16	85	89	-216
1	9	16	89	183	-226
-2	10	16	338	316	-105
-1	10	16	82	81	-208
0	10	16	226	231	-113
-5	1	17	175	23	-112
-4	1	17	90	58	-227
-3	1	17	77	11	-196
-2	1	17	117	131	-127
-1	1	17	72	62	-183
0	1	17	71	65	-179
1	1	17	80	218	-203
2	1	17	210	58	-113
3	1	17	112	191	-284
-5	2	17	209	116	-108
-4	2	17	148	61	-126
-3	2	17	504	461	72
-2	2	17	79	158	-201
-1	2	17	134	122	-124
0	2	17	93	190	-236

H	K	L	$10F_o$	$10F_c$	10σ

Table 68. F_o F_c Tables for $K_2[Pt(NO_2)_2(br)_2]$, 3, F(obs), F(calc), and σ_F ($-\sigma_F$ indicates omitted data).

H	K	L	$10F_o$	$10F_c$	10σ
2	0	0	132	119	10
4	0	0	954	1052	27
6	0	0	997	1006	20
8	0	0	255	299	28
10	0	0	511	431	29
1	1	0	1300	1217	13
2	1	0	793	820	11
3	1	0	2100	2195	36
4	1	0	298	338	12
5	1	0	249	234	13
6	1	0	168	201	21
7	1	0	842	851	17
8	1	0	137	160	-33
9	1	0	413	425	20
10	1	0	57	52	-106
11	1	0	139	201	-79
0	2	0	2144	1908	18
1	2	0	398	463	21
2	2	0	1099	1128	54
3	2	0	381	444	27
4	2	0	1003	1000	24
5	2	0	210	215	18
6	2	0	944	968	15
7	2	0	76	38	-38
8	2	0	378	400	18
9	2	0	123	104	-44
10	2	0	272	295	42
11	2	0	65	60	-122
1	3	0	1542	1513	15
2	3	0	263	202	26
3	3	0	1096	1084	30
4	3	0	62	110	-33
5	3	0	924	996	21
6	3	0	179	183	22
7	3	0	357	375	29
8	3	0	138	115	-34
9	3	0	504	506	17
10	3	0	58	54	-107
11	3	0	186	206	-92
0	4	0	1308	939	24
1	4	0	492	451	13
2	4	0	1668	1778	23
3	4	0	70	21	-26
4	4	0	483	489	48
5	4	0	95	138	-30
6	4	0	678	724	62
7	4	0	126	107	26
8	4	0	565	550	25
9	4	0	80	41	-62
10	4	0	101	203	-89
11	4	0	92	15	-79
1	5	0	1433	1311	66
2	5	0	444	452	19
3	5	0	628	590	14
4	5	0	538	599	30
5	5	0	1010	1035	50
6	5	0	299	332	15
7	5	0	322	361	23
8	5	0	110	41	-43
9	5	0	449	437	30
10	5	0	59	33	-110
11	5	0	159	198	-68
0	6	0	1272	1091	27
1	6	0	1148	1084	67
2	6	0	1005	963	73
3	6	0	389	401	26
4	6	0	717	722	24
5	6	0	153	150	26
6	6	0	518	577	33
7	6	0	187	183	-41
8	6	0	423	426	20
9	6	0	161	93	-50
10	6	0	243	248	47
11	6	0	112	22	-74
1	7	0	952	824	36
2	7	0	249	232	15
3	7	0	1017	983	90
4	7	0	420	384	55
5	7	0	362	407	26
6	7	0	239	241	22
7	7	0	533	543	23
8	7	0	48	13	-89
9	7	0	290	265	48
10	7	0	137	48	-63
0	8	0	1046	977	21
1	8	0	151	147	20

Table 68. (continued)

H	K	L	$10F_o$	$10F_c$	10σ
2	8	0	574	479	40
3	8	0	118	82	-31
4	8	0	812	820	89
5	8	0	153	147	-42
6	8	0	456	472	42
7	8	0	104	48	-45
8	8	0	195	280	-45
9	8	0	99	10	-57
10	8	0	233	264	-69
1	9	0	692	635	26
2	9	0	77	37	-42
3	9	0	698	663	38
4	9	0	117	113	-32
5	9	0	434	434	55
6	9	0	149	115	-37
7	9	0	455	440	26
8	9	0	115	95	-60
9	9	0	149	208	-68
0	10	0	565	576	20
1	10	0	197	208	21
2	10	0	657	632	29
3	10	0	187	153	24
4	10	0	496	471	22
5	10	0	109	111	-49
6	10	0	300	311	33
7	10	0	83	17	-77
8	10	0	295	312	-78
9	10	0	62	32	-114
1	11	0	626	606	32
2	11	0	172	139	33
3	11	0	304	287	20
4	11	0	86	80	-53
5	11	0	533	505	19
6	11	0	56	16	-104
7	11	0	146	255	-71
8	11	0	132	73	-64
0	12	0	99	122	-53
1	12	0	44	57	-81
2	12	0	629	588	16
3	12	0	47	6	-87
4	12	0	384	406	15
5	12	0	59	40	-109
6	12	0	189	250	-84
7	12	0	58	28	-108
1	13	0	391	400	21
2	13	0	53	81	-99
3	13	0	243	276	41
4	13	0	59	34	-109
5	13	0	352	376	32
6	13	0	63	56	-116
7	13	0	171	199	-67
0	14	0	283	297	42
1	14	0	89	57	-77
2	14	0	356	333	35
3	14	0	94	70	-76
4	14	0	285	304	56
5	14	0	62	10	-115
1	15	0	238	279	39
2	15	0	72	13	-83
3	15	0	294	254	-88
4	15	0	59	11	-110
0	16	0	301	256	43
1	16	0	62	14	-116
-11	0	1	388	367	57
-9	0	1	361	355	27
-7	0	1	890	869	22
-5	0	1	580	535	17
-3	0	1	1388	1481	16
-1	0	1	1475	1368	9
1	0	1	1863	1708	15
3	0	1	884	1008	22
5	0	1	179	151	20
7	0	1	933	958	25
9	0	1	203	262	43
11	0	1	259	221	-60
-12	1	1	61	171	-159
-11	1	1	59	47	-155
-10	1	1	408	393	51
-9	1	1	111	127	-68
-8	1	1	627	634	24
-7	1	1	233	237	27
-6	1	1	623	641	17
-5	1	1	33	9	-87
-4	1	1	1199	1204	20
-3	1	1	558	587	14
-2	1	1	1349	1225	4
-1	1	1	458	537	11
0	1	1	1778	1777	10
1	1	1	409	439	16
2	1	1	356	254	19
3	1	1	592	637	19
4	1	1	1218	1272	24
5	1	1	152	151	26
6	1	1	633	642	18
7	1	1	92	105	-59
8	1	1	310	322	22

Table 68. (continued)

H	K	L	$10F_o$	$10F_c$	10σ
9	1	1	47	55	-124
10	1	1	420	399	46
11	1	1	58	25	-152
-12	2	1	61	39	-160
-11	2	1	329	341	52
-10	2	1	108	7	-89
-9	2	1	375	399	24
-8	2	1	234	188	28
-7	2	1	527	567	21
-6	2	1	490	508	18
-5	2	1	1248	1206	24
-4	2	1	877	937	20
-3	2	1	1053	1058	17
-2	2	1	693	719	15
-1	2	1	1176	1121	4
0	2	1	94	29	20
1	2	1	1051	965	21
2	2	1	657	688	18
3	2	1	934	885	18
4	2	1	553	648	18
5	2	1	753	819	22
6	2	1	309	326	22
7	2	1	609	641	21
8	2	1	134	124	-42
9	2	1	292	290	33
10	2	1	55	34	-144
11	2	1	140	218	-86
-11	3	1	139	63	-68
-10	3	1	96	257	-126
-9	3	1	116	160	-66
-8	3	1	669	716	24
-7	3	1	239	243	24
-6	3	1	565	571	18
-5	3	1	77	19	-37
-4	3	1	646	636	17
-3	3	1	380	449	12
-2	3	1	2358	2447	15
-1	3	1	1309	1377	16
0	3	1	214	102	16
1	3	1	947	917	23
2	3	1	1421	1335	26
3	3	1	91	100	-38
4	3	1	855	838	20
5	3	1	34	22	-89
6	3	1	543	534	21
7	3	1	41	24	-108
8	3	1	474	481	27
9	3	1	47	22	-124
10	3	1	196	261	-90
11	3	1	57	36	-151
-11	4	1	217	286	-79
-10	4	1	61	88	-159
-9	4	1	492	495	26
-8	4	1	82	37	-57
-7	4	1	214	269	31
-6	4	1	98	104	-32
-5	4	1	1354	1372	23
-4	4	1	110	147	21
-3	4	1	438	402	14
-2	4	1	143	129	19
-1	4	1	1370	1386	19
0	4	1	279	223	14
1	4	1	1820	1620	25
2	4	1	77	111	-72
3	4	1	228	167	18
4	4	1	34	47	-91
5	4	1	1048	1068	21
6	4	1	67	89	-60
7	4	1	347	371	26
8	4	1	111	61	-52
9	4	1	422	366	43
10	4	1	59	24	-154
11	4	1	189	222	-77
-11	5	1	64	32	-167
-10	5	1	126	248	-94
-9	5	1	52	26	-137
-8	5	1	552	599	25
-7	5	1	111	120	-36
-6	5	1	568	630	19
-5	5	1	41	87	-108
-4	5	1	692	655	18
-3	5	1	66	80	-49
-2	5	1	1319	1409	21
-1	5	1	118	130	-29
0	5	1	593	502	15
1	5	1	573	547	16
2	5	1	1323	1178	29
3	5	1	466	451	20
4	5	1	769	713	18
5	5	1	113	136	-41
6	5	1	503	503	20
7	5	1	119	42	-39
8	5	1	484	471	25
9	5	1	110	113	-88
10	5	1	132	232	-116
11	5	1	72	35	-189

H	K	L	$10F_o$	$10F_c$	10σ
-11	6	1	196	223	-73
-10	6	1	77	67	-99
-9	6	1	397	373	45
-8	6	1	140	81	-50
-7	6	1	537	522	22
-6	6	1	189	202	31
-5	6	1	601	656	18
-4	6	1	113	162	-33
-3	6	1	925	907	18
-2	6	1	306	355	19
-1	6	1	868	857	18
0	6	1	296	248	17
1	6	1	1210	1031	27
2	6	1	85	28	-49
3	6	1	783	684	18
4	6	1	255	230	23
5	6	1	575	593	20
6	6	1	351	343	21
7	6	1	481	495	26
8	6	1	221	178	38
9	6	1	259	279	-57
10	6	1	53	49	-139
-10	7	1	237	326	-98
-9	7	1	89	21	-103
-8	7	1	265	299	30
-7	7	1	48	102	-125
-6	7	1	565	592	21
-5	7	1	39	11	-101
-4	7	1	748	767	21
-3	7	1	37	43	-98
-2	7	1	672	619	16
-1	7	1	72	119	-51
0	7	1	1325	1259	28
1	7	1	468	447	19
2	7	1	473	397	16
3	7	1	349	354	22
4	7	1	855	797	24
5	7	1	125	115	-38
6	7	1	463	462	23
7	7	1	49	8	-129
8	7	1	178	316	-105
9	7	1	62	83	-162
10	7	1	255	263	-59
-10	8	1	60	37	-158
-9	8	1	160	261	-92
-8	8	1	49	69	-128
-7	8	1	586	578	26
-6	8	1	100	60	-49
-5	8	1	245	290	35
-4	8	1	78	63	-52
-3	8	1	1026	1073	22
-2	8	1	108	18	-38
-1	8	1	546	538	19
0	8	1	35	58	-92
1	8	1	555	503	19
2	8	1	225	187	24
3	8	1	1056	973	22
4	8	1	121	93	-44
5	8	1	337	326	25
6	8	1	87	80	-73
7	8	1	548	484	25
8	8	1	64	54	-169
9	8	1	167	212	-71
10	8	1	164	39	-80
-10	9	1	204	262	-69
-9	9	1	62	39	-164
-8	9	1	152	239	-64
-7	9	1	53	85	-138
-6	9	1	498	531	25
-5	9	1	91	59	-64
-4	9	1	679	664	22
-3	9	1	226	242	27
-2	9	1	340	329	20
-1	9	1	555	519	21
0	9	1	1012	944	22
1	9	1	307	292	22
2	9	1	491	474	25
3	9	1	128	80	-36
4	9	1	592	547	24
5	9	1	46	67	-122
6	9	1	475	439	25
7	9	1	136	34	-69
8	9	1	197	264	-84
-9	10	1	193	276	-80
-8	10	1	120	104	-79
-7	10	1	353	366	49
-6	10	1	198	165	39
-5	10	1	369	365	25
-4	10	1	271	251	28
-3	10	1	546	530	22
-2	10	1	48	87	-125
-1	10	1	649	662	20
0	10	1	98	68	-64
1	10	1	611	581	22
2	10	1	213	196	26
3	10	1	525	514	21

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
4	10	1	261	229	29	2	13	1	388	466	50
5	10	1	469	388	21	3	13	1	57	104	-149
6	10	1	106	71	-60	4	13	1	119	245	-109
7	10	1	169	269	-86	5	13	1	54	5	-141
8	10	1	61	18	-160	6	13	1	196	267	-71
9	10	1	203	261	-90	-6	14	1	159	53	-81
-8	11	1	186	262	-71	-5	14	1	168	219	-71
-7	11	1	57	96	-151	-4	14	1	57	64	-150
-6	11	1	277	374	-70	-3	14	1	207	309	-72
-5	11	1	45	42	-118	-2	14	1	90	73	-93
-4	11	1	336	407	32	-1	14	1	338	357	54
-3	11	1	171	166	33	0	14	1	46	26	-122
-2	11	1	508	509	22	1	14	1	251	289	-64
-1	11	1	161	148	34	2	14	1	56	83	-146
0	11	1	417	432	20	3	14	1	300	327	47
1	11	1	119	62	-35	4	14	1	71	36	-185
2	11	1	704	661	20	5	14	1	221	227	-57
3	11	1	47	51	-122	-4	15	1	191	266	-87
4	11	1	270	261	27	-3	15	1	59	39	-154
5	11	1	113	11	-54	-2	15	1	101	165	-108
6	11	1	250	344	-89	-1	15	1	54	49	-143
7	11	1	54	68	-141	0	15	1	344	363	43
8	11	1	312	270	48	1	15	1	65	37	-169
-8	12	1	56	25	-146	2	15	1	190	260	-73
-7	12	1	69	244	-182	3	15	1	53	15	-138
-6	12	1	62	35	-162	4	15	1	194	201	-79
-5	12	1	410	429	43	-1	16	1	205	223	-56
-4	12	1	55	13	-144	0	16	1	84	5	-108
-3	12	1	293	335	26	1	16	1	157	211	-69
-2	12	1	76	5	-61	-12	0	2	170	175	-83
-1	12	1	477	486	21	-10	0	2	612	557	34
0	12	1	86	20	-55	-8	0	2	262	275	23
1	12	1	338	344	23	-6	0	2	628	599	16
2	12	1	43	45	-114	-4	0	2	1489	1540	19
3	12	1	352	391	23	-2	0	2	254	142	10
4	12	1	92	27	-85	0	0	2	2018	2152	10
5	12	1	502	440	33	2	0	2	1268	1037	22
6	12	1	81	47	-100	4	0	2	867	912	23
7	12	1	91	152	-100	6	0	2	613	603	21
-7	13	1	74	4	-194	8	0	2	485	497	23
-6	13	1	261	277	-68	10	0	2	355	314	62
-5	13	1	58	12	-153	-12	1	2	135	1	-76
-4	13	1	327	364	41	-11	1	2	217	263	-57
-3	13	1	56	77	-147	-10	1	2	54	33	-143
-2	13	1	366	353	40	-9	1	2	312	326	30
-1	13	1	48	50	-126	-8	1	2	192	165	34
0	13	1	292	309	25	-7	1	2	932	933	23
1	13	1	53	65	-99	-6	1	2	283	283	18

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
-5	1	2	352	336	18	-4	3	2	481	550	15
-4	1	2	392	394	14	-3	3	2	545	504	13
-3	1	2	1345	1380	16	-2	3	2	473	509	12
-2	1	2	602	643	14	-1	3	2	1810	1857	15
-1	1	2	1270	1172	11	0	3	2	342	305	11
0	1	2	127	71	11	1	3	2	796	769	15
1	1	2	918	809	16	2	3	2	81	23	-42
2	1	2	704	692	18	3	3	2	744	629	21
3	1	2	1311	1295	30	4	3	2	554	573	22
4	1	2	418	444	18	5	3	2	1225	1235	24
5	1	2	784	804	24	6	3	2	405	413	23
6	1	2	205	233	35	7	3	2	272	278	24
7	1	2	549	566	27	8	3	2	120	127	-67
8	1	2	118	139	-71	9	3	2	313	381	-83
9	1	2	279	309	32	10	3	2	58	31	-151
10	1	2	89	16	-98	11	3	2	81	251	-212
11	1	2	182	286	-85	-11	4	2	53	6	-140
-12	2	2	234	222	-68	-10	4	2	167	283	-79
-11	2	2	139	73	-73	-9	4	2	52	117	-137
-10	2	2	403	408	25	-8	4	2	534	575	25
-9	2	2	175	120	38	-7	4	2	38	8	-99
-8	2	2	388	403	23	-6	4	2	414	460	20
-7	2	2	199	160	23	-5	4	2	206	211	18
-6	2	2	715	671	20	-4	4	2	839	861	22
-5	2	2	34	5	-88	-3	4	2	84	69	-23
-4	2	2	1217	1260	20	-2	4	2	1381	1478	17
-3	2	2	307	347	12	-1	4	2	298	265	12
-2	2	2	976	952	14	0	4	2	311	186	13
-1	2	2	930	1043	13	1	4	2	318	305	15
0	2	2	497	437	12	2	4	2	1827	1822	28
1	2	2	1323	1444	19	3	4	2	139	64	-33
2	2	2	1565	1470	26	4	4	2	542	465	21
3	2	2	698	691	19	5	4	2	38	9	-100
4	2	2	1035	972	23	6	4	2	544	571	26
5	2	2	106	115	-50	7	4	2	100	93	-55
6	2	2	604	625	22	8	4	2	567	526	25
7	2	2	130	149	-47	9	4	2	143	52	-70
8	2	2	484	503	25	10	4	2	132	202	-77
9	2	2	149	127	-89	-11	5	2	153	249	-115
10	2	2	149	232	-91	-10	5	2	55	50	-145
-12	3	2	63	21	-166	-9	5	2	376	391	33
-11	3	2	146	280	-100	-8	5	2	146	137	-45
-10	3	2	53	3	-139	-7	5	2	446	476	21
-9	3	2	416	424	29	-6	5	2	317	326	21
-8	3	2	128	77	-39	-5	5	2	954	959	25
-7	3	2	396	416	18	-4	5	2	331	369	15
-6	3	2	234	267	20	-3	5	2	475	481	15
-5	3	2	1025	1083	23	-2	5	2	98	103	-23

Table 68. (continued)

H	K	L	$10F_o$	$10F_c$	10σ
-1	5	2	1037	1060	21
0	5	2	241	205	17
1	5	2	1062	1046	26
2	5	2	359	319	17
3	5	2	839	680	23
4	5	2	61	67	-66
5	5	2	991	903	25
6	5	2	41	39	-108
7	5	2	288	327	29
8	5	2	79	20	-88
9	5	2	341	352	51
10	5	2	65	71	-171
-11	6	2	62	73	-163
-10	6	2	178	312	-110
-9	6	2	198	177	33
-8	6	2	373	426	25
-7	6	2	108	84	-46
-6	6	2	499	531	21
-5	6	2	171	187	24
-4	6	2	763	828	19
-3	6	2	649	681	18
-2	6	2	709	719	18
-1	6	2	599	660	18
0	6	2	1050	1005	26
1	6	2	139	152	26
2	6	2	942	829	24
3	6	2	125	133	-54
4	6	2	778	672	20
5	6	2	43	33	-114
6	6	2	547	533	24
7	6	2	47	30	-122
8	6	2	308	352	39
9	6	2	67	31	-176
10	6	2	162	252	-93
-11	7	2	132	242	-107
-10	7	2	55	42	-143
-9	7	2	127	266	-103
-8	7	2	159	119	-41
-7	7	2	595	587	23
-6	7	2	305	310	21
-5	7	2	286	323	21
-4	7	2	247	287	28
-3	7	2	1052	1054	25
-2	7	2	34	42	-89
-1	7	2	813	798	19
0	7	2	139	146	-30
1	7	2	658	603	18
2	7	2	244	212	25
3	7	2	1035	933	23
4	7	2	77	64	-76
5	7	2	318	340	43
6	7	2	116	47	-56
7	7	2	602	519	24
8	7	2	101	7	-114
9	7	2	124	243	-108
10	7	2	69	51	-181
-10	8	2	252	305	-77
-9	8	2	140	100	-71
-8	8	2	142	271	-63
-7	8	2	45	9	-118
-6	8	2	520	555	24
-5	8	2	103	141	-53
-4	8	2	689	732	23
-3	8	2	87	125	-47
-2	8	2	364	380	19
-1	8	2	78	33	-42
0	8	2	1159	1133	29
1	8	2	151	131	29
2	8	2	321	263	20
3	8	2	41	68	-109
4	8	2	853	778	26
5	8	2	47	54	-123
6	8	2	521	473	25
7	8	2	105	44	-66
8	8	2	103	216	-129
9	8	2	58	5	-152
-10	9	2	60	38	-157
-9	9	2	205	274	-69
-8	9	2	52	22	-136
-7	9	2	420	437	28
-6	9	2	155	75	-40
-5	9	2	356	387	22
-4	9	2	184	184	36
-3	9	2	736	780	24
-2	9	2	181	152	26
-1	9	2	449	431	18
0	9	2	184	181	28
1	9	2	727	652	19
2	9	2	121	120	-40
3	9	2	806	729	19
4	9	2	248	208	29
5	9	2	283	276	31
6	9	2	204	178	41
7	9	2	453	419	40
8	9	2	64	67	-167
9	9	2	75	216	-198

H	K	L	10F_o	10F_c	10σ	H	K	L	10F_o	10F_c	10σ
-9	10	2	58	16	-151	-5	13	2	351	385	43
-8	10	2	270	338	53	-4	13	2	58	38	-153
-7	10	2	54	65	-141	-3	13	2	279	321	53
-6	10	2	381	415	25	-2	13	2	59	79	-154
-5	10	2	122	67	-48	-1	13	2	336	346	27
-4	10	2	340	345	26	0	13	2	83	2	-61
-3	10	2	63	21	-76	1	13	2	420	411	32
-2	10	2	648	630	20	2	13	2	61	93	-160
-1	10	2	243	236	24	3	13	2	257	282	46
0	10	2	712	682	20	4	13	2	55	27	-144
1	10	2	424	362	19	5	13	2	303	283	45
2	10	2	512	480	22	6	13	2	173	36	-64
3	10	2	191	161	32	-6	14	2	175	234	-76
4	10	2	418	410	26	-5	14	2	59	6	-156
5	10	2	51	54	-133	-4	14	2	182	224	-66
6	10	2	352	352	46	-3	14	2	58	45	-153
7	10	2	63	39	-165	-2	14	2	310	351	47
8	10	2	118	242	-111	-1	14	2	59	43	-156
-9	11	2	194	269	-73	0	14	2	311	366	43
-8	11	2	57	36	-149	1	14	2	138	78	-69
-7	11	2	60	217	-158	2	14	2	188	254	-70
-6	11	2	118	7	-67	3	14	2	54	91	-142
-5	11	2	500	512	24	4	14	2	252	263	55
-4	11	2	71	73	-69	5	14	2	166	2	-62
-3	11	2	323	361	25	-4	15	2	125	29	-73
-2	11	2	170	136	31	-3	15	2	257	266	42
-1	11	2	463	483	24	-2	15	2	110	45	-84
0	11	2	70	55	-65	-1	15	2	154	224	-67
1	11	2	613	624	21	-9	0	3	496	462	24
2	11	2	68	55	-76	-7	0	3	928	914	20
3	11	2	345	332	22	-5	0	3	170	104	20
4	11	2	158	87	-40	-3	0	3	2566	2691	16
5	11	2	372	359	48	-1	0	3	542	433	14
6	11	2	59	34	-154	1	0	3	1606	1530	15
7	11	2	185	257	-85	3	0	3	1740	1770	27
8	11	2	61	62	-159	5	0	3	36	73	-93
-8	12	2	248	284	-60	7	0	3	721	724	27
-7	12	2	59	30	-154	9	0	3	298	327	51
-6	12	2	297	345	46	-12	1	3	159	234	-78
-4	12	2	64	255	-169	-11	1	3	103	71	-88
-3	12	2	52	48	-136	-10	1	3	397	400	27
-2	12	2	622	594	22	-9	1	3	200	110	32
-1	12	2	47	43	-123	-8	1	3	276	305	27
0	12	2	239	269	28	-7	1	3	117	104	-49
1	12	2	100	8	-41	-6	1	3	1271	1232	24
2	12	2	479	444	22	-5	1	3	69	79	-42
3	12	2	45	11	-118	-4	1	3	1010	1014	18
-6	13	2	55	59	-145	-3	1	3	506	528	13

Table 68. (continued)

H	K	L	$10F_o$	$10F_c$	10σ
-2	1	3	597	478	16
-1	1	3	436	519	10
0	1	3	2578	2719	14
1	1	3	320	422	12
2	1	3	594	484	15
3	1	3	421	449	20
4	1	3	1120	1088	26
5	1	3	40	114	-106
6	1	3	668	652	26
-11	2	3	152	240	-80
-10	2	3	53	77	-138
-9	2	3	475	510	24
-8	2	3	226	204	27
-7	2	3	561	568	19
-6	2	3	390	384	16
-5	2	3	969	962	21
-4	2	3	447	508	12
-3	2	3	1509	1512	16
-2	2	3	124	164	12
-1	2	3	802	805	15
0	2	3	399	345	12
1	2	3	1271	1207	18
2	2	3	213	254	17
3	2	3	1440	1364	32
4	2	3	204	196	30
5	2	3	625	579	22
6	2	3	275	202	39
7	2	3	443	469	27
8	2	3	168	128	-53
9	2	3	340	346	-81
10	2	3	95	32	-100
-12	3	3	299	297	47
-11	3	3	58	90	-151
-10	3	3	141	233	-73
-9	3	3	106	82	-72
-8	3	3	519	528	22
-7	3	3	42	91	-110
-6	3	3	862	861	18
0	3	3	1224	1063	18
1	3	3	171	227	19
2	3	3	1221	1211	26
3	3	3	37	72	-97
4	3	3	736	645	23
5	3	3	44	36	-116
6	3	3	666	641	26
7	3	3	114	29	-48
8	3	3	319	372	35
9	3	3	89	9	-97

H	K	L	$10F_o$	$10F_c$	10σ
10	3	3	63	219	-166
-12	4	3	116	20	-80
-11	4	3	199	253	-68
-10	4	3	52	27	-136
-9	4	3	539	531	24
-8	4	3	47	97	-124
-7	4	3	267	263	21
-6	4	3	90	64	-36
-5	4	3	1223	1273	24
-4	4	3	289	276	15
-3	4	3	722	687	20
-2	4	3	362	363	12
-1	4	3	1242	1304	18
0	4	3	29	16	-77
1	4	3	1217	1245	23
2	4	3	147	145	27
3	4	3	795	686	19
4	4	3	177	180	38
5	4	3	958	82^Y	

Table 69. F_o F_c Tables for $K_2[Pt(NO_2)_2Cl_4]$, 4, F(obs), F(calc), and σ_F ($-\sigma_F$ indicates omitted data).

H	K	L	$10F_o$	$10F_c$	10σ
4	0	0	7504	7543	88
8	0	0	3912	3850	107
2	2	0	1160	1074	77
6	2	0	1741	1629	124
0	4	0	6074	6175	67
4	4	0	4525	4643	105
8	4	0	1772	1810	136
2	6	0	2961	2796	99
6	6	0	3078	3025	101
0	8	0	7821	7607	92
4	8	0	6629	6568	116
8	8	0	2669	2597	135
2	10	0	801	648	154
6	10	0	1009	975	160
0	12	0	5689	5479	120
4	12	0	3205	3302	103
2	14	0	2639	2596	111
6	14	0	2056	1975	137
0	16	0	3699	3680	108
4	16	0	2646	2703	128
2	18	0	463	781	-335
1	1	1	4397	4307	51
3	1	1	1571	1545	81
5	1	1	2956	3082	86
7	1	1	1099	1114	132
9	1	1	1391	1654	179
1	3	1	4568	4429	67
3	3	1	4154	4260	94
5	3	1	4100	4132	122
7	3	1	1323	1278	136
9	3	1	1934	2143	152
1	5	1	4714	4607	80
3	5	1	1903	1884	85
5	5	1	3086	3109	99
7	5	1	1460	1430	165
9	5	1	1914	1748	164
1	7	1	2650	2698	73
3	7	1	1291	1305	117
5	7	1	2390	2404	112
7	7	1	576	819	-272
1	9	1	3073	3192	110
3	9	1	2989	2927	92
5	9	1	3101	3039	104
7	9	1	1040	1017	195
1	11	1	3348	3391	87
3	11	1	1827	1843	114
5	11	1	2637	2621	118
7	11	1	1411	1446	145
1	13	1	1883	1900	109
3	13	1	1224	1337	164
5	13	1	1919	1861	143
7	13	1	788	689	-222
1	15	1	1782	1706	130
3	15	1	1395	1551	155
5	15	1	1683	1760	163
1	17	1	2040	2367	131
3	17	1	1539	1516	160
5	17	1	1976	1839	151
1	19	1	1158	1297	207
2	0	2	6207	6312	63
6	0	2	4412	4388	127
0	2	2	5786	5923	49
2	2	2	143	153	-350
4	2	2	5456	5352	23
6	2	2	220	54	-542
8	2	2	1892	2159	158
2	4	2	1257	1177	90
4	4	2	194	113	-476
6	4	2	1383	1339	136
8	4	2	226	6	-557
0	6	2	9514	9555	79
2	6	2	359	50	-195
4	6	2	4799	4771	114
6	6	2	416	134	-299
8	6	2	2986	2978	126
2	8	2	4497	4411	23
4	8	2	207	118	-509
6	8	2	2651	2729	118
8	8	2	214	117	-525
0	10	2	3367	3396	117
2	10	2	218	181	-534
4	10	2	2635	2695	108
6	10	2	204	81	-501
8	10	2	1696	1507	177

Table 69. (continued)

H	K	L	$10F_O$	$10F_C$	σ_F	H	K	L	$10F_O$	$10F_C$	σ_F
2	12	2	2144	2074	115	0	0	4	8109	8342	53
4	12	2	179	112	-440	4	0	4	4006	3835	95
6	12	2	1898	1964	127	8	0	4	2915	3141	127
0	14	2	3973	4074	134	2	2	4	6698	6674	73
4	14	2	4003	4017	108	4	2	4	211	8	-517
6	14	2	473	127	-261	6	2	4	3276	3130	103
2	16	2	1668	1878	144	8	2	4	215	122	-528
4	16	2	307	145	-324	0	4	4	748	722	95
0	18	2	2184	2224	130	2	4	4	332	377	-210
2	18	2	216	45	-532	4	4	4	1424	1510	109
4	18	2	1375	1540	194	6	4	4	432	15	-302
1	1	3	3718	3803	59	8	4	4	1258	1280	193
3	1	3	2432	2434	67	2	6	4	7045	6941	92
5	1	3	1897	1881	109	4	6	4	211	40	-518
7	1	3	1751	1923	143	6	6	4	4292	4236	99
9	1	3	863	1114	-257	8	6	4	335	33	-333
1	3	3	4035	4027	69	0	8	4	3076	3044	105
3	3	3	5239	5057	91	2	8	4	208	82	-511
5	3	3	3095	3102	94	4	8	4	3860	3849	132
7	3	3	1897	2016	130	8	8	4	2050	2084	162
9	3	3	1479	1582	175	2	10	4	3436	3464	88
1	5	3	3788	3729	82	4	10	4	201	176	-493
3	5	3	2558	2582	80	6	10	4	2135	2007	128
5	5	3	2261	2247	109	8	10	4	255	43	-627
7	5	3	2016	2094	129	0	12	4	2448	2494	107
9	5	3	1155	1253	229	2	12	4	222	18	-546
1	7	3	2418	2418	76	4	12	4	1554	1540	118
3	7	3	2221	2211	92	6	12	4	581	182	-230
5	7	3	1644	1742	134	2	14	4	4415	4432	138
7	7	3	1233	1454	173	4	14	4	218	88	-534
1	9	3	2636	2583	79	6	14	4	2674	2660	128
3	9	3	3325	3323	92	0	16	4	1928	1818	128
5	9	3	2207	2225	112	2	16	4	447	129	-249
7	9	3	1624	1612	156	4	16	4	1466	1521	161
1	11	3	3276	3383	90	2	18	4	1875	1942	144
3	11	3	2548	2461	105	1	1	5	2831	2838	74
5	11	3	2013	2003	135	3	1	5	3239	3254	90
7	11	3	1922	1924	146	5	1	5	1230	1339	134
1	13	3	1448	1568	132	7	1	5	2656	2451	115
3	13	3	1456	1514	139	9	1	5	430	622	-396
5	13	3	1298	1240	173	1	3	5	3246	3296	78
7	13	3	805	1085	-228	3	3	5	5337	5366	91
1	15	3	1494	1809	134	5	3	5	2127	2157	103
3	15	3	1994	1959	125	7	3	5	2752	2612	118
5	15	3	1349	1391	185	9	3	5	947	1055	-256
1	17	3	1958	2016	136	1	5	5	3607	3602	86
3	17	3	1624	1612	165	3	5	5	3144	3198	110
1	19	3	1056	1331	188	5	5	5	1259	1297	160

Table 69. (continued)

H	K	L	$10F_o$	$10F_c$	σ_F
7	5	5	2719	2675	115
9	5	5	276	786	-677
1	7	5	2165	2203	77
3	7	5	2482	2458	92
5	7	5	601	855	-302
7	7	5	2100	1971	132
1	9	5	2769	2604	82
3	9	5	3816	3645	86
5	9	5	1719	1636	127
7	9	5	1978	2019	140
1	11	5	2776	2768	97
3	11	5	2701	2633	105
5	11	5	1448	1487	136
7	11	5	2324	2244	135
1	13	5	1395	1459	125
3	13	5	2012	2015	111
5	13	5	745	964	-257
1	15	5	1367	1415	155
3	15	5	2082	2082	130
5	15	5	936	1003	-201
1	17	5	1810	2030	146
3	17	5	1779	1873	152
1	19	5	687	1164	-336
2	0	6	9896	10015	73
6	0	6	5160	5377	123
0	2	6	677	624	93
2	2	6	621	430	98
4	2	6	2100	2074	89
6	2	6	226	32	-555
8	2	6	1767	1488	152
2	4	6	5189	5343	87
4	4	6	184	54	-451
6	4	6	2591	2673	107
8	4	6	561	114	-270
0	6	6	3909	3925	91
2	6	6	176	90	-432
4	6	6	1997	2101	106
6	6	6	420	72	-295
8	6	6	2320	2231	150
2	8	6	6756	6899	105
4	8	6	217	50	-534
6	8	6	3591	3667	111
8	8	6	253	83	-621
0	10	6	686	617	-221
2	10	6	217	187	-533
4	10	6	831	880	-193
6	10	6	176	144	-433
2	12	6	4091	4012	92

H	K	L	$10F_o$	$10F_c$	σ_F
4	12	6	414	95	-264
6	12	6	2646	2667	130
0	14	6	1893	1932	118
2	14	6	211	73	-516
4	14	6	2564	2442	120
6	14	6	452	20	-361
2	16	6	3151	3102	116
4	16	6	338	36	-331
0	18	6	1241	974	156
2	18	6	212	77	-520
1	1	7	3333	3197	78
3	1	7	2621	2699	70
5	1	7	1273	1197	113
7	1	7	2075	2212	124
9	1	7	663	745	-319
1	3	7	3254	3238	84
3	3	7	4341	4487	97
5	3	7	2294	2236	102
7	3	7	2245	2267	129
9	3	7	1113	1162	214
1	5	7	3050	3119	95
3	5	7	2952	2882	81
5	5	7	1680	1753	130
7	5	7	2348	2242	126
1	7	7	1922	1792	87
3	7	7	2325	2302	93
5	7	7	1293	1267	151
7	7	7	2014	1720	138
1	9	7	2514	2439	90
3	9	7	3337	3361	93
5	9	7	1763	1730	126
7	9	7	1833	1826	156
1	11	7	2628	2663	96
3	11	7	2375	2319	108
5	11	7	1566	1431	141
7	11	7	1901	2014	155
1	13	7	1488	1684	129
3	13	7	1860	1734	131
5	13	7	679	961	-335
1	15	7	1385	1454	134
3	15	7	1760	1766	135
5	15	7	607	1032	-309
1	17	7	1957	1941	123
3	17	7	1578	1741	153
0	0	8	7216	7201	76
4	0	8	3815	3781	107
8	0	8	2642	2640	123
2	2	8	4695	4731	87

H	K	L	$10F_o$	$10F_c$	σ_F
4	2	8	185	70	-454
6	2	8	2791	2775	102
8	2	8	203	138	-498
0	4	8	1464	1448	77
2	4	8	173	381	-426
4	4	8	1782	1862	110
6	4	8	186	171	-458
8	4	8	964	1135	194
2	6	8	5027	5172	103
4	6	8	202	169	-496
6	6	8	3699	3612	102
8	6	8	228	100	-559
0	8	8	3375	3438	110
2	8	8	210	295	-517
4	8	8	3624	3565	93
6	8	8	214	99	-526
8	8	8	1725	1814	160
2	10	8	2892	2698	93
4	10	8	212	25	-521
6	10	8	1824	1827	129
0	12	8	2757	2638	100
2	12	8	378	164	-262
4	12	8	1628	1690	140
6	12	8	204	1	-501
2	14	8	3680	3558	106
4	14	8	438	150	-309
6	14	8	2187	2347	159
0	16	8	2003	1962	128
2	16	8	390	30	-276
4	16	8	1472	1566	146
2	18	8	1279	1609	206
1	1	9	2709	2702	67
3	1	9	2014	1891	82
5	1	9	2409	2380	101
7	1	9	957	1239	-201
1	3	9	3373	3266	94
3	3	9	3203	3345	110
5	3	9	2907	2873	94
7	3	9	1389	1449	171
1	5	9	3049	3212	104
3	5	9	1898	1869	100
5	5	9	2109	2043	115
7	5	9	1391	1511	163
1	7	9	2495	2496	86
3	7	9	1523	1541	123
5	7	9	1765	1694	112
7	7	9	1119	1036	176
1	9	9	2268	2421	100

H	K	L	$10F_o$	$10F_c$	σ_F
3	9	9	2301	2238	107
5	9	9	1901	2151	126
7	9	9	942	1128	-254
1	11	9	2559	2671	101
3	11	9	1983	1878	118
5	11	9	1955	2061	136
7	11	9	1183	1362	236
1	13	9	1308	1335	134
3	13	9	1190	1264	156
5	13	9	1358	1413	174
1	15	9	1815	1574	128
3	15	9	1428	1585	171
5	15	9	1533	1430	164
1	17	9	1660	1740	137
3	17	9	1489	1272	175
2	0	10	3489	3598	100
6	0	10	3228	3113	98
0	2	10	5093	5129	19
2	2	10	353	426	-253
4	2	10	4371	4263	113
6	2	10	184	21	-453
8	2	10	1589	1776	173
2	4	10	1019	1021	128
4	4	10	200	38	-493
6	4	10	1300	1229	154
8	4	10	245	158	-602
0	6	10	6650	6646	99
2	6	10	215	102	-529
4	6	10	4032	4054	126
6	6	10	184	62	-451
8	6	10	2383	2276	150
2	8	10	2799	2761	92
4	8	10	197	78	-483
6	8	10	2017	2136	135
0	10	10	3401	3333	91
2	10	10	209	190	-513
4	10	10	2515	2536	113
6	10	10	449	206	-277
2	12	10	1588	1465	135
4	12	10	377	141	-314
6	12	10	1351	1545	163
0	14	10	3584	3564	106
2	14	10	219	100	-539
4	14	10	3265	3219	115
2	16	10	1386	1390	143
4	16	10	468	23	-274
0	18	10	2175	2037	132
1	1	11	2949	2996	105

H	K	L	$10F_o$	$10F_c$	σ_F
3	1	11	1078	1315	139
5	1	11	2259	2243	103
7	1	11	644	862	-248
1	3	11	3003	3076	77
3	3	11	2547	2406	86
5	3	11	2905	2974	100
7	3	11	1119	917	178
1	5	11	2778	2754	83
3	5	11	1500	1525	114
5	5	11	2583	2632	105
7	5	11	602	914	-312
1	7	11	1882	1946	104
3	7	11	1293	1261	132
5	7	11	2089	2173	118
7	7	11	540	630	-237
1	9	11	2155	2275	104
3	9	11	1742	1959	114
5	9	11	2364	2327	127
7	9	11	842	842	-204
1	11	11	2605	2452	100
3	11	11	1509	1408	144
5	11	11	1935	1958	142
1	13	11	1657	1651	123
3	13	11	711	970	-221
5	13	11	1570	1474	143
1	15	11	1525	1532	157
3	15	11	1033	1123	-229
1	17	11	1777	1679	147
0	0	12	7371	7571	97
4	0	12	4995	4818	116
8	0	12	2971	2663	125
2	2	12	1350	1440	110
4	2	12	552	7	-224
6	2	12	1278	1347	162
8	2	12	388	174	-332
0	4	12	3934	4101	104
2	4	12	382	377	-277
4	4	12	3263	3304	89
6	4	12	646	77	-204
8	4	12	1532	1539	170
2	6	12	1974	2045	99
4	6	12	399	33	-260
6	6	12	1897	1978	133
0	8	12	5004	4830	117
2	8	12	187	164	-459
4	8	12	4162	4155	96
6	8	12	189	43	-465
2	10	12	803	862	-202
6	10	12	796	916	-274
0	12	12	3595	3581	101
2	12	12	204	41	-501
4	12	12	2684	2512	118
2	14	12	1696	1813	154
4	14	12	419	20	-288
0	16	12	2616	2627	124
2	16	12	364	133	-358
1	1	13	2255	2154	86
3	1	13	1685	1658	109
5	1	13	2271	2052	106
7	1	13	1105	965	154
1	3	13	2495	2474	83
3	3	13	2473	2384	98
5	3	13	2230	2265	114
7	3	13	645	1153	-300
1	5	13	2550	2564	90
3	5	13	1558	1670	126
5	5	13	1615	1740	139
7	5	13	1037	1164	210
1	7	13	2047	1928	98
3	7	13	1122	1253	160
5	7	13	1294	1438	164
7	7	13	612	859	-280
1	9	13	2171	2156	103
3	9	13	1797	1837	116
5	9	13	1792	1828	141
1	11	13	1838	1900	123
3	11	13	1471	1430	146
5	11	13	1625	1670	158
1	13	13	1497	1330	140
3	13	13	1367	1226	154
5	13	13	1405	1290	192
1	15	13	933	1187	-200
3	15	13	767	1208	-305
2	0	14	3637	3612	119
6	0	14	2436	2492	119
0	2	14	3033	2912	83
2	2	14	538	280	-191
4	2	14	2753	2780	99
6	2	14	196	51	-481
2	4	14	1944	1947	104
4	4	14	509	104	-240
6	4	14	954	1254	-205
0	6	14	3736	3784	124
2	6	14	455	4	-237
4	6	14	2780	2775	104
6	6	14	207	166	-509

H	K	L	$10F_o$	$10F_c$	σ_F
2	8	14	2976	2855	97
4	8	14	182	72	-445
6	8	14	1951	1846	144
0	10	14	2009	2025	115
2	10	14	205	243	-504
4	10	14	2008	1781	128
6	10	14	235	36	-577
2	12	14	1725	1804	132
4	12	14	210	24	-516
0	14	14	2451	2339	121
2	14	14	192	6	-472
1	1	15	2127	1957	96
3	1	15	1780	1893	113
5	1	15	943	929	174
7	1	15	1649	1489	154
1	3	15	2087	2081	98
3	3	15	2337	2457	106
5	3	15	1188	1418	159
7	3	15	1558	1504	161
1	5	15	1653	1746	117
3	5	15	1937	1896	109
5	5	15	1050	1254	201
7	5	15	1597	1410	157
1	7	15	1551	1433	128
3	7	15	1548	1767	142
5	7	15	1148	1076	185
1	9	15	1626	1518	125
3	9	15	1848	1967	136
5	9	15	1299	1133	170
1	11	15	1956	1757	122
3	11	15	1500	1676	146
5	11	15	1075	1020	-221
1	13	15	1062	1147	174
3	13	15	1166	1157	191
1	15	15	1356	1235	169
0	0	16	2502	2395	91
4	0	16	1886	1932	125
2	2	16	3494	3564	90
4	2	16	199	2	-489
6	2	16	2054	2047	130
0	4	16	680	812	-171
2	4	16	191	244	-469

H	K	L	$10F_o$	$10F_c$	σ_F

Table 70. F_o F_c Tables for $K_2[Pt(Cl)_2(PO_3)_2]$, 5, F(obs), F(calc), and σ_F ($-\sigma_F$ indicates omitted data).

H	K	L	$10F_o$	$10F_c$	10σ
2	0	0	2219	1850	13
4	0	0	2567	2493	111
6	0	0	888	938	86
8	0	0	179	218	33
10	0	0	47	22	-83
3	1	0	3127	3251	532
4	1	0	90	41	-41
5	1	0	992	1063	154
6	1	0	316	349	21
7	1	0	739	767	101
8	1	0	48	74	-84
9	1	0	183	156	-39
10	1	0	86	24	-63
11	1	0	307	308	57
0	2	0	3484	3157	6
1	2	0	62	51	-24
5	2	0	258	266	-60
6	2	0	932	977	129
7	2	0	345	380	28
8	2	0	426	409	60
9	2	0	117	117	-58
10	2	0	121	76	-64
11	2	0	51	86	-90
1	3	0	1347	1262	126
2	3	0	369	333	61
4	3	0	513	526	-118
5	3	0	884	831	183
6	3	0	514	510	-106
7	3	0	749	759	82
8	3	0	318	349	35
9	3	0	109	70	-67
10	3	0	196	231	-42
11	3	0	431	456	35
0	4	0	2941	2689	9
1	4	0	692	605	69
2	4	0	1133	1160	175
3	4	0	698	714	138
5	4	0	145	99	24
6	4	0	516	495	64
7	4	0	642	677	111
8	4	0	172	96	-51
9	4	0	525	486	49
10	4	0	97	108	-78
11	4	0	448	461	28
1	5	0	2614	2479	132
2	5	0	158	199	30
3	5	0	1764	1760	308
4	5	0	205	272	26
5	5	0	782	774	147
6	5	0	714	701	95
7	5	0	499	453	47
8	5	0	642	638	50
9	5	0	86	30	-72
10	5	0	678	603	25
11	5	0	353	336	61
0	6	0	3072	2842	11
1	6	0	247	162	17
2	6	0	1948	1945	189
3	6	0	1000	983	151
4	6	0	1556	1615	299
5	6	0	425	431	87
6	6	0	792	775	151
7	6	0	1051	970	133
8	6	0	140	129	-60
9	6	0	627	571	24
10	6	0	157	59	-64
11	6	0	569	535	27
1	7	0	2210	2082	84
2	7	0	843	838	94
3	7	0	1861	1860	251
4	7	0	1069	1087	178
5	7	0	872	891	145
6	7	0	978	1005	183
7	7	0	833	746	106
8	7	0	850	746	76
9	7	0	194	176	39
10	7	0	460	427	29
0	8	0	1871	1814	14
1	8	0	147	118	23
2	8	0	1321	1242	91
3	8	0	1413	1411	166
4	8	0	1194	1191	172
5	8	0	783	791	132
6	8	0	876	880	130

H	K	L	$10F_o$	$10F_c$	10σ
7	8	0	1120	1062	150
8	8	0	164	156	-51
9	8	0	639	558	23
10	8	0	252	191	37
1	9	0	863	817	24
2	9	0	596	595	48
3	9	0	1049	1046	98
4	9	0	625	556	101
5	9	0	515	489	89
6	9	0	933	943	159
7	9	0	465	473	49
8	9	0	1011	924	63
9	9	0	175	114	-46
10	9	0	740	648	24
0	10	0	578	498	17
1	10	0	311	346	14
2	10	0	604	635	47
3	10	0	591	607	35
4	10	0	396	387	67
5	10	0	680	633	92
6	10	0	484	477	78
7	10	0	1020	1015	143
8	10	0	154	129	-48
9	10	0	954	831	91
1	11	0	614	587	13
2	11	0	448	448	39
3	11	0	646	651	60
4	11	0	712	695	103
5	11	0	93	77	-52
6	11	0	949	898	179
7	11	0	178	143	-39
8	11	0	1112	996	78
9	11	0	181	144	-61
0	12	0	849	865	19
1	12	0	42	48	-73
2	12	0	800	775	58
3	12	0	1016	979	85
4	12	0	204	186	37
5	12	0	944	943	121
6	12	0	312	315	62
7	12	0	1121	1042	154
8	12	0	296	286	39
9	12	0	839	772	105
1	13	0	679	646	32
2	13	0	684	669	53
3	13	0	633	648	39
4	13	0	977	977	101
5	13	0	210	170	38
6	13	0	1008	1035	141
7	13	0	304	247	-85
8	13	0	989	905	95
0	14	0	233	258	37
1	14	0	306	275	35
2	14	0	372	385	26
3	14	0	776	762	40
4	14	0	210	207	-43
5	14	0	853	889	115
6	14	0	608	587	109
7	14	0	1004	949	110
1	15	0	155	162	-40
2	15	0	386	395	20
3	15	0	364	314	20
4	15	0	669	666	80
5	15	0	87	58	-53
6	15	0	865	871	118
7	15	0	375	371	-81
0	16	0	216	187	33
1	16	0	149	132	-35
2	16	0	73	72	-77
3	16	0	479	446	20
4	16	0	266	234	35
5	16	0	680	688	93
6	16	0	175	164	-46
1	17	0	207	213	31
2	17	0	253	298	27
3	17	0	165	98	-57
4	17	0	495	484	23
5	17	0	416	416	36
0	18	0	137	214	-72
1	18	0	164	201	-47
2	18	0	167	201	-69
3	18	0	423	442	53
-11	0	1	1231	1112	28
-9	0	1	656	658	27
-7	0	1	1492	1472	22
-5	0	1	1070	1078	20
-3	0	1	581	466	19
-1	0	1	461	331	13
1	0	1	1078	883	14
3	0	1	2366	2345	18
5	0	1	1649	1868	20
7	0	1	1763	2122	23
9	0	1	768	908	26
11	0	1	803	907	30
-11	1	1	154	92	-57
-10	1	1	827	809	28

Table 70. (continued)

H	K	L	$10F_o$	$10F_c$	10σ
-9	1	1	175	206	-66
-8	1	1	1633	1582	23
-7	1	1	421	437	32
-6	1	1	838	802	22
-5	1	1	106	68	-75
-4	1	1	1410	1229	18
-3	1	1	189	217	24
-2	1	1	329	310	18
-1	1	1	816	716	9
0	1	1	725	629	7
1	1	1	428	519	10
2	1	1	1305	1948	-14
3	1	1	79	85	-44
4	1	1	1739	2010	19
5	1	1	322	336	28
6	1	1	1511	1712	22
7	1	1	227	348	-54
8	1	1	1208	1366	25
9	1	1	109	209	-79
10	1	1	928	1038	27
11	1	1	111	118	-96
-11	2	1	1308	1238	27
-10	2	1	114	190	-82
-9	2	1	987	989	25
-8	2	1	97	154	-88
-7	2	1	1679	1591	23
-6	2	1	368	314	27
-5	2	1	1293	1202	19
-4	2	1	317	269	21
-3	2	1	884	805	14
-2	2	1	175	144	20
-1	2	1	699	661	9
1	2	1	608	627	9
2	2	1	155	224	22
3	2	1	1343	1902	-15
4	2	1	42	101	-103
5	2	1	889	1054	21
6	2	1	250	309	28
7	2	1	1536	1746	23
8	2	1	262	237	45
9	2	1	684	757	28
10	2	1	223	264	-51
11	2	1	846	881	29
-11	3	1	165	113	-93
-10	3	1	1136	1100	26
-9	3	1	115	153	-72
-8	3	1	1826	1755	24
-7	3	1	276	236	35
-6	3	1	842	802	22
-5	3	1	524	496	20
-4	3	1	1600	1532	16
-3	3	1	337	306	15
-2	3	1	259	232	14
-1	3	1	564	470	10
0	3	1	623	631	9
1	3	1	388	409	11
2	3	1	336	377	14
3	3	1	427	510	16
4	3	1	1064	1337	17
5	3	1	119	155	-47
6	3	1	948	1089	23
7	3	1	200	169	39
8	3	1	1025	1053	25
9	3	1	49	107	-122
10	3	1	989	985	29
11	3	1	179	181	-69
-11	4	1	1230	1217	28
-10	4	1	117	30	-90
-9	4	1	1057	1004	26
-8	4	1	759	702	26
-7	4	1	1654	1537	23
-6	4	1	563	502	24
-5	4	1	977	855	18
-4	4	1	1446	1356	15
-3	4	1	490	448	14
-2	4	1	877	891	12
-1	4	1	440	488	11
0	4	1	755	637	11
1	4	1	723	848	11
2	4	1	388	484	14
3	4	1	768	890	14
4	4	1	762	899	17
5	4	1	709	811	20
6	4	1	236	303	32
7	4	1	1491	1573	23
8	4	1	315	339	35
9	4	1	702	715	30
10	4	1	65	108	-160
11	4	1	836	782	31
-11	5	1	216	26	-47
-10	5	1	780	752	30
-9	5	1	440	435	33
-8	5	1	1386	1279	24
-7	5	1	681	618	26
-6	5	1	937	823	20
-5	5	1	1518	1393	17

H	K	L	$10F_o$	$10F_c$	10σ
-4	5	1	1410	1269	15
-3	5	1	1071	885	14
-2	5	1	266	235	17
-1	5	1	2345	2194	11
0	5	1	600	550	12
1	5	1	888	880	12
2	5	1	546	569	13
3	5	1	760	866	15
4	5	1	1501	1811	16
5	5	1	563	632	21
6	5	1	1172	1312	22
7	5	1	382	344	30
8	5	1	1053	995	27
9	5	1	171	135	-62
10	5	1	901	851	30
-11	6	1	712	706	32
-10	6	1	62	14	-155
-9	6	1	696	601	28
-8	6	1	662	584	27
-7	6	1	1139	1004	23
-6	6	1	517	472	24
-5	6	1	1229	1115	18
-4	6	1	1769	1591	16
-3	6	1	499	419	15
-2	6	1	1440	1392	13
-1	6	1	405	415	14
0	6	1	1968	1806	12
1	6	1	1160	1161	13
2	6	1	973	1069	14
3	6	1	1788	2076	15
4	6	1	922	1137	17
5	6	1	1039	1178	19
6	6	1	46	66	-113
7	6	1	1560	1565	23
8	6	1	329	250	33
9	6	1	789	648	30
10	6	1	219	261	-62
-11	7	1	58	124	-144
-10	7	1	526	522	37
-9	7	1	264	258	50
-8	7	1	1049	947	26
-7	7	1	253	222	35
-6	7	1	674	569	22
-5	7	1	1120	985	19
-4	7	1	878	827	17
-3	7	1	1020	955	15
-2	7	1	128	56	25
-1	7	1	1920	1678	13
0	7	1	937	869	14
1	7	1	1454	1529	14
2	7	1	813	861	15
3	7	1	984	1110	16
4	7	1	1489	1703	17
5	7	1	384	423	22
6	7	1	1085	1185	21
7	7	1	135	40	-46
8	7	1	984	924	27
9	7	1	319	252	59
10	7	1	855	774	32
-10	8	1	224	181	-54
-9	8	1	818	706	29
-8	8	1	390	342	33
-7	8	1	742	674	24
-6	8	1	407	328	29
-5	8	1	700	620	19
-4	8	1	1209	1141	17
-3	8	1	337	344	20
-2	8	1	1075	952	15
-1	8	1	65	76	-69
0	8	1	1787	1720	14
1	8	1	756	771	15
2	8	1	999	1018	15
3	8	1	746	796	18
4	8	1	727	821	18
5	8	1	602	681	20
6	8	1	151	92	-42
7	8	1	1047	1118	25
8	8	1	88	3	-97
9	8	1	783	674	31
10	8	1	614	498	37
-10	9	1	771	690	33
-9	9	1	366	277	49
-8	9	1	1016	901	26
-7	9	1	262	242	35
-6	9	1	473	431	24
-5	9	1	1191	1053	20
-4	9	1	337	261	22
-3	9	1	1192	1142	17
-2	9	1	80	100	-60
-1	9	1	1496	1417	15
0	9	1	695	700	16
1	9	1	1156	1118	15
2	9	1	197	195	23
3	9	1	795	854	17
4	9	1	538	673	19
5	9	1	350	399	30

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
6	9	1	589	577	24	-4	12	1	1466	1350	20
7	9	1	53	29	-132	-3	12	1	106	48	-46
8	9	1	588	605	30	-2	12	1	1737	1650	18
9	9	1	167	182	-95	-1	12	1	581	565	20
-10	10	1	180	59	-92	0	12	1	1758	1732	18
-9	10	1	738	621	31	1	12	1	543	542	20
-8	10	1	675	586	28	2	12	1	1307	1346	19
-7	10	1	637	555	25	3	12	1	339	375	25
-6	10	1	1013	890	22	4	12	1	1005	1141	21
-5	10	1	905	854	20	5	12	1	481	562	27
-4	10	1	1445	1325	18	6	12	1	351	325	31
-3	10	1	48	39	-119	7	12	1	440	456	32
-2	10	1	1347	1255	16	8	12	1	216	255	-70
-1	10	1	448	392	18	-8	13	1	154	170	-78
0	10	1	1663	1622	16	-7	13	1	477	410	29
1	10	1	420	437	20	-6	13	1	126	98	-50
2	10	1	667	668	18	-5	13	1	1197	1122	22
3	10	1	365	360	22	-4	13	1	45	28	-112
4	10	1	905	964	20	-3	13	1	1453	1410	20
5	10	1	324	408	30	-1	13	1	1773	1761	19
6	10	1	175	180	-40	0	13	1	328	350	25
7	10	1	533	575	29	1	13	1	1752	1792	19
8	10	1	224	300	-60	2	13	1	123	78	-47
9	10	1	418	362	37	3	13	1	1029	1070	21
-9	11	1	659	534	33	4	13	1	526	548	24
-8	11	1	630	557	29	5	13	1	549	664	27
-7	11	1	790	678	26	6	13	1	296	313	37
-6	11	1	538	482	25	7	13	1	84	61	-95
-5	11	1	1519	1391	20	8	13	1	276	282	45
-4	11	1	739	678	20	-8	14	1	279	294	55
-3	11	1	1641	1527	18	-7	14	1	180	75	-47
-2	11	1	473	475	22	-6	14	1	726	641	27
-1	11	1	1530	1444	17	-5	14	1	211	177	40
0	11	1	268	261	24	-4	14	1	1135	1038	22
1	11	1	1263	1251	17	-3	14	1	581	534	23
2	11	1	104	120	-46	-2	14	1	1526	1517	20
3	11	1	1068	1114	19	-1	14	1	52	68	-128
4	11	1	768	838	21	0	14	1	1545	1509	20
5	11	1	712	797	23	1	14	1	389	449	26
6	11	1	342	391	30	2	14	1	1119	1213	21
7	11	1	267	325	42	3	14	1	42	32	-105
8	11	1	334	316	49	4	14	1	739	801	24
9	11	1	62	32	-155	5	14	1	256	246	34
-9	12	1	218	225	-73	6	14	1	54	80	-133
-8	12	1	714	640	29	7	14	1	205	162	-46
-7	12	1	300	230	38	-7	15	1	493	441	36
-6	12	1	1096	956	23	-6	15	1	58	62	-144
-5	12	1	647	644	25	-5	15	1	980	922	25

H	K	L	10F_o	10F_c	10σ	H	K	L	10F_o	10F_c	10σ
-4	15	1	151	155	-78	4	0	2	717	710	22
-3	15	1	971	1034	24	6	0	2	44	62	-109
-1	15	1	1069	1085	22	8	0	2	266	313	36
0	15	1	333	311	25	10	0	2	619	724	34
1	15	1	1147	1153	22	-12	1	2	125	169	-127
2	15	1	84	120	-79	-11	1	2	232	210	-64
3	15	1	604	624	25	-10	1	2	47	64	-118
4	15	1	96	82	-80	-9	1	2	736	675	26
5	15	1	462	508	35	-8	1	2	115	185	-77
6	15	1	50	56	-123	-7	1	2	1067	1054	23
-6	16	1	834	793	28	-6	1	2	247	249	33
-5	16	1	223	172	41	-5	1	2	2337	2153	20
-4	16	1	906	863	26	-4	1	2	593	489	20
-3	16	1	187	261	-57	-3	1	2	2474	2319	15
-2	16	1	1101	1101	23	-2	1	2	840	768	13
-1	16	1	177	245	-64	0	1	2	731	674	9
0	16	1	671	735	24	1	1	2	1101	1421	-11
1	16	1	49	120	-122	2	1	2	280	382	20
2	16	1	793	794	24	3	1	2	1647	2101	-18
3	16	1	295	286	39	4	1	2	167	179	-43
4	16	1	602	620	30	5	1	2	301	369	30
5	16	1	84	10	-98	6	1	2	148	218	-61
6	16	1	287	298	41	7	1	2	251	274	41
-5	17	1	864	863	27	8	1	2	84	42	-72
-4	17	1	87	67	-104	9	1	2	220	295	-48
-3	17	1	1014	1042	25	10	1	2	85	61	-75
-2	17	1	306	256	40	11	1	2	618	627	31
-1	17	1	941	960	24	-11	2	2	276	257	43
0	17	1	122	73	-77	-10	2	2	372	376	44
1	17	1	951	1008	25	-9	2	2	208	205	43
2	17	1	251	268	34	-8	2	2	1312	1300	24
3	17	1	591	618	27	-7	2	2	477	480	29
4	17	1	53	43	-132	-6	2	2	1418	1315	21
-3	18	1	52	56	-129	-5	2	2	619	587	21
-2	18	1	1295	1311	25	-4	2	2	2913	2716	16
-1	18	1	371	395	36	-3	2	2	801	690	14
0	18	1	1012	1047	25	-2	2	2	1800	1666	11
1	18	1	117	39	-67	-1	2	2	742	651	10
2	18	1	914	1039	27	1	2	2	424	490	12
3	18	1	180	229	-57	2	2	2	1291	1715	-13
-12	0	2	187	57	-57	3	2	2	277	361	20
-10	0	2	414	374	31	4	2	2	531	623	20
-8	0	2	948	930	24	5	2	2	137	262	-65
-6	0	2	1119	1216	22	6	2	2	415	452	31
-4	0	2	2991	2770	19	7	2	2	213	202	39
-2	0	2	2849	2371	16	8	2	2	124	126	-77
0	0	2	3196	3890	9	9	2	2	150	38	-61
2	0	2	2308	2096	18	10	2	2	548	605	32

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
-11	3	2	64	97	-159	-6	5	2	184	193	-40
-10	3	2	208	303	-80	-5	5	2	1673	1595	17
-9	3	2	628	593	29	-4	5	2	82	29	-53
-8	3	2	607	560	27	-3	5	2	1724	1532	14
-7	3	2	1521	1435	23	-2	5	2	1362	1184	13
-6	3	2	311	291	27	0	5	2	772	821	12
-5	3	2	2382	2160	18	1	5	2	1401	1400	12
-4	3	2	872	863	16	2	5	2	867	869	14
-3	3	2	1742	1581	13	3	5	2	1198	1365	15
-2	3	2	576	558	12	4	5	2	649	767	18
-1	3	2	2829	3075	11	5	5	2	256	280	30
0	3	2	58	117	-30	6	5	2	823	894	23
1	3	2	727	782	11	7	5	2	187	216	-64
2	3	2	593	715	13	8	5	2	794	697	28
3	3	2	1000	1200	15	9	5	2	292	274	-63
4	3	2	274	321	25	10	5	2	627	527	34
5	3	2	427	519	24	-11	6	2	483	493	46
6	3	2	379	357	28	-10	6	2	456	443	47
7	3	2	75	19	-88	-9	6	2	398	379	39
8	3	2	192	238	-60	-8	6	2	800	745	27
9	3	2	56	132	-139	-7	6	2	689	637	24
10	3	2	62	126	-153	-6	6	2	738	662	21
-11	4	2	394	451	45	-5	6	2	215	211	27
-10	4	2	338	319	41	-4	6	2	2181	2057	16
-9	4	2	534	445	31	-3	6	2	148	119	27
-8	4	2	1003	939	26	-2	6	2	1582	1503	13
-7	4	2	580	553	27	-1	6	2	660	581	15
-6	4	2	1254	1130	20	1	6	2	933	1017	13
-5	4	2	288	253	24	2	6	2	1675	1820	14
-4	4	2	2726	2529	15	3	6	2	1038	1126	16
-3	4	2	285	229	16	4	6	2	610	690	19
-2	4	2	2063	2025	12	5	6	2	897	983	20
-1	4	2	777	649	12	6	6	2	196	211	-42
1	4	2	982	1059	11	7	6	2	1066	1016	25
2	4	2	1124	1238	13	8	6	2	413	381	38
3	4	2	584	750	16	9	6	2	541	496	33
4	4	2	474	582	21	10	6	2	571	505	36
5	4	2	338	372	26	-11	7	2	275	281	-60
6	4	2	167	151	-47	-10	7	2	449	420	38
7	4	2	629	630	27	-9	7	2	378	333	39
8	4	2	157	130	-53	-8	7	2	796	735	26
9	4	2	367	342	41	-7	7	2	1194	1082	22
10	4	2	537	481	33	-6	7	2	554	515	23
-11	5	2	143	214	-94	-5	7	2	1228	1112	18
-10	5	2	340	392	46	-4	7	2	1038	992	17
-9	5	2	381	327	34	-3	7	2	1625	1559	15
-8	5	2	609	581	29	-2	7	2	415	450	16
-7	5	2	1142	1025	24	0	7	2	115	83	-30

Table 70. (continued)

H	K	L	$10F_o$	$10F_c$	10σ
1	7	2	1322	1381	14
2	7	2	1299	1354	15
3	7	2	1094	1173	17
4	7	2	1028	1138	18
5	7	2	269	297	35
6	7	2	907	1036	23
7	7	2	53	102	-132
8	7	2	720	660	30
10	7	2	400	338	45
-10	8	2	392	362	40
-9	8	2	793	678	29
-8	8	2	703	650	27
-7	8	2	1053	955	23
-6	8	2	1113	970	21
-5	8	2	789	755	20
-4	8	2	1735	1646	17
-3	8	2	798	754	16
-2	8	2	1314	1264	15
-1	8	2	282	279	24
1	8	2	392	346	17
2	8	2	697	703	16
3	8	2	1131	1251	17
4	8	2	329	327	28
5	8	2	794	866	21
6	8	2	275	307	41
7	8	2	904	887	26
8	8	2	201	165	-61
9	8	2	387	320	51
-10	9	2	851	780	30
-9	9	2	193	152	-61
-8	9	2	1253	1071	25
-7	9	2	1181	1074	23
-6	9	2	668	627	23
-5	9	2	995	945	20
-4	9	2	668	596	19
-3	9	2	1313	1203	17
-2	9	2	132	72	-34
-1	9	2	1223	1246	16
0	9	2	145	118	-39
1	9	2	460	437	18
2	9	2	936	963	17
3	9	2	491	520	20
4	9	2	614	649	20
5	9	2	121	193	-54
6	9	2	851	899	24
7	9	2	52	11	-128
8	9	2	702	648	30
9	9	2	62	60	-154

H	K	L	$10F_o$	$10F_c$	10σ
-10	10	2	256	259	-55
-9	10	2	970	888	29
-8	10	2	482	415	36
-7	10	2	1006	903	24
-6	10	2	650	602	23
-5	10	2	307	254	37
-4	10	2	1031	1003	19
-3	10	2	99	166	-74
-2	10	2	749	692	18
-1	10	2	883	848	17
0	10	2	794	748	17
1	10	2	464	469	22
2	10	2	611	665	18
3	10	2	850	908	19
4	10	2	108	121	-60
5	10	2	771	817	23
6	10	2	355	375	30
7	10	2	870	901	27
8	10	2	202	214	-62
9	10	2	725	583	36
-9	11	2	62	70	-153
-8	11	2	1029	879	27
-7	11	2	626	582	29
-6	11	2	487	455	26
-5	11	2	267	228	31
-4	11	2	179	128	-43
-3	11	2	771	729	20
-2	11	2	579	554	21
-1	11	2	832	770	19
0	11	2	760	740	19
1	11	2	721	673	18
2	11	2	1321	1389	19
3	11	2	522	566	23
4	11	2	838	920	22
5	11	2	171	245	-54
6	11	2	1057	1063	25
7	11	2	156	194	-56
8	11	2	934	854	31
-9	12	2	697	637	33
-8	12	2	117	95	-108
-7	12	2	724	685	26
-6	12	2	188	172	-44
-5	12	2	331	280	28
-4	12	2	581	547	22
-3	12	2	159	103	32
-2	12	2	641	596	20
-1	12	2	910	884	20
0	12	2	639	663	20

H	K	L	10F_O	10F_C	10σ	H	K	L	10F_O	10F_C	10σ
1	12	2	930	973	19	1	15	2	132	137	-51
2	12	2	840	840	20	2	15	2	702	753	24
3	12	2	1447	1445	20	3	15	2	92	41	-74
4	12	2	46	51	-113	4	15	2	693	793	26
5	12	2	1133	1243	23	5	15	2	150	185	-72
6	12	2	52	204	-130	6	15	2	753	785	30
7	12	2	1133	1121	27	-6	16	2	169	14	-63
8	12	2	316	325	49	-5	16	2	436	430	35
-8	13	2	640	591	31	-4	16	2	129	56	-68
-7	13	2	466	439	33	-3	16	2	188	126	-42
-6	13	2	617	536	27	-2	16	2	56	32	-138
-5	13	2	140	134	-77	-1	16	2	347	366	29
-4	13	2	395	369	28	0	16	2	205	181	-43
-3	13	2	568	573	22	1	16	2	588	596	25
-2	13	2	239	212	31	2	16	2	106	116	-66
-1	13	2	550	527	22	3	16	2	615	645	27
0	13	2	500	503	23	4	16	2	63	279	-155
1	13	2	303	348	26	5	16	2	625	700	31
2	13	2	1239	1299	20	-5	17	2	340	339	41
3	13	2	229	269	-51	-4	17	2	108	128	-103
4	13	2	1203	1287	22	-3	17	2	154	99	-70
5	13	2	185	128	-41	-2	17	2	188	191	-51
6	13	2	1191	1270	25	-1	17	2	50	62	-124
7	13	2	144	165	-64	0	17	2	511	501	29
-8	14	2	245	204	-56	1	17	2	49	47	-122
-7	14	2	857	744	29	2	17	2	664	699	27
-6	14	2	366	327	32	3	17	2	53	57	-131
-5	14	2	427	403	29	4	17	2	636	710	33
-4	14	2	304	343	36	-3	18	2	150	21	-56
-3	14	2	361	365	30	-2	18	2	205	179	-45
-2	14	2	147	208	-51	-1	18	2	289	304	34
-1	14	2	286	296	29	0	18	2	141	219	-97
0	14	2	129	38	-41	1	18	2	648	698	29
1	14	2	626	631	22	2	18	2	104	149	-72
2	14	2	184	302	-56	-11	0	3	840	789	31
3	14	2	999	1052	22	-9	0	3	773	763	27
4	14	2	227	220	35	-7	0	3	56	131	-138
5	14	2	1044	1129	25	-5	0	3	644	677	23
6	14	2	292	363	41	-3	0	3	640	561	22
7	14	2	959	919	28	-1	0	3	2196	1956	17
-7	15	2	485	430	34	1	0	3	1160	1064	19
-6	15	2	838	762	27	3	0	3	2746	2860	20
-5	15	2	52	28	-129	5	0	3	1694	1894	22
-4	15	2	408	393	28	7	0	3	1530	1780	24
-3	15	2	234	212	36	9	0	3	759	817	28
-2	15	2	114	100	-64	-12	1	3	1068	1087	31
-1	15	2	148	118	-50	-11	1	3	112	76	-107
0	15	2	275	342	39	-10	1	3	460	454	30

Table 70. (continued)

H	K	L	$10F_o$	$10F_c$	10σ
-9	1	3	165	110	-42
-8	1	3	1198	1218	24
-7	1	3	84	47	-76
-6	1	3	140	150	-80
-5	1	3	228	172	35
-4	1	3	48	185	-119
-3	1	3	576	572	19
-2	1	3	572	461	17
-1	1	3	794	777	13
1	1	3	351	347	16
2	1	3	1520	2255	-16
3	1	3	376	520	24
4	1	3	1551	1834	21
5	1	3	43	65	-106
6	1	3	1653	1971	23
7	1	3	90	23	-76
8	1	3	773	826	27
9	1	3	151	98	-58
10	1	3	715	797	30
-12	2	3	182	156	-73
-11	2	3	963	1048	30
-10	2	3	214	225	-71
-9	2	3	1301	1311	25
-8	2	3	167	171	-52
-7	2	3	741	669	27
-6	2	3	246	283	38
-5	2	3	950	929	21
-4	2	3	336	302	23
-3	2	3	969	912	15
-2	2	3	1152	1089	13
-1	2	3	1722	1525	11
0	2	3	843	733	11
1	2	3	1317	1462	12
2	2	3	427	528	-17
3	2	3	1688	2263	-17
4	2	3	440	542	26
5	2	3	804	947	23
6	2	3	123	127	-61
7	2	3	1168	1299	26
8	2	3	123	58	-58
9	2	3	620	620	29
10	2	3	134	182	-79
-11	3	3	91	27	-113
-10	3	3	919	931	29
-9	3	3	531	529	31
-8	3	3	1710	1611	24
-7	3	3	314	301	38
-6	3	3	667	664	23
-5	3	3	851	814	20
-4	3	3	77	2	-84
-3	3	3	531	497	15
-1	3	3	557	433	12
0	3	3	1501	1400	11
1	3	3	810	905	12
2	3	3	1293	1622	14
3	3	3	242	323	26
4	3	3	856	978	20
5	3	3	43	61	-106
6	3	3	1157	1292	23
7	3	3	47	58	-117
8	3	3	513	504	36
9	3	3	239	239	-53
10	3	3	696	691	34
-11	4	3	961	1030	31
-10	4	3	236	236	-52
-9	4	3	1300	1231	25
-8	4	3	517	509	31
-7	4	3	844	777	24
-6	4	3	983	886	21
-5	4	3	549	467	21
-4	4	3	935	884	17
-3	4	3	242	187	19
-2	4	3	807	753	14
-1	4	3	879	756	12
0	4	3	453	409	13
1	4	3	859	970	13
2	4	3	113	100	-26
3	4	3	1470	1695	16
4	4	3	175	240	32
5	4	3	833	923	23
6	4	3	171	218	-52
7	4	3	1116	1121	27
8	4	3	49	40	-123
9	4	3	706	628	34
10	4	3	270	268	53
-11	5	3	64	133	-159
-10	5	3	600	550	35
-9	5	3	493	503	36
-8	5	3	933	888	25
-7	5	3	607	587	26
-6	5	3	432	419	26
-5	5	3	1481	1405	18
-4	5	3	190	219	24
-3	5	3	710	591	15
-2	5	3	332	356	19
-1	5	3	1098	1101	13

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
0	5	3	1203	1213	12	5	7	3	42	33	-104
1	5	3	181	186	21	6	7	3	1385	1433	23
2	5	3	1266	1357	14	7	7	3	215	152	43
3	5	3	74	92	-42	8	7	3	673	602	31
4	5	3	1310	1464	18	9	7	3	695	588	32
5	5	3	232	299	34	-10	8	3	539	511	35
6	5	3	1583	1580	23	-9	8	3	775	712	28
7	5	3	144	30	-50	-8	8	3	710	696	29
8	5	3	672	634	31	-7	8	3	260	247	34
9	5	3	280	310	-67	-6	8	3	1039	986	21
10	5	3	705	589	32	-5	8	3	107	75	-53
-11	6	3	597	554	34	-4	8	3	1323	1242	17
-10	6	3	387	319	38	-3	8	3	594	577	17
-9	6	3	693	632	29	-2	8	3	1395	1346	16
-8	6	3	521	457	29	-1	8	3	1077	998	15
-7	6	3	204	226	-46	1	8	3	819	797	16
-6	6	3	990	886	20	2	8	3	856	855	17
-5	6	3	511	478	21	3	8	3	1280	1355	18
-4	6	3	1148	1054	16	4	8	3	645	707	21
-3	6	3	330	351	18	5	8	3	724	831	23
-2	6	3	1234	1227	14	6	8	3	218	251	-49
-1	6	3	1087	1050	14	7	8	3	707	728	28
0	6	3	858	811	14	8	8	3	216	222	-51
1	6	3	1209	1205	14	9	8	3	818	653	35
2	6	3	301	310	18	-10	9	3	575	617	40
3	6	3	1891	2153	3	-9	9	3	914	863	30
4	6	3	270	335	27	-8	9	3	748	686	28
5	6	3	1187	1274	20	-7	9	3	848	852	25
6	6	3	429	431	26	-6	9	3	482	436	26
7	6	3	1249	1192	26	-5	9	3	1732	1569	19
8	6	3	57	148	-142	-4	9	3	443	420	20
9	6	3	804	678	31	-3	9	3	1585	1559	17
10	6	3	615	467	37	-2	9	3	157	144	-42
-11	7	3	217	126	-62	0	9	3	988	1003	17
-10	7	3	396	389	39	1	9	3	807	762	17
-9	7	3	850	773	28	2	9	3	629	633	19
-8	7	3	525	511	28	3	9	3	753	783	19
-7	7	3	446	441	31	4	9	3	484	556	22
-6	7	3	286	234	34	5	9	3	84	98	-62
-5	7	3	1176	1096	19	6	9	3	686	693	25
-4	7	3	290	234	22	7	9	3	55	47	-136
-3	7	3	991	978	16	8	9	3	426	370	37
-2	7	3	664	613	15	9	9	3	395	396	46
0	7	3	1515	1502	14	-10	10	3	406	413	42
1	7	3	1061	1080	15	-9	10	3	760	695	30
2	7	3	1472	1486	16	-8	10	3	841	847	28
3	7	3	764	820	18	-7	10	3	455	434	28
4	7	3	1102	1277	19	-6	10	3	1657	1564	21

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
-5	10	3	490	478	23	7	12	3	339	336	39
-4	10	3	1562	1540	19	-8	13	3	170	78	-76
-3	10	3	172	119	32	-7	13	3	781	712	27
-2	10	3	1492	1371	18	-6	13	3	157	83	-63
-1	10	3	370	359	21	-5	13	3	1127	1078	23
0	10	3	1295	1279	17	-4	13	3	475	411	25
1	10	3	437	417	20	-3	13	3	1279	1229	21
2	10	3	270	266	29	-2	13	3	53	152	-131
3	10	3	665	681	20	-1	13	3	1376	1351	20
4	10	3	266	315	34	0	13	3	569	582	25
5	10	3	403	390	33	1	13	3	886	917	21
6	10	3	104	189	-81	2	13	3	146	192	-65
7	10	3	379	316	33	3	13	3	606	637	24
8	10	3	89	87	-94	4	13	3	563	578	26
-9	11	3	866	797	30	5	13	3	92	97	-67
-8	11	3	336	321	50	6	13	3	338	390	41
-7	11	3	951	910	24	7	13	3	339	276	52
-6	11	3	594	569	26	-8	14	3	758	686	31
-5	11	3	1619	1522	21	-7	14	3	230	161	46
-4	11	3	44	32	-109	-6	14	3	1049	997	26
-3	11	3	1404	1343	19	-5	14	3	47	3	-118
-2	11	3	324	328	24	-4	14	3	1267	1243	23
-1	11	3	1200	1189	18	-3	14	3	488	468	24
0	11	3	464	465	20	-2	14	3	1374	1338	22
1	11	3	622	590	20	-1	14	3	438	407	25
2	11	3	402	400	22	0	14	3	1173	1198	21
3	11	3	453	501	25	1	14	3	338	327	28
4	11	3	552	535	23	2	14	3	727	699	23
5	11	3	47	141	-117	3	14	3	274	276	32
6	11	3	474	514	29	4	14	3	342	364	36
7	11	3	61	72	-152	5	14	3	171	202	-56
8	11	3	212	241	-57	6	14	3	234	223	47
-9	12	3	137	199	-92	-7	15	3	1006	992	29
-8	12	3	808	724	29	-6	15	3	152	146	-65
-7	12	3	59	64	-145	-5	15	3	1257	1222	25
-6	12	3	1149	1053	23	-4	15	3	555	486	26
-5	12	3	275	288	32	-3	15	3	1340	1336	22
-4	12	3	1259	1227	21	-2	15	3	60	36	-149
-3	12	3	45	69	-113	-1	15	3	1140	1129	23
-2	12	3	1100	1081	19	0	15	3	542	550	24
-1	12	3	48	90	-120	1	15	3	842	867	23
0	12	3	1271	1260	19	2	15	3	41	39	-103
1	12	3	246	266	32	3	15	3	462	483	28
2	12	3	552	539	23	4	15	3	51	50	-127
3	12	3	547	558	23	5	15	3	141	56	-72
4	12	3	306	332	33	-6	16	3	1179	1187	27
5	12	3	587	625	26	-5	16	3	184	207	-52
6	12	3	151	255	-93	-4	16	3	1274	1257	25

H	K	L	$10F_o$	$10F_c$	10σ
-3	16	3	54	114	-133
-2	16	3	1087	1146	24
-1	16	3	147	107	-57
0	16	3	869	884	24
1	16	3	142	96	-48
2	16	3	492	492	28
3	16	3	104	123	-77
4	16	3	312	299	36
5	16	3	150	84	-57
-5	17	3	1007	1038	28
-4	17	3	89	17	-82
-3	17	3	1127	1216	25
-2	17	3	648	607	27
-1	17	3	804	825	25
0	17	3	125	85	-57
1	17	3	743	741	27
2	17	3	397	421	37
3	17	3	240	264	43
-2	18	3	979	997	26
-1	18	3	348	387	34
0	18	3	689	781	28
1	18	3	249	298	51
-12	0	4	379	399	41
-10	0	4	650	666	30
-8	0	4	1214	1244	24
-6	0	4	1501	1543	23
-4	0	4	1506	1335	22
-2	0	4	2361	2111	20
0	0	4	951	1122	13
2	0	4	649	621	25
4	0	4	80	128	-89
6	0	4	719	814	25
8	0	4	515	600	32
10	0	4	905	990	30
-12	1	4	130	138	-81
-11	1	4	536	614	35
-10	1	4	106	55	-93
-9	1	4	1183	1195	27
-8	1	4	45	13	-111
-7	1	4	1061	1108	26
-6	1	4	166	193	-58
-5	1	4	2281	2108	21
-4	1	4	429	435	25
-2	1	4	692	609	17
0	1	4	136	59	21
1	1	4	503	595	16
2	1	4	116	80	-38
3	1	4	318	448	33
4	1	4	262	334	43
5	1	4	313	374	33
6	1	4	350	363	34
7	1	4	577	654	27
8	1	4	49	105	-121
9	1	4	785	870	29
10	1	4	89	17	-101
-12	2	4	407	380	41
-11	2	4	183	122	-60
-10	2	4	792	832	30
-9	2	4	55	128	-138
-8	2	4	1636	1612	25
-7	2	4	139	18	-49
-6	2	4	1924	1901	22
-5	2	4	269	186	29
-4	2	4	2390	2297	18
-3	2	4	289	297	20
-2	2	4	2182	1891	14
-1	2	4	94	72	-28
0	2	4	1455	1444	12
1	2	4	83	57	-37
2	2	4	677	848	17
3	2	4	403	521	23
4	2	4	39	13	-98
5	2	4	298	345	31
6	2	4	415	490	39
7	2	4	327	330	37
8	2	4	304	354	46
9	2	4	120	67	-76
10	2	4	775	747	31
-11	3	4	638	656	33
-10	3	4	251	267	45
-9	3	4	1285	1321	27
-8	3	4	285	356	41
-7	3	4	1674	1664	24
-6	3	4	152	92	-63
-5	3	4	3132	3010	19
-4	3	4	91	21	-60
-2	3	4	661	570	15
-1	3	4	2614	2335	12
0	3	4	625	597	14
1	3	4	800	891	14
2	3	4	580	701	16
3	3	4	300	322	22
4	3	4	170	174	-36
5	3	4	42	65	-105
6	3	4	461	474	33
7	3	4	326	303	49

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
8	3	4	116	72	-73	-6	6	4	777	705	22
9	3	4	457	478	38	-5	6	4	240	219	27
-11	4	4	347	324	41	-4	6	4	1200	1119	17
-10	4	4	765	757	32	-3	6	4	430	379	18
-9	4	4	538	516	31	-2	6	4	1500	1444	15
-8	4	4	1637	1637	25	-1	6	4	841	768	15
-7	4	4	320	289	31	0	6	4	831	757	15
-6	4	4	1970	1851	21	1	6	4	919	959	15
-5	4	4	132	130	-40	2	6	4	827	871	16
-4	4	4	2580	2491	16	3	6	4	1026	1136	18
-3	4	4	889	900	15	4	6	4	58	16	-61
-2	4	4	2571	2377	5	5	6	4	718	734	23
-1	4	4	981	804	13	6	6	4	478	497	30
0	4	4	1058	927	13	7	6	4	742	696	30
1	4	4	866	883	14	8	6	4	710	593	33
2	4	4	850	988	16	9	6	4	267	235	52
3	4	4	717	820	18	-11	7	4	458	495	40
4	4	4	43	11	-106	-10	7	4	287	317	-65
5	4	4	163	245	-60	-9	7	4	705	647	30
6	4	4	294	335	34	-8	7	4	423	409	34
7	4	4	305	357	39	-7	7	4	701	711	25
8	4	4	172	191	-87	-6	7	4	91	62	-70
9	4	4	136	145	-80	-5	7	4	1336	1310	19
-11	5	4	664	671	34	-4	7	4	246	193	32
-10	5	4	296	328	47	-3	7	4	606	576	17
-9	5	4	948	958	28	-2	7	4	821	796	16
-8	5	4	437	433	32	-1	7	4	1219	1156	15
-7	5	4	1234	1165	23	0	7	4	612	559	16
-6	5	4	193	153	35	1	7	4	587	581	17
-5	5	4	2045	1992	18	2	7	4	1304	1346	17
-4	5	4	247	201	31	3	7	4	33	40	-82
-3	5	4	1226	1135	15	4	7	4	784	819	21
-1	5	4	2125	2065	14	5	7	4	138	137	-42
0	5	4	823	759	14	6	7	4	1007	1009	25
1	5	4	851	848	15	7	7	4	732	687	30
2	5	4	1015	1048	16	8	7	4	499	359	34
3	5	4	299	353	22	9	7	4	662	546	37
4	5	4	558	615	23	-10	8	4	266	269	-57
5	5	4	43	72	-107	-9	8	4	473	511	38
6	5	4	636	667	27	-8	8	4	1078	1043	25
7	5	4	543	504	32	-7	8	4	217	240	44
8	5	4	318	224	43	-6	8	4	1057	989	21
9	5	4	613	594	36	-5	8	4	121	119	-51
-11	6	4	277	342	52	-4	8	4	1355	1260	18
-10	6	4	571	558	34	-3	8	4	280	249	21
-9	6	4	434	398	42	-2	8	4	1339	1304	16
-8	6	4	1144	1111	26	-1	8	4	703	692	17
-7	6	4	206	138	-49	0	8	4	234	189	23

Table 70. (continued)

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
1	8	4	1018	1031	17	-7	11	4	586	586	28
2	8	4	327	291	21	-6	11	4	49	53	-120
3	8	4	991	1067	19	-5	11	4	716	705	23
4	8	4	264	327	40	-4	11	4	306	268	31
5	8	4	848	919	24	-3	11	4	627	589	21
6	8	4	340	326	30	-2	11	4	1281	1278	19
7	8	4	806	759	28	-1	11	4	840	821	19
8	8	4	365	279	43	0	11	4	1034	1004	19
-10	9	4	483	541	39	1	11	4	825	824	20
-9	9	4	525	552	41	2	11	4	1483	1525	20
-8	9	4	810	731	28	3	11	4	143	160	-42
-7	9	4	1109	1017	23	4	11	4	902	889	23
-6	9	4	53	87	-132	5	11	4	345	409	38
-5	9	4	1629	1598	20	6	11	4	778	795	28
-4	9	4	112	53	-42	7	11	4	381	375	40
-3	9	4	1059	1038	18	-9	12	4	451	424	39
-2	9	4	923	872	18	-8	12	4	561	501	32
-1	9	4	929	888	17	-7	12	4	305	310	39
0	9	4	771	735	18	-6	12	4	110	160	-88
1	9	4	435	407	19	-5	12	4	140	111	-46
2	9	4	1305	1317	19	-4	12	4	431	408	26
3	9	4	159	185	-35	-3	12	4	680	663	22
4	9	4	820	849	21	-2	12	4	581	587	22
5	9	4	41	58	-103	-1	12	4	925	956	20
6	9	4	859	892	26	0	12	4	256	259	30
7	9	4	71	302	-175	1	12	4	1344	1356	20
8	9	4	524	399	35	2	12	4	597	583	23
-10	10	4	389	347	48	3	12	4	1121	1129	22
-9	10	4	680	654	35	4	12	4	41	20	-103
-8	10	4	1032	977	26	5	12	4	1035	1036	25
-7	10	4	474	421	33	6	12	4	90	80	-106
-6	10	4	853	809	23	7	12	4	832	765	31
-5	10	4	132	62	-42	-8	13	4	401	353	40
-4	10	4	1213	1179	20	-7	13	4	333	271	37
-3	10	4	755	709	20	-6	13	4	60	140	-148
-2	10	4	1134	1063	18	-5	13	4	93	152	-92
-1	10	4	1167	1151	18	-4	13	4	101	55	-55
0	10	4	496	500	19	-3	13	4	270	236	44
1	10	4	1157	1162	19	-2	13	4	780	771	22
2	10	4	679	713	20	-1	13	4	128	119	-46
3	10	4	1079	1096	21	0	13	4	724	746	22
4	10	4	47	21	-116	1	13	4	148	176	-44
5	10	4	785	843	24	2	13	4	1233	1271	22
6	10	4	55	49	-135	3	13	4	313	294	31
7	10	4	691	656	30	4	13	4	1148	1190	25
8	10	4	144	126	-88	5	13	4	150	138	-51
-9	11	4	459	417	38	6	13	4	970	965	29
-8	11	4	723	707	30	-8	14	4	269	231	46

Table 70. (continued)

H	K	L	10F$_o$	10F$_c$	10σ
-7	14	4	307	294	58
-6	14	4	58	85	-143
-5	14	4	107	124	-80
-4	14	4	180	152	-50
-3	14	4	257	290	34
-2	14	4	57	80	-142
-1	14	4	621	607	25
0	14	4	313	281	27
1	14	4	1111	1091	22
2	14	4	76	29	-74
3	14	4	970	1025	25
4	14	4	356	304	41
5	14	4	1116	1072	27
6	14	4	162	90	-53
-7	15	4	207	168	-49
-6	15	4	61	104	-152
-4	15	4	117	99	-69
-3	15	4	124	148	-62
-2	15	4	780	784	24
-1	15	4	265	230	34
0	15	4	810	864	24
1	15	4	95	63	-82
2	15	4	977	991	24
3	15	4	370	392	33
4	15	4	901	961	27
5	15	4	124	178	-83
-6	16	4	145	15	-67
-5	16	4	116	78	-77
-4	16	4	117	66	-64
-3	16	4	568	597	29
-2	16	4	54	87	-133
-1	16	4	758	815	27
0	16	4	86	62	-95
1	16	4	1089	1115	25
2	16	4	140	117	-61
3	16	4	753	800	28
4	16	4	51	28	-126
-4	17	4	229	257	46
-3	17	4	55	73	-136
-2	17	4	654	703	28
-1	17	4	86	58	-84
0	17	4	893	925	27
1	17	4	262	307	38
2	17	4	769	836	28
-2	18	4	65	73	-160
-1	18	4	490	548	31
0	18	4	53	46	-132
-11	0	5	409	411	34
-9	0	5	612	656	32
-7	0	5	331	390	36
-5	0	5	482	447	34
-3	0	5	501	413	27
-1	0	5	2048	1874	22
1	0	5	1221	1265	23
3	0	5	1697	1800	24
5	0	5	1346	1557	25
7	0	5	697	739	28
9	0	5	499	482	32
-12	1	5	836	893	35
-11	1	5	252	268	48
-10	1	5	524	543	32
-9	1	5	284	287	43
-8	1	5	285	268	40
-7	1	5	304	327	50
-6	1	5	171	144	-64
-5	1	5	241	225	41
-4	1	5	1034	995	22
-3	1	5	220	281	34
-2	1	5	1547	1345	17
-1	1	5	446	408	17
0	1	5	1213	1219	14
1	1	5	291	314	19
2	1	5	1757	2497	-20
3	1	5	326	436	33
4	1	5	829	934	26
5	1	5	50	56	-123
6	1	5	1253	1434	27
7	1	5	189	116	-45
8	1	5	399	394	33
9	1	5	141	101	-77
-11	2	5	505	537	38
-10	2	5	366	492	48
-9	2	5	904	924	28
-8	2	5	397	443	42
-7	2	5	46	23	-115
-6	2	5	494	489	27
-5	2	5	521	525	27
-4	2	5	349	290	24
-3	2	5	1408	1303	17
-2	2	5	619	625	17
0	2	5	804	726	14
1	2	5	1654	1852	15
2	2	5	309	354	22
3	2	5	1229	1532	21
4	2	5	326	324	33
5	2	5	1063	1246	26

H	K	L	$10F_o$	$10F_c$	10σ
6	2	5	49	68	-121
7	2	5	530	527	30
8	2	5	174	139	-58
9	2	5	504	475	36
-11	3	5	210	293	-64
-10	3	5	696	715	33
-9	3	5	492	473	32
-8	3	5	372	374	36
-7	3	5	462	475	33
-6	3	5	122	101	-61
-5	3	5	802	788	22
-3	3	5	379	340	21
-2	3	5	2446	2229	15
-1	3	5	812	727	15
0	3	5	1734	1635	14
1	3	5	152	228	-33
2	3	5	2008	2392	17
3	3	5	305	318	27
4	3	5	834	884	23
5	3	5	263	304	39
6	3	5	1121	1139	27
7	3	5	42	55	-103
8	3	5	410	338	36
9	3	5	253	277	-53
-11	4	5	361	404	44
-10	4	5	359	389	58
-9	4	5	724	755	31
-8	4	5	411	429	34
-7	4	5	136	99	-69
-6	4	5	708	694	25
-5	4	5	567	597	21
-4	4	5	927	928	19
-3	4	5	907	904	17
-2	4	5	532	484	17
-1	4	5	2196	2054	14
0	4	5	130	108	27
1	4	5	1570	1583	15
2	4	5	275	320	24
3	4	5	1451	1670	19
4	4	5	298	326	27
5	4	5	1203	1257	24
6	4	5	324	328	46
7	4	5	646	569	31
8	4	5	283	293	-65
9	4	5	537	465	39
-11	5	5	131	106	-110
-10	5	5	448	428	35
-9	5	5	374	391	37

H	K	L	$10F_o$	$10F_c$	10σ
-8	5	5	86	55	-102
-7	5	5	781	717	25
-6	5	5	194	148	35
-5	5	5	1019	975	20
-4	5	5	756	661	19
-3	5	5	530	561	18
-2	5	5	1263	1237	15
-1	5	5	488	426	17
0	5	5	1186	1111	15
1	5	5	636	624	16
2	5	5	1768	1853	17
3	5	5	156	124	31
4	5	5	997	1039	21
5	5	5	759	814	25
6	5	5	1265	1180	26
7	5	5	125	143	-95
8	5	5	583	458	34
9	5	5	580	434	36
-11	6	5	293	351	-68
-10	6	5	617	602	41
-9	6	5	497	481	36
-8	6	5	533	543	30
-7	6	5	159	133	-52
-6	6	5	878	785	22
-5	6	5	495	495	21
-4	6	5	899	874	18
-3	6	5	638	624	18
-2	6	5	552	538	17
-1	6	5	1166	1068	16
0	6	5	227	188	22
1	6	5	1175	1233	17
2	6	5	37	29	-91
3	6	5	1146	1217	19
4	6	5	360	348	25
5	6	5	1073	1099	24
6	6	5	362	372	35
7	6	5	641	560	35
8	6	5	500	469	42
-11	7	5	507	545	38
-10	7	5	447	446	45
-9	7	5	857	857	29
-8	7	5	113	124	-85
-7	7	5	790	795	24
-6	7	5	155	27	-47
-5	7	5	967	922	20
-4	7	5	674	687	20
-3	7	5	572	500	18
-2	7	5	791	746	17

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
-1	7	5	1218	1187	17	-9	10	5	360	344	41
0	7	5	1173	1143	17	-8	10	5	946	986	27
1	7	5	255	249	24	-7	10	5	105	21	-78
2	7	5	1210	1243	18	-6	10	5	1674	1628	22
3	7	5	475	505	21	-5	10	5	324	303	27
4	7	5	699	731	22	-4	10	5	1413	1400	20
5	7	5	379	459	30	-3	10	5	575	548	21
6	7	5	895	819	26	-2	10	5	1170	1109	19
7	7	5	412	267	45	-1	10	5	1086	1046	19
8	7	5	341	358	61	0	10	5	446	466	22
-10	8	5	1017	1003	32	1	10	5	812	753	19
-9	8	5	587	552	33	2	10	5	43	37	-106
-8	8	5	856	888	28	3	10	5	755	755	22
-7	8	5	117	57	-76	4	10	5	335	380	30
-6	8	5	1287	1244	22	5	10	5	625	576	26
-5	8	5	279	270	30	6	10	5	396	355	32
-4	8	5	1047	1024	19	7	10	5	185	250	-91
-3	8	5	716	682	19	-9	11	5	909	895	32
-2	8	5	1080	1002	18	-8	11	5	221	183	-46
-1	8	5	1226	1221	17	-7	11	5	912	984	26
0	8	5	1081	1026	17	-6	11	5	197	106	38
1	8	5	934	925	18	-5	11	5	1382	1325	22
2	8	5	472	456	23	-4	11	5	639	606	23
3	8	5	1069	1026	20	-3	11	5	1081	1053	21
4	8	5	45	79	-113	-2	11	5	270	262	28
5	8	5	663	724	26	-1	11	5	738	750	21
7	8	5	294	272	49	0	11	5	646	641	22
8	8	5	596	481	36	1	11	5	97	98	-63
-10	9	5	417	430	44	2	11	5	583	604	23
-9	9	5	1129	1094	29	3	11	5	46	57	-114
-8	9	5	101	186	-95	4	11	5	553	587	26
-7	9	5	1246	1223	24	5	11	5	612	642	29
-6	9	5	164	149	-48	6	11	5	448	407	35
-5	9	5	1620	1554	20	7	11	5	473	405	45
-4	9	5	665	658	21	-9	12	5	123	44	-86
-3	9	5	1291	1251	19	-8	12	5	779	751	31
-2	9	5	901	872	18	-7	12	5	110	167	-104
-1	9	5	1224	1181	18	-6	12	5	1100	1041	24
0	9	5	1205	1142	18	-5	12	5	305	295	32
1	9	5	154	137	-40	-4	12	5	906	875	23
2	9	5	953	999	20	-3	12	5	124	112	-49
3	9	5	323	370	29	-2	12	5	700	716	22
4	9	5	649	652	23	-1	12	5	412	403	28
5	9	5	425	479	30	0	12	5	467	485	24
6	9	5	397	426	35	1	12	5	241	251	31
7	9	5	218	176	-67	2	12	5	100	48	-56
8	9	5	412	309	52	3	12	5	413	483	28
-10	10	5	749	782	36	4	12	5	312	340	37

H	K	L	10F$_o$	10F$_c$	10σ	H	K	L	10F$_o$	10F$_c$	10σ
5	12	5	540	540	30	2	16	5	53	72	-131
6	12	5	546	532	33	3	16	5	60	10	-148
-8	13	5	163	164	-56	-4	17	5	56	110	-139
-7	13	5	912	904	27	-3	17	5	1038	1032	26
-6	13	5	191	185	-49	-2	17	5	339	365	39
-5	13	5	939	921	24	-1	17	5	474	526	30
-4	13	5	374	368	29	0	17	5	57	110	-141
-3	13	5	778	782	23	1	17	5	268	263	41
-2	13	5	135	118	-49	-10	0	6	1057	1127	30
-1	13	5	782	757	23	-8	0	6	1300	1361	27
0	13	5	281	303	30	-6	0	6	1799	1805	25
1	13	5	228	236	33	-4	0	6	703	647	29
2	13	5	243	226	34	-2	0	6	1225	1076	26
3	13	5	49	105	-121	0	0	6	76	64	-41
4	13	5	325	361	35	2	0	6	46	98	-113
5	13	5	359	445	35	4	0	6	552	595	27
6	13	5	119	128	-82	6	0	6	689	762	29
-7	14	5	62	131	-155	8	0	6	719	768	33
-6	14	5	1113	1139	26	-11	1	6	851	891	32
-5	14	5	57	113	-141	-10	1	6	260	214	-67
-4	14	5	967	1023	25	-9	1	6	1581	1647	27
-3	14	5	77	23	-90	-8	1	6	279	287	39
-2	14	5	870	880	24	-7	1	6	1070	1084	28
-1	14	5	439	470	27	-6	1	6	491	466	31
0	14	5	588	593	26	-5	1	6	1954	1824	25
1	14	5	113	79	-83	-4	1	6	130	68	-52
2	14	5	266	240	41	-3	1	6	901	898	22
3	14	5	61	124	-151	-2	1	6	137	128	-47
4	14	5	117	132	-97	-1	1	6	847	747	17
5	14	5	58	56	-144	0	1	6	37	33	-92
-6	15	5	353	333	39	1	1	6	98	45	-40
-5	15	5	1178	1224	26	2	1	6	266	410	39
-4	15	5	345	382	43	3	1	6	250	313	39
-3	15	5	1106	1136	24	4	1	6	262	337	45
-2	15	5	52	18	-130	5	1	6	649	814	30
-1	15	5	844	817	25	6	1	6	360	359	33
0	15	5	242	322	-53	7	1	6	533	603	38
1	15	5	391	397	35	8	1	6	164	157	-58
2	15	5	47	16	-117	-11	2	6	122	66	-98
3	15	5	193	46	-58	-10	2	6	1105	1102	28
4	15	5	83	28	-97	-9	2	6	192	257	-67
-5	16	5	57	72	-141	-8	2	6	1318	1373	28
-4	16	5	1161	1252	26	-7	2	6	393	387	32
-3	16	5	62	132	-155	-6	2	6	2070	2037	25
-2	16	5	886	931	26	-5	2	6	327	388	42
-1	16	5	239	206	39	-4	2	6	1298	1223	21
0	16	5	587	585	28	-3	2	6	622	610	20
1	16	5	121	151	-103	-2	2	6	1664	1650	18

Table 70. (continued)

H	K	L	$10F_O$	$10F_C$	10σ
-1	2	6	155	103	26
0	2	6	230	252	20
1	2	6	414	510	20
2	2	6	104	113	-41
3	2	6	411	482	26
4	2	6	503	615	29
5	2	6	378	480	35
6	2	6	785	862	30
7	2	6	248	287	-53
8	2	6	650	645	33
-11	3	6	652	775	37
-10	3	6	114	93	-110
-9	3	6	1577	1579	28
-8	3	6	55	56	-138
-7	3	6	1438	1426	26
-6	3	6	451	419	37
-5	3	6	2164	2204	22
-4	3	6	337	345	29
-3	3	6	1593	1491	17
-2	3	6	887	816	18
-1	3	6	1137	1057	17
0	3	6	616	625	17
1	3	6	36	29	-89
2	3	6	551	614	20
3	3	6	386	461	26
4	3	6	184	210	-48
5	3	6	719	801	29
6	3	6	349	375	47
7	3	6	584	496	34
8	3	6	144	49	-81
-11	4	6	161	272	-92
-10	4	6	1057	1057	30
-9	4	6	367	366	44
-8	4	6	1465	1464	27
-7	4	6	84	140	-103
-6	4	6	1900	1903	22
-5	4	6	148	133	-41
-4	4	6	1321	1362	20
-3	4	6	886	800	18
-2	4	6	1651	1544	16
-1	4	6	728	654	17
0	4	6	42	65	-105
1	4	6	904	902	17
2	4	6	151	55	31
3	4	6	270	307	28
4	4	6	474	489	25
5	4	6	211	277	-51
6	4	6	764	688	28
7	4	6	53	51	-131
8	4	6	562	504	38
-11	5	6	740	812	38
-10	5	6	397	338	56
-9	5	6	1316	1384	28
-8	5	6	354	367	37
-7	5	6	1120	1113	25
-6	5	6	168	156	-38
-5	5	6	1466	1472	21
-4	5	6	128	166	-57
-3	5	6	927	849	18
-2	5	6	1172	1107	16
-1	5	6	503	500	19
0	5	6	591	557	17
1	5	6	369	356	21
2	5	6	775	832	19
3	5	6	293	327	27
4	5	6	221	253	-46
5	5	6	520	536	28
6	5	6	272	263	42
7	5	6	619	489	38
8	5	6	115	124	-112
-11	6	6	130	264	-126
-10	6	6	919	928	35
-9	6	6	281	296	44
-8	6	6	914	963	29
-7	6	6	203	147	-47
-6	6	6	1228	1171	22
-5	6	6	218	197	34
-4	6	6	404	422	24
-3	6	6	706	694	20
-2	6	6	953	873	18
-1	6	6	527	505	19
0	6	6	258	273	23
1	6	6	967	974	18
2	6	6	108	46	-44
3	6	6	510	534	22
4	6	6	148	188	-46
5	6	6	491	523	32
6	6	6	793	750	29
7	6	6	240	184	-57
8	6	6	749	589	35
-10	7	6	66	86	-163
-9	7	6	968	1026	32
-8	7	6	57	29	-142
-7	7	6	712	707	26
-6	7	6	615	630	24
-5	7	6	1133	1075	20

H	K	L	$10F_o$	$10F_c$	10σ
-4	7	6	559	546	22
-3	7	6	614	610	20
-2	7	6	1097	1036	18
-1	7	6	223	206	24
0	7	6	611	617	19
1	7	6	373	358	22
2	7	6	1013	1044	19
3	7	6	437	451	25
4	7	6	589	575	25
5	7	6	574	504	27
6	7	6	678	701	31
7	7	6	570	526	37
-10	8	6	520	543	41
-9	8	6	108	42	-109
-8	8	6	971	911	27
-7	8	6	545	562	31
-6	8	6	1193	1204	23
-5	8	6	581	616	25
-4	8	6	758	727	20
-3	8	6	1285	1234	19
-2	8	6	966	912	18
-1	8	6	847	815	19
0	8	6	96	46	-44
1	8	6	1332	1312	19
2	8	6	414	409	26
3	8	6	855	839	23
4	8	6	260	291	33
5	8	6	835	861	26
6	8	6	680	628	31
7	8	6	590	469	35
-10	9	6	121	93	-86
-9	9	6	794	840	31
-8	9	6	65	60	-162
-7	9	6	882	869	26
-6	9	6	697	691	25
-5	9	6	1137	1127	22
-4	9	6	737	766	22
-3	9	6	1100	1101	20
-2	9	6	1424	1372	19
-1	9	6	105	86	-63
0	9	6	1254	1205	19
1	9	6	238	235	28
2	9	6	1391	1379	21
3	9	6	537	562	24
4	9	6	882	825	24
5	9	6	310	322	44
6	9	6	781	699	29
7	9	6	350	320	54
-9	10	6	296	325	50
-8	10	6	770	757	32
-7	10	6	312	283	37
-6	10	6	868	889	24
-5	10	6	207	291	-59
-4	10	6	652	667	23
-3	10	6	1309	1318	21
-2	10	6	767	726	21
-1	10	6	1292	1279	20
0	10	6	282	303	30
1	10	6	1433	1459	20
2	10	6	83	161	-95
3	10	6	1009	979	23
4	10	6	109	48	-66
5	10	6	623	642	29
6	10	6	483	454	38
-9	11	6	562	636	34
-8	11	6	375	351	43
-7	11	6	444	487	39
-6	11	6	373	361	34
-5	11	6	413	436	29
-4	11	6	660	653	23
-3	11	6	484	530	24
-2	11	6	1204	1216	21
-1	11	6	140	135	-37
0	11	6	1272	1215	21
1	11	6	500	507	25
2	11	6	1074	1102	22
3	11	6	182	174	-48
4	11	6	658	621	26
5	11	6	84	48	-81
6	11	6	521	472	33
-8	12	6	410	455	40
-7	12	6	264	212	46
-6	12	6	336	314	45
-5	12	6	228	307	44
-4	12	6	150	171	-50
-3	12	6	963	961	22
-2	12	6	77	124	-95
-1	12	6	863	869	22
0	12	6	203	201	36
1	12	6	1078	1043	23
2	12	6	50	13	-125
3	12	6	750	752	25
4	12	6	154	128	-49
5	12	6	613	570	31
-8	13	6	161	13	-61
-7	13	6	334	223	52

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
-6	13	6	420	470	33	5	0	7	847	986	31
-5	13	6	99	122	-80	7	0	7	161	180	-68
-4	13	6	594	593	29	-11	1	7	191	232	-102
-3	13	6	225	244	35	-10	1	7	283	291	52
-2	13	6	758	778	24	-9	1	7	252	288	-53
-1	13	6	237	243	34	-8	1	7	363	353	40
0	13	6	847	872	24	-7	1	7	91	53	-108
1	13	6	186	219	-45	-6	1	7	974	921	29
2	13	6	968	895	25	-5	1	7	131	62	-71
3	13	6	320	325	35	-4	1	7	1115	1082	26
4	13	6	809	808	28	-3	1	7	163	205	-61
5	13	6	111	39	-97	-2	1	7	1930	1851	21
-7	14	6	322	361	49	-1	1	7	315	297	25
-6	14	6	70	146	-174	0	1	7	1060	1036	17
-5	14	6	464	501	31	1	1	7	98	110	-46
-4	14	6	242	184	38	2	1	7	1054	1507	-25
-3	14	6	896	906	25	3	1	7	48	84	-119
-2	14	6	52	46	-129	4	1	7	696	785	32
-1	14	6	833	860	25	5	1	7	135	25	-65
0	14	6	53	20	-130	6	1	7	420	495	35
1	14	6	1079	1061	25	7	1	7	42	36	-105
2	14	6	272	285	40	8	1	7	209	162	-68
3	14	6	990	989	27	-11	2	7	136	172	-85
4	14	6	56	44	-138	-10	2	7	376	398	45
-6	15	6	453	456	38	-9	2	7	60	53	-149
-5	15	6	67	114	-165	-8	2	7	202	287	-65
-4	15	6	817	823	26	-7	2	7	557	554	35
-3	15	6	324	301	33	-6	2	7	159	216	-71
-2	15	6	1096	1083	25	-5	2	7	1312	1271	25
-1	15	6	96	135	-78	-4	2	7	224	167	37
0	15	6	1200	1267	25	-3	2	7	1875	1790	20
1	15	6	99	127	-88	-2	2	7	48	85	-120
2	15	6	1000	1008	27	-1	2	7	1840	1734	17
3	15	6	275	325	47	0	2	7	191	179	28
-4	16	6	50	64	-125	1	2	7	1854	2085	18
-3	16	6	1033	1086	27	2	2	7	77	136	-55
-2	16	6	55	44	-137	3	2	7	667	729	26
-1	16	6	1155	1194	25	4	2	7	53	114	-132
0	16	6	54	83	-135	5	2	7	874	987	31
1	16	6	1154	1159	26	6	2	7	106	65	-91
-11	0	7	123	268	-101	7	2	7	183	137	-52
-9	0	7	58	27	-144	8	2	7	195	226	-82
-7	0	7	693	695	32	-11	3	7	317	320	48
-5	0	7	871	803	29	-10	3	7	233	224	-78
-3	0	7	1645	1487	28	-9	3	7	244	370	-73
-1	0	7	1042	952	28	-8	3	7	401	399	48
1	0	7	1464	1598	27	-7	3	7	232	283	-50
3	0	7	733	675	28	-6	3	7	913	928	28

H	K	L	$10F_O$	$10F_C$	10σ
-5	3	7	577	569	27
-4	3	7	1413	1366	21
-3	3	7	148	104	-36
-1	3	7	247	258	24
0	3	7	1848	1777	17
1	3	7	45	121	-112
2	3	7	1636	1813	20
3	3	7	132	148	-69
4	3	7	901	906	26
5	3	7	391	368	33
6	3	7	495	472	35
7	3	7	260	219	47
-11	4	7	128	64	-98
-10	4	7	463	424	40
-9	4	7	60	93	-149
-8	4	7	357	431	40
-7	4	7	685	607	29
-6	4	7	806	781	26
-5	4	7	1229	1244	23
-4	4	7	409	408	25
-3	4	7	1723	1581	18
-2	4	7	812	796	20
-1	4	7	1865	1744	17
0	4	7	266	270	25
1	4	7	2011	2014	18
2	4	7	192	169	31
3	4	7	930	985	22
4	4	7	548	572	31
5	4	7	964	955	28
6	4	7	352	262	44
7	4	7	236	202	-82
-11	5	7	272	367	-65
-10	5	7	145	195	-109
-9	5	7	507	583	37
-8	5	7	592	604	34
-7	5	7	781	745	27
-6	5	7	775	807	25
-5	5	7	890	902	24
-4	5	7	1036	1021	22
-3	5	7	437	430	22
-2	5	7	1745	1665	18
-1	5	7	336	323	26
0	5	7	1060	1003	18
1	5	7	313	343	29
2	5	7	1314	1350	20
3	5	7	290	333	36
4	5	7	764	775	26
5	5	7	437	487	41
6	5	7	502	501	38
7	5	7	270	242	-60
-10	6	7	810	799	37
-9	6	7	66	103	-163
-8	6	7	656	663	33
-7	6	7	321	378	34
-6	6	7	895	873	24
-4	6	7	401	429	24
-3	6	7	1035	969	19
-2	6	7	527	521	21
-1	6	7	936	861	19
0	6	7	275	283	30
1	6	7	967	976	20
2	6	7	100	61	-59
3	6	7	539	534	26
4	6	7	523	541	30
5	6	7	733	706	28
6	6	7	217	238	-60
7	6	7	203	203	-85
-10	7	7	255	387	-80
-9	7	7	846	856	31
-8	7	7	313	312	42
-7	7	7	687	742	28
-6	7	7	452	448	30
-5	7	7	687	672	23
-4	7	7	722	713	23
-3	7	7	135	155	-50
-2	7	7	1101	1049	20
-1	7	7	360	362	26
0	7	7	734	698	20
1	7	7	184	187	-50
2	7	7	774	796	22
3	7	7	45	94	-111
4	7	7	494	485	30
5	7	7	498	490	31
6	7	7	354	262	53
7	7	7	528	391	36
-10	8	7	1032	1004	33
-9	8	7	58	43	-144
-8	8	7	623	735	34
-7	8	7	126	71	-91
-6	8	7	965	937	24
-5	8	7	681	703	24
-4	8	7	349	362	28
-3	8	7	744	724	22
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-1	8	7	1164	1109	20
0	8	7	209	190	31

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3	8	7	630	634	25
4	8	7	612	582	26
5	8	7	441	418	35
6	8	7	474	383	33
-9	9	7	827	920	32
-8	9	7	233	245	45
-7	9	7	963	954	27
-6	9	7	278	300	37
-5	9	7	938	929	22
-4	9	7	629	670	23
-3	9	7	486	491	24
-2	9	7	1228	1187	20
-1	9	7	262	241	30
0	9	7	1121	1046	21
1	9	7	361	391	25
2	9	7	1016	999	22
3	9	7	372	348	29
4	9	7	476	511	28
5	9	7	671	664	30
6	9	7	175	155	-82
-9	10	7	188	209	-66
-8	10	7	842	888	30
-7	10	7	152	159	-65
-6	10	7	1188	1190	24
-5	10	7	978	970	24
-4	10	7	771	792	23
-3	10	7	619	619	23
-2	10	7	610	581	23
-1	10	7	1176	1149	21
0	10	7	203	203	41
1	10	7	855	835	23
2	10	7	357	333	33
3	10	7	553	573	28
4	10	7	825	802	26
5	10	7	467	439	35
6	10	7	541	465	33
-8	11	7	500	508	39
-7	11	7	1007	1028	27
-6	11	7	434	438	31
-5	11	7	939	972	25
-4	11	7	710	692	25
-3	11	7	684	680	25
-2	11	7	706	704	25
-1	11	7	452	420	28
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1	11	7	411	402	34
2	11	7	495	513	28
3	11	7	406	422	32
4	11	7	566	490	28
5	11	7	663	710	33
-8	12	7	788	895	34
-7	12	7	65	119	-161
-6	12	7	974	975	27
-5	12	7	641	670	28
-4	12	7	652	677	26
-3	12	7	56	85	-140
-2	12	7	467	494	31
-1	12	7	484	451	25
0	12	7	98	6	-80
1	12	7	188	199	-59
2	12	7	142	181	-96
3	12	7	265	313	47
4	12	7	581	583	29
-7	13	7	989	1018	29
-6	13	7	184	49	-49
-5	13	7	686	713	28
-4	13	7	125	130	-61
-3	13	7	424	394	31
-2	13	7	238	209	37
-1	13	7	139	239	-76
0	13	7	47	71	-117
1	13	7	182	201	-57
2	13	7	249	180	38
3	13	7	241	195	41
4	13	7	163	216	-90
-6	14	7	831	827	29
-5	14	7	240	194	41
-4	14	7	654	677	29
-3	14	7	184	162	-53
-2	14	7	233	199	43
-1	14	7	275	311	39
0	14	7	54	18	-134
1	14	7	55	80	-136
2	14	7	162	168	-62
3	14	7	54	44	-134
-5	15	7	716	797	30
-4	15	7	147	29	-54
-3	15	7	489	510	32
-2	15	7	94	147	-92
-1	15	7	217	240	43
0	15	7	196	144	-45
1	15	7	214	238	-45
-3	16	7	159	148	-53
-2	16	7	319	375	57

H	K	L	$10F_o$	$10F_c$	10σ
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-4	0	8	283	286	43
-2	0	8	304	242	47
0	0	8	281	335	28
2	0	8	334	389	46
4	0	8	511	602	36
6	0	8	516	511	36
-11	1	8	1002	1081	34
-10	1	8	71	149	-177
-9	1	8	1418	1532	30
-8	1	8	380	349	41
-7	1	8	1343	1313	31
-6	1	8	360	360	43
-5	1	8	714	737	33
-4	1	8	283	247	44
-3	1	8	853	790	26
-2	1	8	208	189	42
-1	1	8	351	317	25
0	1	8	101	108	-49
1	1	8	345	369	32
2	1	8	46	135	-113
3	1	8	413	549	46
4	1	8	148	133	-69
5	1	8	723	877	36
6	1	8	250	171	42
7	1	8	445	494	41
-11	2	8	150	123	-79
-10	2	8	1164	1295	32
-9	2	8	196	236	-106
-8	2	8	712	743	35
-7	2	8	603	607	35
-6	2	8	1633	1614	27
-5	2	8	229	307	-49
-4	2	8	404	417	31
-3	2	8	714	696	23
-2	2	8	560	539	23
-1	2	8	127	151	-53
0	2	8	348	364	25
1	2	8	176	256	-40
2	2	8	733	793	24
3	2	8	164	203	-74
4	2	8	847	992	31
5	2	8	159	246	-84
6	2	8	815	775	33
7	2	8	111	108	-90
-11	3	8	645	707	36
-10	3	8	64	68	-158
-9	3	8	980	1021	32
-8	3	8	183	203	-63
-7	3	8	1170	1151	29
-6	3	8	473	471	41
-5	3	8	760	728	26
-4	3	8	566	548	24
-3	3	8	770	764	23
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-1	3	8	209	207	28
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1	3	8	662	686	23
2	3	8	240	250	30
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4	3	8	170	195	-55
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6	3	8	61	158	-150
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-10	4	8	1144	1167	33
-9	4	8	167	209	-108
-8	4	8	711	738	34
-7	4	8	130	256	-94
-6	4	8	1208	1246	27
-5	4	8	178	148	-45
-4	4	8	381	383	27
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-2	4	8	48	105	-119
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3	4	8	297	262	40
4	4	8	936	887	27
5	4	8	154	153	-78
6	4	8	743	694	35
-10	5	8	68	69	-169
-9	5	8	1091	1179	32
-8	5	8	162	56	-69
-7	5	8	985	1048	28
-6	5	8	161	138	-55
-5	5	8	494	504	28
-4	5	8	561	523	24
-3	5	8	432	389	24
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-1	5	8	372	352	23
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H	K	L	$10F_o$	$10F_c$	10σ
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6	5	8	132	69	-86
-10	6	8	1166	1238	34
-9	6	8	111	106	-112
-8	6	8	773	899	32
-7	6	8	653	619	28
-5	6	8	316	334	32
-4	6	8	334	323	30
-3	6	8	1049	976	21
-2	6	8	223	163	30
-1	6	8	552	502	23
0	6	8	153	128	-44
1	6	8	801	798	21
2	6	8	424	428	28
3	6	8	364	288	37
4	6	8	339	406	36
5	6	8	277	296	48
6	6	8	585	488	36
-10	7	8	67	148	-165
-9	7	8	959	1045	33
-8	7	8	569	562	32
-7	7	8	903	957	28
-6	7	8	764	792	28
-5	7	8	638	640	26
-4	7	8	1032	1044	23
-3	7	8	590	561	24
-2	7	8	876	807	21
-1	7	8	183	89	32
0	7	8	728	700	22
1	7	8	246	196	28
2	7	8	506	497	25
3	7	8	287	297	36
4	7	8	396	345	33
5	7	8	696	613	29
6	7	8	331	334	40
-9	8	8	146	220	-103
-8	8	8	751	765	31
-7	8	8	1008	1069	28
-6	8	8	845	877	27
-5	8	8	763	818	26
-4	8	8	554	585	25
-3	8	8	1333	1310	21
-2	8	8	273	201	28
-1	8	8	877	797	21
0	8	8	92	41	-56
1	8	8	913	855	22
2	8	8	583	579	25
3	8	8	450	452	30
4	8	8	416	437	34
5	8	8	546	499	34
-9	9	8	506	605	42
-8	9	8	423	482	38
-7	9	8	620	643	30
-6	9	8	658	753	32
-5	9	8	527	531	28
-4	9	8	1119	1127	23
-3	9	8	437	459	26
-2	9	8	1188	1152	22
-1	9	8	52	108	-128
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1	9	8	283	323	32
2	9	8	926	906	25
3	9	8	556	508	28
4	9	8	490	442	35
5	9	8	704	606	31
-8	10	8	400	390	39
-7	10	8	588	632	32
-6	10	8	456	407	30
-5	10	8	535	574	32
-4	10	8	244	303	44
-3	10	8	1318	1299	23
-2	10	8	146	101	-51
-1	10	8	1081	1100	22
0	10	8	51	28	-128
1	10	8	1301	1210	23
2	10	8	669	632	26
3	10	8	652	586	28
4	10	8	444	362	35
-8	11	8	186	245	-56
-7	11	8	309	335	40
-6	11	8	538	572	31
-5	11	8	165	66	-48
-4	11	8	986	997	25
-3	11	8	146	78	-50
-2	11	8	1039	1032	23
-1	11	8	202	214	41
0	11	8	1085	1059	24
1	11	8	237	240	46
2	11	8	825	809	27
3	11	8	154	232	-90
4	11	8	349	337	37
-7	12	8	626	659	33
-6	12	8	62	168	-155

H	K	L	10F$_o$	10F$_c$	10σ	H	K	L	10F$_o$	10F$_c$	10σ
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-4	12	8	146	142	-53	3	1	9	98	59	-94
-3	12	8	1033	1026	25	4	1	9	494	510	36
-2	12	8	375	337	32	5	1	9	56	30	-138
-1	12	8	883	871	25	6	1	9	58	64	-143
0	12	8	54	83	-134	-10	2	9	169	263	-86
1	12	8	839	790	28	-9	2	9	561	600	38
2	12	8	244	278	40	-8	2	9	134	146	-93
3	12	8	486	449	33	-7	2	9	1022	1012	32
-6	13	8	708	772	32	-6	2	9	174	60	-64
-5	13	8	98	111	-84	-5	2	9	1248	1217	28
-4	13	8	1000	990	27	-4	2	9	478	417	34
-3	13	8	187	193	-58	-3	2	9	1706	1722	24
-2	13	8	913	911	26	-2	2	9	236	260	40
-1	13	8	57	94	-142	-1	2	9	1204	1111	21
0	13	8	772	762	27	0	2	9	478	429	23
1	13	8	51	28	-127	1	2	9	1255	1355	22
2	13	8	677	657	30	2	2	9	125	191	-71
-5	14	8	794	866	29	3	2	9	361	428	43
-4	14	8	305	375	46	4	2	9	121	198	-111
-3	14	8	1038	1050	26	5	2	9	306	346	47
-2	14	8	64	27	-159	6	2	9	149	109	-88
-1	14	8	930	950	27	-10	3	9	285	293	-69
0	14	8	246	300	41	-9	3	9	133	139	-90
1	14	8	801	803	28	-8	3	9	636	687	43
-3	15	8	345	325	38	-7	3	9	261	286	52
-2	15	8	1035	1082	28	-6	3	9	1031	1050	29
-1	15	8	52	70	-130	-5	3	9	101	75	-93
-9	0	9	687	706	36	-4	3	9	1326	1301	24
-7	0	9	1313	1303	33	-3	3	9	117	87	-65
-5	0	9	1420	1306	34	-1	3	9	270	231	30
-3	0	9	2051	1816	33	0	3	9	1395	1351	21
-1	0	9	1044	942	31	1	3	9	270	257	31
1	0	9	1122	1229	32	2	3	9	828	832	24
3	0	9	357	300	39	3	3	9	273	323	40
5	0	9	345	381	55	4	3	9	524	526	34
-10	1	9	204	269	-77	5	3	9	361	338	44
-9	1	9	214	149	-60	6	3	9	68	45	-168
-8	1	9	921	934	35	-10	4	9	440	428	58
-7	1	9	58	29	-144	-9	4	9	562	601	41
-6	1	9	1461	1387	32	-8	4	9	300	295	44
-5	1	9	192	251	-62	-7	4	9	827	823	32
-4	1	9	1522	1481	29	-6	4	9	583	556	33
-3	1	9	386	371	40	-5	4	9	1021	1072	26
-2	1	9	1537	1454	24	-4	4	9	241	279	41
-1	1	9	429	396	26	-3	4	9	1755	1612	22
0	1	9	1265	1196	21	-2	4	9	393	364	27
1	1	9	153	145	-47	-1	4	9	1090	1000	21

H	K	L	$10F_o$	$10F_c$	10σ
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3	4	9	375	413	37
4	4	9	533	512	36
5	4	9	321	264	43
-10	5	9	119	268	-140
-9	5	9	362	444	49
-8	5	9	734	777	33
-7	5	9	679	684	36
-6	5	9	1184	1246	27
-5	5	9	512	488	30
-4	5	9	1187	1130	23
-3	5	9	378	384	28
-2	5	9	1302	1273	21
-1	5	9	44	34	-109
0	5	9	998	963	21
1	5	9	196	134	34
2	5	9	518	512	26
3	5	9	349	370	32
4	5	9	360	425	47
5	5	9	402	346	51
-9	6	9	591	674	39
-8	6	9	502	560	42
-7	6	9	860	930	34
-6	6	9	598	630	31
-5	6	9	1208	1202	25
-4	6	9	170	155	-48
-3	6	9	1350	1302	22
-2	6	9	145	131	-45
-1	6	9	710	660	23
0	6	9	350	346	27
1	6	9	788	763	23
2	6	9	190	171	-52
3	6	9	255	255	-55
4	6	9	516	486	33
5	6	9	412	261	47
-9	7	9	594	639	37
-8	7	9	474	543	38
-7	7	9	613	675	36
-6	7	9	1195	1182	30
-5	7	9	136	111	-54
-4	7	9	788	794	25
-3	7	9	97	47	-82
-2	7	9	1128	1086	23
-1	7	9	356	353	29
0	7	9	885	778	23
1	7	9	535	442	26

H	K	L	$10F_o$	$10F_c$	10σ
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4	7	9	425	404	38
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-9	8	9	508	510	49
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-6	8	9	444	436	34
-5	8	9	673	740	30
-4	8	9	187	202	-51
-3	8	9	1142	1078	23
-2	8	9	81	140	-72
-1	8	9	725	732	25
0	8	9	822	775	23
1	8	9	975	899	24
2	8	9	399	371	34
3	8	9	398	396	35
4	8	9	708	720	30
-8	9	9	208	216	-67
-7	9	9	513	548	34
-6	9	9	625	677	29
-5	9	9	190	225	-52
-4	9	9	524	516	28
-3	9	9	84	73	-91
-2	9	9	943	964	24
-1	9	9	442	418	26
0	9	9	858	832	25
1	9	9	597	586	27
2	9	9	477	513	32
3	9	9	733	701	30
4	9	9	369	339	42
-8	10	9	495	583	40
-7	10	9	319	293	37
-6	10	9	604	628	38
-5	10	9	635	672	30
-4	10	9	203	181	-43
-3	10	9	712	702	26
-2	10	9	63	119	-157
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0	10	9	567	568	27
1	10	9	560	545	28
2	10	9	498	461	29
3	10	9	303	296	50
-7	11	9	664	692	32
-6	11	9	691	750	30
-5	11	9	539	590	31
-4	11	9	353	388	36
-3	11	9	251	246	39

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
-2	11	9	536	566	29	-5	2	10	309	336	46
-1	11	9	52	83	-129	-4	2	10	215	174	-63
0	11	9	323	281	34	-3	2	10	258	247	45
1	11	9	439	441	30	-2	2	10	403	405	31
2	11	9	211	132	-46	-1	2	10	54	40	-135
-6	12	9	676	710	31	0	2	10	841	779	23
-5	12	9	543	551	30	1	2	10	50	31	-125
-4	12	9	238	262	40	2	2	10	672	761	31
-3	12	9	318	331	38	3	2	10	56	149	-139
-2	12	9	220	159	38	4	2	10	1005	1098	34
-1	12	9	317	258	37	5	2	10	58	24	-144
0	12	9	455	451	32	-9	3	10	333	389	59
1	12	9	192	139	-50	-8	3	10	352	370	52
2	12	9	303	315	56	-7	3	10	647	685	39
-5	13	9	348	416	47	-6	3	10	314	316	47
-4	13	9	60	134	-148	-5	3	10	60	67	-148
-3	13	9	61	62	-150	-4	3	10	341	382	35
-2	13	9	352	353	34	-3	3	10	54	42	-135
-1	13	9	210	258	-49	-2	3	10	276	263	33
0	13	9	126	184	-75	-1	3	10	611	567	25
-10	0	10	1279	1385	34	0	3	10	284	246	32
-8	0	10	971	955	34	1	3	10	928	935	25
-6	0	10	700	583	38	2	3	10	177	108	-46
-4	0	10	172	28	-79	3	3	10	862	900	29
-2	0	10	648	591	40	4	3	10	65	43	-161
0	0	10	662	725	24	-9	4	10	228	265	-68
2	0	10	488	573	52	-8	4	10	321	429	-69
4	0	10	698	811	35	-7	4	10	373	341	56
-10	1	10	72	65	-180	-6	4	10	270	281	-62
-9	1	10	671	800	41	-5	4	10	281	370	45
-8	1	10	243	155	-64	-4	4	10	50	8	-124
-7	1	10	1077	1066	35	-3	4	10	595	582	29
-6	1	10	258	196	-61	-2	4	10	622	551	25
-5	1	10	70	49	-174	-1	4	10	500	472	26
-4	1	10	194	200	-64	0	4	10	727	698	23
-3	1	10	92	111	-111	1	4	10	515	513	31
-2	1	10	115	25	-71	2	4	10	748	755	27
-1	1	10	642	590	26	3	4	10	134	155	-109
0	1	10	48	30	-120	4	4	10	1043	951	32
1	1	10	760	868	26	-9	5	10	587	671	38
2	1	10	129	124	-97	-8	5	10	620	588	37
3	1	10	618	679	40	-7	5	10	714	753	33
4	1	10	118	100	-96	-6	5	10	185	312	-61
5	1	10	672	664	39	-5	5	10	145	88	-66
-9	2	10	65	131	-162	-4	5	10	836	765	27
-8	2	10	537	561	41	-3	5	10	231	255	47
-7	2	10	191	278	-93	-2	5	10	683	646	25
-6	2	10	394	442	48	-1	5	10	629	583	25

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
0	5	10	666	681	27	-2	9	10	704	686	26
1	5	10	808	772	25	-1	9	10	227	208	47
2	5	10	502	440	29	0	9	10	673	642	27
3	5	10	568	591	31	1	9	10	497	507	31
4	5	10	112	151	-88	2	9	10	335	303	42
-9	6	10	285	404	-65	-6	10	10	188	53	-51
-8	6	10	721	746	35	-5	10	10	623	683	30
-7	6	10	697	726	32	-4	10	10	102	63	-98
-6	6	10	432	432	36	-3	10	10	974	957	27
-5	6	10	753	760	28	-2	10	10	315	362	38
-4	6	10	60	7	-148	-1	10	10	766	741	27
-3	6	10	860	846	26	0	10	10	289	274	39
-2	6	10	418	426	37	1	10	10	748	724	29
-1	6	10	633	570	25	2	10	10	583	534	31
0	6	10	580	572	27	-6	11	10	582	719	35
1	6	10	589	568	27	-5	11	10	57	93	-141
2	6	10	587	541	28	-4	11	10	982	1029	29
3	6	10	107	75	-81	-3	11	10	206	240	-43
4	6	10	599	582	38	-2	11	10	823	834	28
-8	7	10	780	854	34	-1	11	10	220	288	-66
-7	7	10	652	725	35	0	11	10	792	788	29
-6	7	10	703	796	33	1	11	10	501	470	31
-5	7	10	127	163	-88	-4	12	10	55	23	-136
-4	7	10	1035	1027	26	-3	12	10	990	1030	28
-3	7	10	55	41	-137	-2	12	10	435	441	34
-2	7	10	658	598	26	-1	12	10	805	747	29
-1	7	10	394	363	38	-9	0	11	950	1078	39
0	7	10	460	442	27	-7	0	11	1512	1514	37
1	7	10	535	556	30	-5	0	11	1647	1432	39
2	7	10	167	169	-78	-3	0	11	1877	1598	37
3	7	10	472	439	33	-1	0	11	737	732	35
-8	8	10	352	432	50	1	0	11	632	609	41
-7	8	10	823	902	33	3	0	11	117	42	-103
-6	8	10	224	307	-51	-9	1	11	73	137	-181
-5	8	10	847	876	30	-8	1	11	1091	1129	38
-4	8	10	69	186	-172	-7	1	11	200	67	-68
-3	8	10	822	844	27	-6	1	11	1411	1406	36
-2	8	10	236	217	40	-5	1	11	67	85	-167
-1	8	10	519	470	28	-4	1	11	1595	1507	34
0	8	10	266	279	38	-3	1	11	272	280	-74
1	8	10	376	406	33	-2	1	11	946	882	30
2	8	10	591	528	29	-1	1	11	204	221	-64
3	8	10	54	57	-135	0	1	11	949	911	25
-7	9	10	199	263	-62	1	1	11	101	93	-83
-6	9	10	536	612	33	2	1	11	130	104	-73
-5	9	10	148	106	-66	3	1	11	57	49	-142
-4	9	10	989	956	27	-9	2	11	776	889	43
-3	9	10	53	34	-132	-8	2	11	210	213	-114

H	K	L	$10F_o$	$10F_c$	10σ
-7	2	11	1196	1205	36
-6	2	11	149	30	-87
-5	2	11	850	895	37
-4	2	11	265	281	-59
-3	2	11	1258	1226	28
-2	2	11	220	223	45
-1	2	11	719	645	27
0	2	11	353	329	37
1	2	11	595	585	28
2	2	11	54	123	-134
3	2	11	155	140	-90
-8	3	11	772	799	45
-7	3	11	68	121	-168
-6	3	11	803	861	33
-5	3	11	55	9	-137
-4	3	11	958	987	30
-3	3	11	133	68	-80
-2	3	11	732	656	26
-1	3	11	348	325	32
0	3	11	836	827	26
1	3	11	167	190	-47
2	3	11	102	145	-102

H	K	L	$10F_o$	$10F_c$	10σ

Table 71. F_o F_c Tables for $[Pt_4(OAc)_6(CO)_2]\cdot 2HOAc$, 6, F(obs), F(calc), and σ_F ($-\sigma_F$ indicates omitted data).

H	K	L	$10F_o$	$10F_c$	10σ
4	0	0	707	475	96
6	0	0	3489	3737	93
8	0	0	2754	2852	65
10	0	0	5322	5538	86
12	0	0	2834	2848	85
14	0	0	2506	2511	98
16	0	0	4519	4463	89
18	0	0	1424	1528	144
20	0	0	783	781	-264
22	0	0	523	191	-216
24	0	0	2457	2496	133
26	0	0	3150	2931	127
28	0	0	372	1521	-369
30	0	0	345	117	-619
32	0	0	316	209	-567
1	1	0	9106	9903	191
3	1	0	3303	3205	38
5	1	0	193	259	-347
7	1	0	2496	2431	87
9	1	0	3692	3933	65
11	1	0	4213	4313	215
13	1	0	466	184	-205
15	1	0	3309	3559	165
17	1	0	3298	3227	160
19	1	0	474	553	-250
21	1	0	589	314	-272
23	1	0	1190	1316	252
25	1	0	2495	2441	155
27	1	0	2067	1917	277
29	1	0	691	624	-360
31	1	0	312	128	-558
33	1	0	330	106	-591
0	2	0	4610	4425	51
2	2	0	4204	4143	91
4	2	0	409	389	-113
6	2	0	2275	2251	115
8	2	0	2657	2652	71
10	2	0	3143	3027	168
12	2	0	1005	1073	170
14	2	0	1195	1161	-369
16	2	0	2462	2617	182
18	2	0	1499	1654	130
20	2	0	661	555	-218
22	2	0	578	755	-331
24	2	0	1533	1336	178
26	2	0	1317	1280	299
28	2	0	527	736	-442
30	2	0	317	188	-568
32	2	0	708	38	-338
1	3	0	1380	1426	59
3	3	0	744	923	92
5	3	0	1900	1901	63
7	3	0	719	726	108
9	3	0	463	150	-158
11	3	0	1082	1069	103
13	3	0	186	436	-335
15	3	0	338	57	-221
17	3	0	596	493	-238
19	3	0	832	905	199
21	3	0	1033	1156	209
23	3	0	638	822	-266
25	3	0	233	312	-417
27	3	0	395	167	-434
29	3	0	729	300	-417
31	3	0	329	272	-590
0	4	0	3355	3316	76
2	4	0	1120	1072	83
4	4	0	1862	1829	69
6	4	0	2498	2473	66
8	4	0	271	340	-218
10	4	0	3545	3457	74
12	4	0	1501	1460	101
14	4	0	713	963	-190
16	4	0	1800	1759	120
18	4	0	170	83	-429
20	4	0	1153	1181	184
22	4	0	1359	1133	-430
24	4	0	321	236	-328
26	4	0	993	851	-372
28	4	0	441	271	-483
30	4	0	749	361	-424
1	5	0	5051	4873	60

H	K	L	$10F_o$	$10F_c$	10σ
3	5	0	297	248	-193
5	5	0	3067	2977	66
7	5	0	937	1036	119
9	5	0	3337	3232	104
11	5	0	3447	3415	109
13	5	0	189	121	-339
15	5	0	2628	2610	114
17	5	0	1692	1539	178
19	5	0	605	531	-262
21	5	0	1157	1282	175
23	5	0	376	144	-433
25	5	0	1258	1463	282
27	5	0	928	1189	-316
29	5	0	493	34	-445
0	6	0	4609	4632	96
2	6	0	2872	3027	114
4	6	0	170	376	-304
6	6	0	951	1049	129
8	6	0	1388	1425	106
10	6	0	3133	2974	160
12	6	0	1428	1478	143
14	6	0	1309	1399	124
16	6	0	1928	2014	270
18	6	0	675	832	-201
20	6	0	407	470	-329
22	6	0	546	22	-313
24	6	0	1264	1216	279
26	6	0	1081	1587	-394
28	6	0	522	677	-497
1	7	0	3710	3514	92
3	7	0	1684	1688	95
5	7	0	172	191	-310
7	7	0	536	641	-193
9	7	0	1914	2039	108
11	7	0	1599	1613	155
13	7	0	371	24	-224
15	7	0	1351	1368	299
17	7	0	1304	1354	166
19	7	0	378	524	-370
21	7	0	264	326	-477
23	7	0	679	775	-355
25	7	0	1112	1282	-461
27	7	0	774	981	-393
0	8	0	2411	2210	134
2	8	0	2347	2282	92
4	8	0	1863	1858	119
6	8	0	1628	1496	110
8	8	0	1157	1133	234

H	K	L	$10F_o$	$10F_c$	10σ
10	8	0	475	525	-258
12	8	0	485	96	-258
14	8	0	208	387	-374
16	8	0	762	583	-289
18	8	0	821	680	-305
20	8	0	722	789	-356
22	8	0	946	828	-374
24	8	0	1277	849	-402
1	9	0	710	1083	-232
3	9	0	1975	2020	110
5	9	0	2239	2385	111
7	9	0	1544	1458	170
9	9	0	207	104	-371
11	9	0	819	814	173
13	9	0	409	271	-223
15	9	0	298	341	-534
17	9	0	282	31	-506
19	9	0	786	879	-416
21	9	0	1341	1186	254
0	10	0	219	270	-553
2	10	0	380	576	-308
4	10	0	2122	2096	117
6	10	0	2085	2007	159
8	10	0	256	384	-460
10	10	0	961	944	-373
12	10	0	290	645	-519
14	10	0	668	413	-384
16	10	0	511	529	-408
18	10	0	792	497	-334
1	11	0	546	558	-398
3	11	0	427	677	-426
5	11	0	1418	1541	-438
7	11	0	867	889	-264
9	11	0	678	443	-358
11	11	0	651	839	-332
13	11	0	300	134	-539
0	12	0	622	688	-406
2	12	0	305	233	-549
4	12	0	726	519	-376
6	12	0	627	557	-325
-33	1	1	314	116	-795
-31	1	1	313	96	-793
-29	1	1	310	278	-784
-27	1	1	1001	900	-278
-25	1	1	946	930	-306
-23	1	1	231	130	-584
-21	1	1	1071	1315	233
-19	1	1	884	1199	-339

Table 71. (continued)

H	K	L	$10F_o$	$10F_c$	10σ
-17	1	1	412	579	-363
-15	1	1	669	773	-270
-13	1	1	756	685	150
-11	1	1	3314	3380	95
-9	1	1	2983	3111	86
-7	1	1	433	184	-187
-5	1	1	481	466	-157
-3	1	1	781	766	73
-1	1	1	5278	4956	39
1	1	1	2973	2828	42
3	1	1	539	174	-151
5	1	1	4656	4695	72
7	1	1	1196	1302	135
9	1	1	192	268	-487
11	1	1	943	1022	231
13	1	1	1217	1290	205
15	1	1	3101	3193	132
17	1	1	2131	2155	150
19	1	1	580	483	-354
21	1	1	644	347	-290
23	1	1	233	193	-590
25	1	1	34	958	-73
27	1	1	263	718	-667
29	1	1	330	11	-835
31	1	1	323	439	-820
33	1	1	316	214	-800
-32	2	1	723	114	-455
-30	2	1	343	82	-867
-28	2	1	975	896	-399
-26	2	1	1456	1733	259
-24	2	1	772	1047	-373
-22	2	1	1007	989	212
-20	2	1	1925	2028	191
-18	2	1	356	500	-369
-16	2	1	1260	1339	176
-14	2	1	198	152	-501
-12	2	1	3694	3845	98
-10	2	1	5733	5789	84
-8	2	1	4233	4254	77
-6	2	1	800	710	111
-4	2	1	617	579	146
-2	2	1	2724	2662	57
0	2	1	6264	6094	52
2	2	1	4108	4020	57
4	2	1	3001	2840	70
6	2	1	3289	3325	84
8	2	1	2072	2067	105
10	2	1	1316	1336	128
12	2	1	342	564	-335
14	2	1	3461	3390	127
16	2	1	4440	4510	128
18	2	1	2210	2239	158
20	2	1	202	108	-512
22	2	1	229	54	-581
24	2	1	904	1097	-322
26	2	1	1894	1596	204
28	2	1	331	536	-839
30	2	1	586	514	-563
32	2	1	722	620	-527
-31	3	1	314	80	-795
-29	3	1	475	453	-500
-27	3	1	1552	1614	344
-25	3	1	1699	1771	198
-23	3	1	457	327	-350
-21	3	1	1536	1678	200
-19	3	1	1285	1393	187
-17	3	1	428	729	-420
-15	3	1	1134	1111	163
-13	3	1	2303	2184	118
-11	3	1	6378	6284	89
-9	3	1	6435	6373	81
-7	3	1	2712	2700	81
-5	3	1	157	139	-399
-3	3	1	2109	2004	69
-1	3	1	5509	5485	64
1	3	1	5527	5794	65
3	3	1	638	591	138
5	3	1	3580	3738	82
7	3	1	2893	2896	91
9	3	1	802	627	150
11	3	1	502	823	-286
13	3	1	2161	2112	145
15	3	1	5272	5245	128
17	3	1	3962	3900	138
19	3	1	1029	1311	-309
21	3	1	179	198	-451
23	3	1	794	685	-297
25	3	1	1817	1712	264
27	3	1	983	1366	-526
29	3	1	298	23	-754
31	3	1	326	736	-825
-30	4	1	283	248	-719
-28	4	1	351	943	-888
-26	4	1	1370	1649	-388
-24	4	1	779	1290	-337
-22	4	1	490	221	-299

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
-20	4	1	1294	1256	186	15	5	1	1787	1937	165
-18	4	1	478	510	-315	17	5	1	2290	2011	181
-16	4	1	917	736	184	19	5	1	1065	1255	-358
-14	4	1	200	647	-505	21	5	1	1062	1183	-311
-12	4	1	3951	3847	103	23	5	1	988	1034	-329
-10	4	1	6106	6014	91	25	5	1	337	862	-851
-8	4	1	4236	3970	85	27	5	1	651	430	-435
-6	4	1	1469	1499	98	29	5	1	674	36	-587
-4	4	1	1037	1000	106	-28	6	1	488	393	-577
-2	4	1	4708	4626	15	-26	6	1	290	168	-736
0	4	1	6418	6450	72	-24	6	1	713	408	-398
2	4	1	3553	3482	80	-22	6	1	1136	780	205
4	4	1	1462	1333	111	-20	6	1	405	568	-395
6	4	1	3399	3323	90	-18	6	1	193	214	-488
8	4	1	1213	878	159	-16	6	1	1015	1060	207
10	4	1	193	416	-487	-14	6	1	1339	1183	152
12	4	1	736	855	-208	-12	6	1	846	870	-222
14	4	1	3545	3629	140	-10	6	1	829	788	175
16	4	1	3839	3870	145	-8	6	1	2515	2245	103
18	4	1	2010	2092	165	-6	6	1	3824	3710	98
20	4	1	253	459	-641	-4	6	1	3100	3011	97
22	4	1	593	518	-322	-2	6	1	1073	1270	156
24	4	1	1172	1369	-313	0	6	1	157	74	-396
26	4	1	924	1478	-471	2	6	1	160	126	-408
28	4	1	675	589	-520	4	6	1	1141	1246	127
30	4	1	837	402	-412	6	6	1	623	603	-209
-29	5	1	370	537	-938	8	6	1	561	524	-315
-27	5	1	751	816	-463	10	6	1	1784	1693	138
-25	5	1	1330	1104	301	12	6	1	1730	1610	166
-23	5	1	904	784	-295	14	6	1	1192	1049	196
-21	5	1	214	50	-540	18	6	1	893	1204	-287
-19	5	1	540	510	-339	20	6	1	972	1522	-429
-17	5	1	485	455	-256	22	6	1	907	1107	-363
-15	5	1	187	456	-471	24	6	1	254	325	-642
-13	5	1	1715	1610	129	26	6	1	354	206	-897
-11	5	1	2913	2819	113	28	6	1	361	84	-912
-9	5	1	3606	3476	97	-27	7	1	339	225	-860
-7	5	1	3514	3481	93	-25	7	1	295	283	-747
-5	5	1	2640	2625	89	-23	7	1	515	527	-509
-3	5	1	2617	2628	93	-21	7	1	1156	1179	-326
-1	5	1	3012	2899	89	-19	7	1	584	565	-326
1	5	1	2841	2994	93	-17	7	1	954	882	219
3	5	1	1088	1158	122	-15	7	1	1573	1617	170
5	5	1	481	379	-212	-13	7	1	395	647	-310
7	5	1	1326	1379	132	-11	7	1	384	858	-388
9	5	1	1009	1095	199	-9	7	1	180	424	-457
11	5	1	739	969	-212	-7	7	1	1890	1853	115
13	5	1	1856	1886	184	-5	7	1	2946	2900	111

Table 71. (continued)

H	K	L	$10F_o$	$10F_c$	10σ
-3	7	1	1266	1248	148
-1	7	1	631	891	-315
1	7	1	1248	1169	133
3	7	1	732	787	-284
5	7	1	2078	2076	135
7	7	1	622	652	-298
9	7	1	1843	1704	164
11	7	1	2517	2478	160
13	7	1	824	1089	-300
15	7	1	237	294	-598
17	7	1	415	216	-361
19	7	1	838	936	-355
21	7	1	1093	1301	-429
23	7	1	585	486	-497
25	7	1	767	541	-421
27	7	1	543	546	-630
-24	8	1	539	150	-516
-22	8	1	339	847	-860
-20	8	1	1036	1070	-387
-18	8	1	272	62	-689
-16	8	1	1494	1337	220
-14	8	1	863	1002	-250
-12	8	1	656	1031	-274
-10	8	1	1947	2086	143
-8	8	1	558	434	-202
-6	8	1	1856	1835	142
-4	8	1	1744	1687	147
0	8	1	2093	2166	148
2	8	1	697	713	-192
4	8	1	1487	1559	151
6	8	1	1849	1881	172
8	8	1	581	649	-333
10	8	1	2468	2331	145
12	8	1	1413	1505	219
14	8	1	236	592	-596
16	8	1	1472	1318	238
18	8	1	257	263	-651
20	8	1	1044	956	-401
22	8	1	335	784	-848
24	8	1	394	376	-999
-21	9	1	639	822	-509
-19	9	1	338	703	-857
-17	9	1	294	257	-744
-15	9	1	826	803	-417
-13	9	1	357	294	-337
-11	9	1	1763	1888	170
-9	9	1	1601	1705	186
-7	9	1	425	64	-247
-5	9	1	1476	1167	178
-3	9	1	178	9	-451
-1	9	1	1659	1748	177
1	9	1	1898	1852	147
3	9	1	346	34	-366
5	9	1	1504	1358	218
7	9	1	204	696	-517
9	9	1	652	966	-291
11	9	1	704	1017	-326
13	9	1	509	390	-330
15	9	1	1008	1321	-416
17	9	1	789	962	-465
19	9	1	303	120	-767
21	9	1	313	500	-793
-18	10	1	303	487	-767
-16	10	1	762	112	-405
-14	10	1	246	114	-625
-12	10	1	465	807	-471
-10	10	1	996	1318	-310
-8	10	1	754	977	-355
-6	10	1	481	418	-245
-4	10	1	206	350	-522
-2	10	1	832	939	-280
0	10	1	1207	1247	192
2	10	1	680	807	-294
4	10	1	246	158	-625
6	10	1	409	613	-349
8	10	1	478	194	-438
10	10	1	292	104	-741
12	10	1	283	389	-717
14	10	1	1099	916	-455
16	10	1	354	974	-897
18	10	1	609	609	-529
-13	11	1	230	585	-584
-11	11	1	607	600	-373
-9	11	1	522	716	-467
-7	11	1	657	946	-514
-5	11	1	749	1169	-453
-3	11	1	709	966	-420
-1	11	1	778	587	-375
1	11	1	320	391	-808
3	11	1	283	363	-717
5	11	1	284	139	-720
7	11	1	264	159	-671
9	11	1	302	465	-765
11	11	1	1138	780	-296
13	11	1	389	821	-987
-6	12	1	983	1397	-441

Table 71. (continued)

H	K	L	10F$_o$	10F$_c$	10σ
-4	12	1	1035	1333	-375
-2	12	1	525	400	-600
0	12	1	266	203	-671
2	12	1	283	129	-719
4	12	1	505	614	-560
-32	0	2	324	108	-820
-30	0	2	711	439	-517
-28	0	2	529	295	-331
-24	0	2	217	396	-549
-22	0	2	2038	2213	184
-20	0	2	3572	3738	144
-18	0	2	2259	2251	160
-16	0	2	508	118	-309
-14	0	2	1377	1333	143
-12	0	2	5498	5794	101
-10	0	2	7333	7712	89
-8	0	2	4661	4789	81
-6	0	2	4361	4306	72
-4	0	2	4242	4308	58
-2	0	2	2373	2259	47
0	0	2	3988	3753	40
2	0	2	889	1002	81
4	0	2	5942	6361	70
6	0	2	6844	7501	81
8	0	2	2967	3125	100
10	0	2	175	49	-444
12	0	2	1238	1083	139
14	0	2	5485	5591	118
16	0	2	5415	5464	125
18	0	2	1687	1679	175
20	0	2	1794	1700	186
22	0	2	1129	1312	279
24	0	2	213	90	-539
26	0	2	737	748	-320
28	0	2	255	160	-646
30	0	2	1474	1435	330
32	0	2	1493	1377	374
-33	1	2	303	209	-767
-31	1	2	317	294	-803
-29	1	2	264	89	-670
-27	1	2	815	814	-333
-25	1	2	568	911	-328
-23	1	2	853	804	-221
-21	1	2	3266	3026	146
-19	1	2	3199	3255	140
-17	1	2	1338	1240	203
-15	1	2	565	529	-277
-13	1	2	2343	2410	108
-11	1	2	5597	5505	90
-9	1	2	6115	6256	80
-7	1	2	1668	1703	94
-5	1	2	3412	3372	61
-3	1	2	1315	1250	63
-1	1	2	3225	3066	47
1	1	2	1774	1647	54
3	1	2	3193	3160	61
5	1	2	6975	7109	71
7	1	2	6488	6783	85
9	1	2	1683	1962	133
11	1	2	467	225	-238
13	1	2	2321	2242	148
15	1	2	5097	5081	123
17	1	2	3234	3352	148
19	1	2	242	77	-611
21	1	2	740	1212	-419
23	1	2	270	542	-686
27	1	2	232	237	-589
29	1	2	671	772	-548
31	1	2	1561	1341	388
-32	2	2	293	91	-742
-30	2	2	277	38	-701
-28	2	2	478	142	-563
-26	2	2	339	351	-425
-24	2	2	200	67	-507
-22	2	2	1432	1294	180
-20	2	2	2028	1998	158
-18	2	2	1772	1678	161
-16	2	2	1072	1146	160
-14	2	2	1770	1770	117
-12	2	2	2431	2529	105
-10	2	2	3605	3675	87
-8	2	2	2517	2515	79
-6	2	2	688	798	125
-4	2	2	165	244	-418
-2	2	2	1808	1789	66
0	2	2	382	336	-162
2	2	2	2064	1995	69
4	2	2	3805	3795	71
6	2	2	4028	4006	81
8	2	2	4151	3977	92
10	2	2	1879	1893	118
12	2	2	1412	1426	150
14	2	2	2598	2475	146
16	2	2	2520	2514	143
18	2	2	853	866	-289
20	2	2	422	139	-392

H	K	L	$10F_o$	$10F_c$	10σ
22	2	2	195	210	-495
24	2	2	229	61	-579
26	2	2	251	105	-635
28	2	2	309	275	-780
30	2	2	715	727	-573
32	2	2	351	740	-890
-31	3	2	301	363	-761
-29	3	2	557	104	-589
-27	3	2	280	390	-709
-23	3	2	364	213	-313
-21	3	2	511	115	-299
-19	3	2	207	219	-521
-17	3	2	1421	1151	148
-15	3	2	1784	1872	127
-13	3	2	1477	1617	146
-11	3	2	722	934	-190
-9	3	2	1062	1136	108
-7	3	2	1799	1701	95
-5	3	2	1647	1536	78
-3	3	2	1024	920	84
-1	3	2	169	460	-428
1	3	2	2348	2316	71
3	3	2	2220	2161	80
5	3	2	751	705	132
7	3	2	694	710	-194
9	3	2	2457	2431	108
11	3	2	1786	1761	129
13	3	2	1750	1751	152
15	3	2	621	747	-349
17	3	2	215	61	-543
19	3	2	234	263	-591
21	3	2	182	524	-460
23	3	2	429	351	-431
25	3	2	262	296	-663
27	3	2	299	374	-758
29	3	2	588	270	-575
31	3	2	344	167	-873
-30	4	2	743	582	-486
-28	4	2	506	96	-500
-26	4	2	783	735	-399
-24	4	2	225	406	-570
-22	4	2	634	739	-289
-20	4	2	1180	1137	184
-18	4	2	209	227	-528
-16	4	2	1602	1757	165
-14	4	2	1418	1431	167
-12	4	2	665	861	-203
-10	4	2	2275	2255	104
-8	4	2	167	132	-423
-6	4	2	2894	2789	87
-4	4	2	3249	3226	82
-2	4	2	552	674	-200
0	4	2	3238	3192	79
2	4	2	3113	3056	83
4	4	2	1939	1912	100
6	4	2	3093	2974	96
8	4	2	290	232	-269
10	4	2	2576	2519	130
12	4	2	1334	1560	186
14	4	2	780	878	-296
16	4	2	1654	1687	222
18	4	2	553	549	-278
20	4	2	1230	1262	249
22	4	2	652	977	-305
24	4	2	232	331	-587
26	4	2	670	1025	-514
28	4	2	555	410	-604
30	4	2	270	366	-682
-29	5	2	362	405	-918
-27	5	2	745	573	-448
-25	5	2	1188	689	-362
-23	5	2	438	592	-362
-21	5	2	2141	2044	165
-19	5	2	1744	1700	191
-17	5	2	607	514	-202
-15	5	2	1816	1762	143
-13	5	2	562	462	-238
-11	5	2	3736	3729	105
-9	5	2	3404	3313	98
-7	5	2	449	617	-255
-5	5	2	3015	3076	96
-3	5	2	1024	970	109
-1	5	2	2465	2497	94
1	5	2	2606	2559	90
3	5	2	1479	1529	118
5	5	2	4899	4874	94
7	5	2	2721	2763	110
9	5	2	1433	1275	134
11	5	2	1680	1747	146
13	5	2	882	692	210
15	5	2	2856	2815	155
17	5	2	1939	2123	174
19	5	2	305	190	-379
21	5	2	864	1245	-343
23	5	2	262	227	-664
27	5	2	387	743	-981

Table 71. (continued)

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
29	5	2	697	286	-489	9	7	2	1604	1468	156
-28	6	2	313	47	-793	11	7	2	999	971	-292
-26	6	2	308	605	-779	13	7	2	1872	1950	172
-24	6	2	575	56	-401	15	7	2	2290	2263	205
-22	6	2	1668	1488	183	17	7	2	1348	1510	293
-20	6	2	2284	2294	178	19	7	2	423	243	-380
-18	6	2	1270	1245	255	21	7	2	265	385	-671
-16	6	2	292	366	-316	23	7	2	587	36	-612
-14	6	2	368	268	-229	25	7	2	598	406	-505
-12	6	2	2487	2407	120	-24	8	2	280	256	-706
-10	6	2	4278	4020	105	-22	8	2	322	492	-815
-8	6	2	2231	2300	117	-20	8	2	475	846	-540
-6	6	2	830	983	173	-18	8	2	1006	1324	-333
-4	6	2	1522	1507	120	-16	8	2	1590	1608	183
-2	6	2	445	332	-241	-14	8	2	1476	1614	191
0	6	2	2164	2178	105	-12	8	2	1754	1696	188
2	6	2	180	111	-455	-10	8	2	1505	1672	167
4	6	2	3509	3548	107	-8	8	2	1085	1083	196
6	6	2	4746	4631	108	-6	8	2	1028	749	190
8	6	2	1809	1856	136	-4	8	2	200	439	-509
10	6	2	222	592	-562	-2	8	2	176	41	-445
12	6	2	200	159	-507	0	8	2	504	549	-253
14	6	2	2290	2205	152	2	8	2	1061	1087	221
16	6	2	2756	2863	164	4	8	2	1371	1417	168
18	6	2	802	1200	-403	6	8	2	1370	1534	176
20	6	2	466	519	-377	8	8	2	1848	1708	177
22	6	2	921	653	-389	10	8	2	1989	1857	170
24	6	2	775	433	-412	12	8	2	2227	1977	189
26	6	2	917	760	-487	14	8	2	1768	1681	192
28	6	2	301	58	-763	16	8	2	616	1060	-410
-27	7	2	311	144	-788	18	8	2	682	548	-368
-25	7	2	295	106	-747	20	8	2	628	292	-447
-23	7	2	305	610	-772	22	8	2	349	151	-884
-21	7	2	1339	1384	291	24	8	2	373	11	-944
-19	7	2	1830	1567	175	-21	9	2	640	24	-552
-17	7	2	943	1118	-252	-19	9	2	272	461	-691
-15	7	2	814	846	-317	-17	9	2	1293	1469	-367
-13	7	2	1747	1673	164	-15	9	2	1666	1854	245
-11	7	2	2808	2856	133	-13	9	2	997	1297	238
-9	7	2	2465	2344	120	-11	9	2	251	538	-635
-7	7	2	353	525	-342	-9	9	2	187	430	-473
-5	7	2	522	383	-244	-7	9	2	1095	1147	194
-3	7	2	175	56	-444	-5	9	2	1642	1581	177
-1	7	2	769	822	-223	-3	9	2	457	574	-366
1	7	2	194	233	-493	-1	9	2	1049	1204	204
3	7	2	1657	1706	146	1	9	2	1681	1699	152
5	7	2	3402	3245	114	3	9	2	740	859	-301
7	7	2	2700	2630	139	5	9	2	201	64	-510

Table 71. (continued)

H	K	L	$10F_o$	$10F_c$	10σ
7	9	2	669	670	-249
9	9	2	2122	1878	176
11	9	2	2301	2278	176
13	9	2	1015	1343	-392
15	9	2	620	298	-499
17	9	2	341	109	-864
19	9	2	354	562	-898
21	9	2	322	650	-815
-18	10	2	832	594	-427
-16	10	2	1324	1586	-353
-14	10	2	1300	1363	307
-12	10	2	603	152	-362
-10	10	2	273	515	-692
-8	10	2	285	343	-722
-6	10	2	1769	1722	195
-4	10	2	1503	1608	168
-2	10	2	205	273	-520
0	10	2	1987	1842	187
2	10	2	1280	1292	262
4	10	2	232	151	-416
6	10	2	290	362	-735
8	10	2	351	870	-889
10	10	2	2126	1935	280
12	10	2	1244	1409	-410
14	10	2	318	105	-805
16	10	2	297	461	-751
18	10	2	307	95	-777
-13	11	2	297	452	-753
-11	11	2	321	474	-812
-9	11	2	241	414	-608
-7	11	2	509	709	-552
-5	11	2	939	1467	-459
-3	11	2	271	649	-686
-1	11	2	684	953	-477
1	11	2	845	1358	-417
3	11	2	331	204	-839
5	11	2	766	674	-407
7	11	2	810	147	-368
9	11	2	1131	1066	-422
11	11	2	1662	1345	263
13	11	2	322	329	-815
-4	12	2	478	596	-496
-2	12	2	246	204	-621
0	12	2	793	740	-433
2	12	2	274	286	-693
4	12	2	522	450	-486
-33	1	3	328	194	-830
-29	1	3	340	493	-861
-27	1	3	215	85	-547
-25	1	3	223	332	-563
-23	1	3	630	849	-298
-21	1	3	1784	1837	180
-19	1	3	1436	1708	183
-17	1	3	395	200	-293
-15	1	3	919	817	201
-13	1	3	738	743	-216
-11	1	3	2921	2858	97
-9	1	3	2188	2185	92
-7	1	3	1324	1319	100
-5	1	3	3288	3201	68
-3	1	3	2626	2617	59
-1	1	3	1337	1390	68
1	1	3	1165	1103	92
3	1	3	3313	3250	69
5	1	3	4428	4493	76
7	1	3	1562	1648	110
9	1	3	1103	1125	168
11	1	3	1576	1708	150
13	1	3	807	873	195
15	1	3	1663	1702	168
17	1	3	1474	1388	168
19	1	3	689	657	-286
21	1	3	1267	1235	214
23	1	3	271	697	-687
25	1	3	250	116	-636
27	1	3	395	43	-366
29	1	3	655	495	-502
31	1	3	548	708	-624
-32	2	3	344	739	-871
-28	2	3	328	260	-831
-26	2	3	514	430	-418
-24	2	3	579	368	-364
-22	2	3	2725	2582	157
-20	2	3	3449	3385	144
-18	2	3	1553	1489	146
-16	2	3	544	765	-336
-14	2	3	494	678	-273
-12	2	3	2813	2920	102
-10	2	3	3564	3597	86
-8	2	3	567	811	-157
-6	2	3	5028	4894	70
-4	2	3	6069	6166	62
-2	2	3	1502	1505	81
0	2	3	1967	2042	71
2	2	3	1205	1238	91
4	2	3	5505	5592	70

Table 71. (continued)

H	K	L	$10F_o$	$10F_c$	10σ
6	2	3	6665	6875	80
8	2	3	2454	2576	100
10	2	3	1207	1346	182
12	2	3	968	1011	-253
14	2	3	1640	1746	167
16	2	3	2260	2438	169
18	2	3	236	344	-598
20	2	3	2129	2046	165
22	2	3	2259	2105	189
24	2	3	260	452	-659
26	2	3	243	270	-616
28	2	3	300	186	-763
32	2	3	1042	984	-457
-31	3	3	395	1080	****
-29	3	3	682	959	-526
-27	3	3	276	24	-700
-25	3	3	231	172	-584
-23	3	3	1475	1567	189
-21	3	3	3729	3571	142
-19	3	3	3145	3209	131
-17	3	3	535	629	-310
-15	3	3	388	772	-310
-13	3	3	598	856	-328
-11	3	3	3308	3252	96
-9	3	3	2118	1978	91
-7	3	3	2713	2792	86
-5	3	3	6612	6611	72
-3	3	3	4084	4064	71
-1	3	3	952	846	97
1	3	3	743	643	99
3	3	3	5156	5101	73
5	3	3	7762	8091	79
7	3	3	6035	6220	89
9	3	3	337	562	-312
11	3	3	1254	1282	154
13	3	3	499	456	-283
15	3	3	2308	2465	169
17	3	3	1529	1318	225
19	3	3	1619	1521	217
21	3	3	2910	2776	167
23	3	3	1391	1544	312
25	3	3	655	49	-309
27	3	3	585	37	-540
29	3	3	674	886	-576
31	3	3	1079	1299	-482
-30	4	3	335	981	-848
-28	4	3	566	743	-530
-26	4	3	243	243	-615
-24	4	3	543	761	-370
-22	4	3	2404	2291	175
-20	4	3	3205	2956	143
-18	4	3	1436	1650	173
-16	4	3	217	199	-551
-14	4	3	355	151	-336
-12	4	3	1873	1831	118
-10	4	3	2979	2852	99
-8	4	3	167	15	-424
-6	4	3	4180	4101	83
-4	4	3	5621	5500	80
-2	4	3	2443	2474	81
0	4	3	1070	1049	108
2	4	3	3328	3263	83
4	4	3	6452	6374	85
6	4	3	5693	5658	91
8	4	3	2440	2293	108
10	4	3	328	316	-368
12	4	3	462	43	-301
14	4	3	1630	1685	160
16	4	3	1604	1594	181
18	4	3	236	427	-595
20	4	3	2313	2215	200
22	4	3	2139	2064	226
24	4	3	696	924	-364
28	4	3	348	639	-880
30	4	3	1217	1077	-531
-29	5	3	345	581	-873
-27	5	3	340	660	-861
-25	5	3	611	801	-491
-23	5	3	907	1238	-390
-21	5	3	1856	1811	169
-19	5	3	1735	1567	174
-17	5	3	1151	1006	195
-15	5	3	470	613	-278
-13	5	3	809	804	189
-11	5	3	984	940	134
-9	5	3	921	837	175
-7	5	3	895	997	166
-5	5	3	2998	2967	91
-3	5	3	3311	3298	90
-1	5	3	2624	2546	90
1	5	3	2526	2553	99
3	5	3	3413	3466	93
5	5	3	3995	4034	99
7	5	3	2915	2901	108
9	5	3	1530	1670	152
11	5	3	798	624	-230

Table 71. (continued)

H	K	L	$10F_o$	$10F_c$	10σ
13	5	3	530	510	-292
15	5	3	179	637	-454
17	5	3	226	118	-571
19	5	3	684	988	-372
21	5	3	961	1425	-388
23	5	3	1221	1225	277
25	5	3	646	798	-450
27	5	3	340	658	-863
29	5	3	750	713	-501
-28	6	3	306	446	-775
-26	6	3	804	824	-461
-24	6	3	625	834	-508
-22	6	3	564	563	-362
-20	6	3	647	668	-332
-18	6	3	944	1264	-274
-16	6	3	2117	1981	159
-14	6	3	1398	1463	159
-12	6	3	187	388	-474
-10	6	3	1275	1225	138
-8	6	3	507	582	-289
-6	6	3	177	36	-448
-4	6	3	383	267	-217
-2	6	3	1774	1795	122
0	6	3	2828	2912	105
2	6	3	2636	2743	119
4	6	3	1909	1797	124
6	6	3	1286	1241	164
8	6	3	1829	1795	134
10	6	3	2021	1961	139
12	6	3	1334	992	216
14	6	3	756	341	-223
16	6	3	814	912	-268
18	6	3	856	796	-336
20	6	3	239	285	-605
22	6	3	362	343	-382
24	6	3	588	730	-456
26	6	3	814	873	-521
28	6	3	993	717	-431
-27	7	3	374	617	-945
-25	7	3	748	863	-481
-23	7	3	589	259	-469
-21	7	3	257	450	-648
-19	7	3	208	56	-526
-17	7	3	1339	1436	230
-15	7	3	2183	2286	159
-11	7	3	1081	1215	198
-9	7	3	1329	1327	174
-7	7	3	197	434	-499
-5	7	3	1268	1365	177
-3	7	3	220	196	-558
-1	7	3	2196	2308	128
1	7	3	2877	2910	114
3	7	3	979	1057	225
5	7	3	957	938	198
7	7	3	393	486	-328
9	7	3	1536	1440	190
11	7	3	1789	1919	160
13	7	3	222	371	-561
15	7	3	910	1217	-388
17	7	3	1191	1249	225
19	7	3	264	28	-669
21	7	3	303	602	-766
23	7	3	596	13	-510
25	7	3	936	819	-439
-24	8	3	440	426	-502
-22	8	3	314	538	-795
-20	8	3	956	1059	-407
-18	8	3	233	11	-591
-16	8	3	1463	1604	220
-14	8	3	1234	1536	209
-12	8	3	230	314	-582
-10	8	3	1337	1427	195
-8	8	3	222	178	-562
-6	8	3	1713	1712	140
-4	8	3	1433	1622	173
-2	8	3	541	626	-266
0	8	3	2159	2352	135
2	8	3	1226	1242	177
4	8	3	1471	1543	150
6	8	3	2221	2176	144
8	8	3	196	260	-496
10	8	3	1795	1552	192
12	8	3	1006	1035	-260
16	8	3	1772	1417	258
18	8	3	693	333	-413
20	8	3	742	841	-498
22	8	3	306	668	-774
-21	9	3	1214	983	-394
-19	9	3	758	841	-471
-17	9	3	256	359	-648
-15	9	3	906	1086	-376
-13	9	3	226	231	-407
-11	9	3	791	1086	-283
-9	9	3	918	899	230
-7	9	3	352	801	-364
-5	9	3	1823	1971	161

Table 71. (continued)

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
-3	9	3	1143	1160	195	2	12	3	1083	1158	-353
-1	9	3	616	484	-237	-32	0	4	1340	1258	-408
1	9	3	643	904	-311	-30	0	4	1637	1871	319
3	9	3	375	805	-387	-28	0	4	932	1162	-397
5	9	3	2100	2173	191	-26	0	4	230	122	-582
7	9	3	1076	1359	243	-24	0	4	267	167	-675
9	9	3	227	327	-574	-22	0	4	2146	1973	197
11	9	3	573	842	-377	-20	0	4	2856	3002	145
13	9	3	280	51	-709	-18	0	4	468	267	-287
15	9	3	1268	1067	308	-16	0	4	2875	2824	130
17	9	3	729	738	-484	-14	0	4	4161	4228	111
21	9	3	761	785	-436	-12	0	4	681	680	-205
-18	10	3	1023	588	-379	-10	0	4	2165	2063	102
-16	10	3	286	41	-724	-8	0	4	1646	1748	103
-14	10	3	316	40	-802	-6	0	4	8013	8135	71
-12	10	3	681	356	-405	-4	0	4	10885	11246	28
-10	10	3	287	567	-726	-2	0	4	6929	6902	57
-8	10	3	248	13	-628	0	0	4	2193	2081	65
-6	10	3	825	901	-360	2	0	4	786	676	155
-4	10	3	1184	1279	171	4	0	4	4760	4635	78
-2	10	3	719	914	-386	6	0	4	4991	5063	90
0	10	3	261	339	-470	8	0	4	896	895	191
2	10	3	994	584	-279	10	0	4	4714	4953	109
4	10	3	1600	1349	203	12	0	4	4015	4196	118
6	10	3	1246	1361	273	14	0	4	239	390	-605
8	10	3	556	562	-551	16	0	4	527	676	-364
10	10	3	532	19	-486	18	0	4	1458	1409	203
12	10	3	802	47	-390	20	0	4	3399	3296	168
14	10	3	640	493	-444	22	0	4	3424	3426	183
16	10	3	341	610	-862	24	0	4	1457	1296	280
18	10	3	294	129	-745	26	0	4	722	174	-347
-13	11	3	684	374	-435	28	0	4	296	101	-750
-11	11	3	272	45	-689	30	0	4	1108	921	-346
-9	11	3	529	251	-453	32	0	4	1104	806	-409
-7	11	3	309	209	-780	-31	1	4	592	1427	-714
-5	11	3	541	331	-464	-29	1	4	987	1354	-397
-3	11	3	571	779	-499	-27	1	4	250	435	-634
-1	11	3	911	1127	-359	-25	1	4	224	166	-566
1	11	3	337	1124	-854	-23	1	4	777	1014	-351
3	11	3	519	933	-498	-21	1	4	2459	2494	164
5	11	3	736	701	-485	-19	1	4	1700	1873	186
7	11	3	335	551	-848	-17	1	4	821	820	-297
9	11	3	508	700	-500	-15	1	4	3249	3239	112
11	11	3	329	736	-835	-13	1	4	2472	2330	121
13	11	3	358	459	-906	-11	1	4	150	129	-379
-4	12	3	269	21	-681	-9	1	4	181	246	-458
-2	12	3	925	823	-416	-7	1	4	5457	5627	74
0	12	3	1349	1372	-343	-5	1	4	8724	8974	12

Table 71. (continued)

H	K	L	$10F_o$	$10F_c$	10σ
-3	1	4	7193	7238	59
-1	1	4	1929	1888	66
1	1	4	764	698	102
3	1	4	2668	2621	71
5	1	4	5599	5547	77
7	1	4	4431	4355	90
9	1	4	1908	1862	115
11	1	4	4784	4803	109
13	1	4	2449	2345	146
15	1	4	229	70	-582
17	1	4	527	454	-298
19	1	4	2267	2259	187
21	1	4	3319	3198	161
23	1	4	2366	2147	183
27	1	4	300	216	-761
29	1	4	349	483	-883
31	1	4	1131	836	-409
-32	2	4	847	590	-463
-30	2	4	549	854	-598
-28	2	4	544	676	-548
-26	2	4	252	320	-638
-24	2	4	566	489	-310
-22	2	4	1151	1372	263
-20	2	4	1542	1522	163
-18	2	4	244	726	-617
-16	2	4	503	890	-392
-14	2	4	1534	1709	140
-12	2	4	1498	1633	141
-10	2	4	807	866	141
-8	2	4	1940	1963	88
-6	2	4	4225	4211	74
-4	2	4	4397	4480	68
-2	2	4	2673	2695	66
0	2	4	661	712	132
2	2	4	173	390	-436
4	2	4	1643	1779	92
6	2	4	3833	3680	87
8	2	4	1370	1205	141
10	2	4	1924	1914	127
12	2	4	2567	2572	130
14	2	4	1051	1120	215
16	2	4	843	883	-302
18	2	4	1317	1324	269
20	2	4	1798	1904	204
22	2	4	1566	1693	243
24	2	4	695	871	-300
26	2	4	465	63	-412
28	2	4	523	112	-491
30	2	4	320	417	-809
-31	3	4	349	49	-885
-29	3	4	335	356	-850
-27	3	4	920	558	-353
-25	3	4	570	721	-347
-23	3	4	454	612	-364
-21	3	4	201	398	-509
-19	3	4	498	174	-247
-17	3	4	190	193	-483
-15	3	4	294	311	-324
-13	3	4	464	592	-271
-11	3	4	848	943	156
-9	3	4	1813	1657	103
-7	3	4	903	894	124
-5	3	4	851	919	117
-3	3	4	270	213	-238
-1	3	4	1434	1455	85
1	3	4	2681	2665	78
3	3	4	731	770	135
5	3	4	408	178	-192
7	3	4	829	800	140
9	3	4	451	397	-274
11	3	4	187	54	-474
13	3	4	382	155	-342
15	3	4	1347	1262	204
17	3	4	1553	1635	233
19	3	4	725	947	-288
21	3	4	228	177	-577
23	3	4	563	302	-333
25	3	4	558	472	-388
27	3	4	365	389	-925
29	3	4	298	120	-755
31	3	4	361	126	-916
-30	4	4	322	494	-814
-28	4	4	517	159	-417
-26	4	4	874	825	-408
-24	4	4	255	681	-646
-22	4	4	182	395	-460
-20	4	4	1163	1218	210
-18	4	4	140	110	-355
-16	4	4	1606	1634	147
-14	4	4	1687	1832	154
-12	4	4	521	449	-245
-10	4	4	2155	2101	105
-8	4	4	740	609	153
-6	4	4	1590	1517	97
-4	4	4	2729	2700	89
-2	4	4	167	81	-422

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
0	4	4	2667	2640	86	-22	6	4	1182	1081	297
2	4	4	1604	1513	112	-20	6	4	1564	1655	231
4	4	4	2084	2081	98	-18	6	4	223	362	-566
6	4	4	2659	2608	97	-16	6	4	1937	1964	155
8	4	4	570	462	-208	-14	6	4	2203	2155	144
10	4	4	1609	1490	138	-12	6	4	158	112	-400
12	4	4	1514	1481	180	-10	6	4	981	992	195
14	4	4	776	733	-274	-8	6	4	859	775	160
16	4	4	1635	1705	173	-6	6	4	3794	3777	109
18	4	4	557	689	-328	-4	6	4	4393	4296	102
22	4	4	637	950	-365	-2	6	4	1615	1537	115
24	4	4	247	182	-626	0	6	4	1618	1538	111
26	4	4	966	671	-450	2	6	4	504	588	-212
28	4	4	330	215	-836	4	6	4	2395	2493	131
30	4	4	324	386	-819	6	6	4	3035	3136	119
-29	5	4	357	609	-903	8	6	4	494	338	-297
-27	5	4	466	328	-437	10	6	4	2194	2227	155
-25	5	4	292	741	-740	12	6	4	2004	2041	157
-23	5	4	223	174	-565	14	6	4	189	181	-480
-21	5	4	1533	1596	219	16	6	4	409	779	-494
-19	5	4	1258	1361	195	18	6	4	264	525	-668
-17	5	4	1047	1023	179	20	6	4	1893	2051	252
-15	5	4	2896	2745	127	22	6	4	1650	1871	400
-13	5	4	1304	1299	151	24	6	4	324	490	-819
-11	5	4	1441	1409	130	26	6	4	497	301	-597
-9	5	4	1275	1289	156	-25	7	4	1021	216	-380
-7	5	4	1534	1701	117	-23	7	4	700	502	-429
-5	5	4	4164	4135	92	-21	7	4	1129	1050	-416
-3	5	4	2798	2773	99	-19	7	4	744	912	-370
-1	5	4	1164	1122	116	-17	7	4	195	414	-491
1	5	4	2494	2532	94	-15	7	4	1527	1488	158
3	5	4	919	1044	160	-13	7	4	1192	1131	184
5	5	4	3768	3735	103	-11	7	4	322	291	-338
7	5	4	2443	2269	113	-7	7	4	1976	2023	130
9	5	4	1390	1216	144	-5	7	4	3349	3347	118
11	5	4	2761	2790	133	-3	7	4	2936	2882	116
13	5	4	917	1045	-265	-1	7	4	1131	1126	174
15	5	4	900	1117	-312	1	7	4	307	237	-349
17	5	4	1070	1075	243	3	7	4	761	1018	188
19	5	4	657	952	-321	5	7	4	1907	2070	146
21	5	4	2187	1941	219	7	7	4	957	1013	217
23	5	4	934	976	-268	9	7	4	440	800	-350
25	5	4	300	357	-761	11	7	4	1644	1467	180
27	5	4	814	453	-449	13	7	4	878	985	-341
29	5	4	644	231	-505	15	7	4	212	283	-538
-28	6	4	298	396	-753	17	7	4	207	560	-524
-26	6	4	353	231	-896	19	7	4	1346	1490	292
-24	6	4	300	40	-761	21	7	4	1493	1725	-406

Table 71. (continued)

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
23	7	4	964	981	-416	-16	10	4	840	844	-400
25	7	4	349	255	-883	-14	10	4	427	572	-536
-24	8	4	790	520	-409	-12	10	4	573	783	-477
-22	8	4	791	444	-400	-10	10	4	1770	1875	243
-20	8	4	268	458	-678	-8	10	4	1205	1370	-387
-18	8	4	291	234	-738	-6	10	4	224	10	-566
-16	8	4	392	320	-308	-4	10	4	547	49	-362
-14	8	4	225	556	-567	-2	10	4	1355	1357	288
-12	8	4	373	715	-295	0	10	4	2288	2264	126
-10	8	4	1280	1271	219	2	10	4	1182	1398	-319
-8	8	4	1478	1727	162	4	10	4	302	239	-765
-6	8	4	1881	1965	150	6	10	4	784	965	-420
-4	8	4	1978	1965	153	8	10	4	248	110	-630
-2	8	4	1849	1927	148	10	10	4	873	822	-412
0	8	4	1666	1782	149	12	10	4	321	430	-814
2	8	4	1746	1632	132	14	10	4	378	896	-959
4	8	4	1254	1281	229	16	10	4	687	1531	-692
8	8	4	183	381	-464	-13	11	4	248	124	-629
10	8	4	779	600	-338	-11	11	4	775	1096	-484
12	8	4	261	626	-660	-9	11	4	582	1312	-468
14	8	4	659	892	-328	-7	11	4	270	179	-686
16	8	4	1189	1088	-393	-5	11	4	966	751	-305
18	8	4	520	1131	-599	-3	11	4	284	59	-720
20	8	4	628	1011	-542	-1	11	4	1109	1203	-369
22	8	4	329	704	-836	1	11	4	784	1342	-557
-21	9	4	297	86	-752	5	11	4	352	808	-891
-19	9	4	665	37	-401	7	11	4	291	536	-737
-17	9	4	680	325	-389	9	11	4	319	494	-806
-15	9	4	281	411	-712	11	11	4	943	735	-470
-13	9	4	290	229	-734	-31	1	5	850	814	-352
-11	9	4	1509	1407	193	-29	1	5	258	487	-652
-9	9	4	1663	1878	188	-27	1	5	836	409	-305
-7	9	4	1020	1187	240	-25	1	5	512	977	-387
-5	9	4	231	656	-584	-23	1	5	201	324	-508
-3	9	4	1333	1386	174	-21	1	5	792	683	-284
-1	9	4	2321	2404	152	-19	1	5	639	321	-273
1	9	4	2229	2298	166	-17	1	5	1264	1375	186
3	9	4	413	1019	-360	-15	1	5	2559	2641	123
5	9	4	204	208	-515	-13	1	5	1505	1589	138
7	9	4	211	496	-535	-11	1	5	165	311	-418
9	9	4	210	43	-532	-9	1	5	162	156	-408
11	9	4	266	243	-476	-7	1	5	2092	2150	84
13	9	4	885	519	-384	-5	1	5	3969	3988	71
15	9	4	1483	1345	300	-3	1	5	241	335	-252
17	9	4	1049	1305	-491	-1	1	5	1662	1570	74
19	9	4	365	686	-925	1	1	5	3370	3292	70
21	9	4	313	252	-794	3	1	5	143	95	-364
-18	10	4	273	181	-693	5	1	5	1325	1321	120

Table 71. (continued)

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
9	1	5	2146	2072	122	-21	3	5	581	878	-312
11	1	5	3187	3103	115	-19	3	5	207	98	-525
13	1	5	1573	1772	166	-17	3	5	2704	2645	136
15	1	5	356	250	-449	-15	3	5	4962	4877	111
17	1	5	270	286	-683	-13	3	5	3694	3563	104
19	1	5	971	1108	-273	-11	3	5	260	374	-322
21	1	5	984	1185	-297	-9	3	5	163	230	-411
23	1	5	259	391	-655	-7	3	5	3572	3538	87
27	1	5	326	574	-826	-5	3	5	6320	6431	79
29	1	5	329	39	-832	-3	3	5	3367	3376	80
31	1	5	329	242	-834	-1	3	5	1197	1291	107
-32	2	5	831	830	-435	1	3	5	3538	3508	81
-30	2	5	1103	1067	-396	3	3	5	1047	1073	114
-28	2	5	312	200	-789	5	3	5	1369	1360	120
-26	2	5	603	997	-382	7	3	5	159	475	-403
-24	2	5	867	878	-299	9	3	5	4243	4283	107
-22	2	5	200	328	-507	11	3	5	5784	5899	113
-20	2	5	844	887	-288	13	3	5	3214	3064	130
-18	2	5	1070	1043	221	15	3	5	215	185	-545
-16	2	5	3920	3854	116	17	3	5	211	104	-534
-14	2	5	3917	3909	109	19	3	5	2056	1897	202
-12	2	5	1333	1541	144	21	3	5	2398	2397	192
-10	2	5	1634	1512	108	23	3	5	1160	1089	260
-8	2	5	1006	1141	141	25	3	5	696	572	-252
-6	2	5	4795	4883	77	27	3	5	743	908	-436
-4	2	5	5175	5141	73	29	3	5	675	183	-495
-2	2	5	386	400	-228	-30	4	5	680	1025	-573
0	2	5	3635	3589	72	-28	4	5	327	382	-828
2	2	5	2695	2666	76	-26	4	5	270	550	-684
4	2	5	343	484	-221	-24	4	5	693	605	-342
6	2	5	1721	1865	108	-22	4	5	200	291	-509
8	2	5	2513	2479	114	-20	4	5	607	521	-283
10	2	5	5185	5160	106	-18	4	5	1197	995	212
12	2	5	4880	4830	117	-16	4	5	3326	3261	125
14	2	5	994	1078	238	-14	4	5	4211	4199	112
16	2	5	863	582	206	-12	4	5	2297	2399	117
18	2	5	1096	830	212	-10	4	5	679	968	-185
20	2	5	2258	2249	171	-8	4	5	2145	2084	112
22	2	5	1678	1861	270	-6	4	5	4766	4725	89
24	2	5	246	93	-626	-4	4	5	4016	4128	87
26	2	5	671	1043	-507	-2	4	5	697	832	169
28	2	5	291	623	-737	0	4	5	1805	1709	94
30	2	5	695	173	-475	2	4	5	1764	1637	97
-31	3	5	1243	1214	-384	4	4	5	156	17	-395
-29	3	5	855	932	-445	6	4	5	169	46	-425
-27	3	5	496	387	-589	8	4	5	1859	1974	141
-25	3	5	317	1131	-804	10	4	5	4538	4429	112
-23	3	5	233	377	-589	12	4	5	3681	3713	127

H	K	L	$10F_o$	$10F_c$	10σ
14	4	5	1584	1629	168
16	4	5	549	517	-335
18	4	5	690	1201	-357
20	4	5	1897	1902	196
22	4	5	670	1441	-419
24	4	5	261	172	-470
26	4	5	770	587	-432
28	4	5	679	456	-512
-29	5	5	975	523	-422
-27	5	5	316	318	-801
-25	5	5	239	24	-606
-23	5	5	405	61	-314
-21	5	5	225	261	-569
-19	5	5	597	524	-280
-17	5	5	1261	1263	171
-15	5	5	2137	2091	132
-13	5	5	2575	2674	126
-11	5	5	2391	2269	116
-9	5	5	2177	2134	127
-7	5	5	2886	2774	108
-5	5	5	2568	2534	101
-3	5	5	2100	1949	103
-1	5	5	467	152	-200
1	5	5	152	208	-386
3	5	5	947	976	188
5	5	5	864	984	195
7	5	5	1063	1165	188
9	5	5	2162	2208	133
11	5	5	2410	2499	137
13	5	5	1726	1977	176
15	5	5	791	1265	-393
17	5	5	1000	1215	250
19	5	5	1099	1204	-353
21	5	5	614	1063	-388
23	5	5	731	432	-396
25	5	5	244	103	-617
27	5	5	321	320	-813
-28	6	5	693	466	-552
-26	6	5	354	628	-898
-24	6	5	298	257	-756
-22	6	5	754	527	-359
-20	6	5	820	1043	-278
-18	6	5	703	588	-288
-16	6	5	177	126	-447
-14	6	5	818	877	-264
-12	6	5	1854	2045	143
-10	6	5	2736	2702	122
-8	6	5	1895	1940	130
-6	6	5	889	824	165
-4	6	5	406	411	-271
-2	6	5	1050	1080	182
0	6	5	1420	1498	131
2	6	5	208	161	-525
4	6	5	1578	1707	164
6	6	5	2156	2122	126
8	6	5	821	1073	-289
10	6	5	216	703	-547
12	6	5	737	839	-311
14	6	5	1506	1564	213
16	6	5	2094	1868	167
18	6	5	687	1089	-360
20	6	5	249	241	-631
22	6	5	290	171	-735
24	6	5	304	8	-773
26	6	5	333	140	-842
-25	7	5	928	858	-435
-23	7	5	573	77	-434
-21	7	5	614	1004	-529
-19	7	5	1140	1015	-405
-17	7	5	456	228	-330
-15	7	5	486	771	-367
-13	7	5	192	441	-484
-11	7	5	2107	2128	143
-9	7	5	2400	2216	136
-7	7	5	316	255	-342
-5	7	5	1301	1445	155
-3	7	5	556	684	-287
-1	7	5	1660	1737	150
1	7	5	2168	2246	131
3	7	5	438	157	-280
5	7	5	2436	2484	140
7	7	5	1923	1968	151
9	7	5	196	134	-496
11	7	5	834	650	-256
13	7	5	415	409	-380
15	7	5	1946	1781	183
17	7	5	1861	1512	224
19	7	5	286	45	-724
21	7	5	828	852	-475
23	7	5	342	444	-866
25	7	5	288	282	-730
-24	8	5	339	666	-860
-22	8	5	295	413	-749
-20	8	5	996	1048	-382
-18	8	5	276	165	-698
-16	8	5	918	1210	228

Table 71. (continued)

H	K	L	$10F_O$	$10F_C$	10σ
-14	8	5	816	1178	-322
-12	8	5	395	567	-317
-10	8	5	1561	1703	168
-8	8	5	613	807	-260
-6	8	5	1070	1356	199
-4	8	5	1766	1893	140
-2	8	5	199	162	-505
0	8	5	2009	2121	153
4	8	5	1142	1289	216
6	8	5	2215	2014	160
8	8	5	259	537	-657
10	8	5	823	1178	-322
12	8	5	645	887	-371
14	8	5	551	602	-339
16	8	5	1399	1303	334
18	8	5	500	361	-527
20	8	5	364	859	-920
22	8	5	639	856	-589
-21	9	5	469	460	-537
-19	9	5	330	302	-836
-17	9	5	310	777	-784
-15	9	5	1733	1502	292
-13	9	5	298	839	-753
-11	9	5	336	439	-303
-9	9	5	589	631	-273
-7	9	5	224	570	-567
-5	9	5	1584	1609	195
-3	9	5	801	956	-269
-1	9	5	806	930	-256
1	9	5	1228	1267	197
3	9	5	237	113	-597
5	9	5	1244	1218	210
7	9	5	233	642	-591
9	9	5	895	921	-312
11	9	5	1306	1507	-350
13	9	5	304	635	-771
15	9	5	306	421	-774
17	9	5	329	368	-832
19	9	5	577	507	-555
-16	10	5	666	825	-490
-14	10	5	561	975	-482
-12	10	5	576	616	-371
-10	10	5	279	271	-707
-8	10	5	909	407	-301
-6	10	5	585	886	-406
-4	10	5	532	994	-419
-2	10	5	252	255	-640
0	10	5	499	476	-458
2	10	5	748	354	-316
4	10	5	269	63	-682
6	10	5	252	37	-639
8	10	5	501	540	-543
10	10	5	751	1112	-535
12	10	5	1031	1035	-371
14	10	5	283	517	-716
16	10	5	338	246	-856
-11	11	5	367	912	-928
-9	11	5	561	816	-593
-7	11	5	662	527	-390
-5	11	5	280	415	-711
-3	11	5	632	444	-468
-1	11	5	258	439	-651
1	11	5	282	206	-715
3	11	5	320	254	-810
5	11	5	967	751	-411
7	11	5	1085	863	-307
9	11	5	941	710	-393
11	11	5	322	636	-815
-32	0	6	1032	576	-364
-30	0	6	337	713	-856
-28	0	6	316	445	-798
-26	0	6	2252	2071	218
-24	0	6	1921	1973	234
-22	0	6	538	506	-366
-20	0	6	199	166	-505
-18	0	6	1654	1660	192
-16	0	6	4704	4771	124
-14	0	6	4821	5058	115
-12	0	6	1478	1431	133
-10	0	6	1886	1849	124
-8	0	6	1435	1403	116
-6	0	6	2675	2631	86
-4	0	6	1183	1175	109
-2	0	6	2966	2820	73
0	0	6	7965	8021	69
2	0	6	5653	5642	73
4	0	6	1599	1614	104
6	0	6	1137	1215	168
8	0	6	2841	2764	119
10	0	6	5878	6138	116
12	0	6	4365	4402	128
14	0	6	1258	1247	209
16	0	6	1548	1633	249
18	0	6	809	939	-264
20	0	6	271	622	-687
22	0	6	656	630	-321

H	K	L	$10F_o$	$10F_c$	10σ
24	0	6	899	1012	-347
26	0	6	2427	2066	295
28	0	6	1460	1413	337
30	0	6	355	357	-898
-31	1	6	844	618	-430
-29	1	6	309	319	-780
-27	1	6	1018	974	-417
-25	1	6	1657	1876	214
-23	1	6	1305	1388	285
-21	1	6	221	505	-560
-19	1	6	383	895	-421
-17	1	6	2582	2832	136
-15	1	6	4210	4280	117
-13	1	6	2990	2927	104
-11	1	6	514	628	-192
-9	1	6	1577	1546	103
-7	1	6	391	414	-232
-5	1	6	2664	2582	82
-3	1	6	211	56	-254
-1	1	6	4499	4503	71
1	1	6	6211	6228	72
3	1	6	4202	4334	79
5	1	6	478	229	-174
7	1	6	1468	1453	120
9	1	6	4278	4350	111
11	1	6	4922	5033	119
13	1	6	2231	2226	145
15	1	6	234	567	-592
17	1	6	1224	1348	237
19	1	6	204	67	-515
21	1	6	1017	936	-336
23	1	6	228	108	-578
25	1	6	1155	1539	-362
27	1	6	1770	1711	358
29	1	6	895	746	-407
31	1	6	390	91	-987
-30	2	6	258	244	-655
-28	2	6	339	246	-859
-26	2	6	877	928	-369
-24	2	6	809	1165	-304
-20	2	6	585	898	-288
-18	2	6	1140	1411	221
-16	2	6	2380	2354	135
-14	2	6	2510	2471	121
-12	2	6	989	1116	198
-10	2	6	345	701	-304
-8	2	6	236	70	-220
-6	2	6	1150	1159	108
-4	2	6	1373	1251	88
-2	2	6	1391	1417	98
0	2	6	3494	3507	78
2	2	6	4309	4264	79
4	2	6	2056	2123	97
6	2	6	1535	1531	105
8	2	6	2682	2820	111
10	2	6	3597	3529	111
12	2	6	2166	2196	137
14	2	6	229	265	-580
16	2	6	223	511	-563
18	2	6	561	292	-292
20	2	6	247	386	-627
22	2	6	278	277	-703
24	2	6	230	640	-582
26	2	6	849	1108	-426
28	2	6	371	754	-941
30	2	6	585	308	-558
-31	3	6	339	116	-859
-29	3	6	317	256	-801
-27	3	6	520	321	-428
-25	3	6	244	244	-440
-23	3	6	215	324	-546
-21	3	6	794	726	-233
-19	3	6	664	991	-328
-17	3	6	683	641	-270
-15	3	6	735	571	174
-13	3	6	632	836	-227
-11	3	6	1415	1484	149
-9	3	6	1314	1368	139
-7	3	6	1135	1126	119
-5	3	6	1248	1133	130
-3	3	6	1690	1645	91
-1	3	6	868	866	135
1	3	6	938	1009	124
3	3	6	1073	1143	107
5	3	6	2444	2466	100
7	3	6	1871	1907	122
9	3	6	1188	1319	160
11	3	6	204	71	-518
13	3	6	203	255	-517
15	3	6	661	864	-374
17	3	6	651	783	-311
19	3	6	246	49	-625
21	3	6	250	484	-633
23	3	6	253	373	-641
25	3	6	342	291	-865
27	3	6	290	96	-734

Table 71. (continued)

H	K	L	$10F_o$	$10F_c$	10σ
29	3	6	317	186	-802
-30	4	6	683	392	-480
-28	4	6	259	65	-657
-26	4	6	652	702	-512
-24	4	6	427	597	-333
-22	4	6	249	532	-631
-20	4	6	727	1221	-332
-18	4	6	200	352	-505
-16	4	6	1378	1418	162
-14	4	6	1319	1081	187
-12	4	6	444	731	-293
-10	4	6	2182	2315	119
-8	4	6	1797	1768	118
-6	4	6	944	1036	189
-4	4	6	2558	2406	95
-2	4	6	326	704	-323
0	4	6	2105	1955	98
2	4	6	1214	1160	119
4	4	6	741	767	152
6	4	6	2013	2116	117
8	4	6	620	711	-225
10	4	6	1456	1421	141
12	4	6	1595	1416	185
14	4	6	361	138	-398
16	4	6	1428	1641	203
18	4	6	499	600	-336
20	4	6	815	748	-297
22	4	6	546	904	-410
24	4	6	307	162	-779
26	4	6	342	486	-865
28	4	6	311	408	-788
-29	5	6	778	173	-461
-27	5	6	691	846	-504
-25	5	6	1107	1472	-441
-23	5	6	638	666	-356
-21	5	6	783	878	-296
-19	5	6	690	780	-280
-17	5	6	1431	1207	193
-15	5	6	2464	2547	138
-13	5	6	786	1079	-262
-11	5	6	1245	1273	186
-9	5	6	1977	1798	125
-7	5	6	345	519	-277
-5	5	6	2693	2796	105
-3	5	6	1151	1033	134
-1	5	6	3169	3157	104
1	5	6	4197	4214	100
3	5	6	1142	1381	177
5	5	6	1651	1569	146
7	5	6	763	1111	-316
9	5	6	1513	1496	184
11	5	6	2875	2900	133
13	5	6	1164	1380	214
15	5	6	498	962	-378
17	5	6	615	1136	-394
19	5	6	461	485	-396
21	5	6	856	1272	-347
23	5	6	309	424	-783
25	5	6	378	695	-957
27	5	6	1033	970	-471
-26	6	6	1173	1262	-418
-24	6	6	1031	1379	-451
-22	6	6	922	360	-328
-20	6	6	235	428	-593
-18	6	6	499	655	-334
-16	6	6	2275	2240	154
-14	6	6	2239	2282	162
-12	6	6	203	451	-514
-10	6	6	1111	1121	178
-8	6	6	429	486	-301
-6	6	6	1386	1465	161
-4	6	6	1819	1830	115
-2	6	6	1470	1381	137
0	6	6	4104	4075	110
2	6	6	3317	3387	111
4	6	6	476	471	-287
6	6	6	507	382	-273
8	6	6	1238	1167	156
10	6	6	3120	3008	132
12	6	6	2708	2688	142
14	6	6	583	275	-257
16	6	6	978	1038	-275
18	6	6	595	270	-334
20	6	6	737	964	-271
22	6	6	981	749	-398
24	6	6	355	371	-898
26	6	6	906	1029	-492
-25	7	6	561	1106	-688
-23	7	6	343	896	-868
-21	7	6	280	356	-710
-19	7	6	604	616	-510
-17	7	6	1878	1735	166
-15	7	6	2359	2264	152
-13	7	6	1293	1472	218
-11	7	6	195	45	-492
-9	7	6	375	717	-405

Table 71. (continued)

H	K	L	$10F_o$	$10F_c$	10σ
-7	7	6	171	129	-435
-5	7	6	905	975	171
-3	7	6	482	117	-206
-1	7	6	2278	2124	124
1	7	6	3085	3072	120
3	7	6	1595	1668	155
5	7	6	659	988	-301
7	7	6	1441	1377	163
9	7	6	2183	2504	161
11	7	6	2529	2577	151
13	7	6	1267	1294	260
15	7	6	464	258	-402
17	7	6	257	399	-467
19	7	6	297	253	-751
21	7	6	599	427	-502
23	7	6	341	111	-864
-22	8	6	712	803	-518
-20	8	6	1029	1009	-444
-18	8	6	1163	1327	-359
-16	8	6	1069	1340	-302
-14	8	6	1232	1086	207
-12	8	6	508	903	-395
-10	8	6	501	671	-399
-8	8	6	534	301	-267
-6	8	6	187	136	-473
-4	8	6	214	590	-543
-2	8	6	859	1175	197
0	8	6	1445	1516	167
2	8	6	852	1350	-263
4	8	6	1279	1450	196
6	8	6	1844	1956	171
8	8	6	1857	1911	174
10	8	6	1462	1454	179
12	8	6	739	1076	-290
14	8	6	275	584	-494
16	8	6	292	377	-741
18	8	6	338	217	-857
20	8	6	311	50	-789
22	8	6	630	386	-587
-19	9	6	676	1237	-513
-17	9	6	529	765	-475
-15	9	6	260	273	-657
-13	9	6	822	644	-348
-11	9	6	773	1353	-446
-9	9	6	1171	1148	-370
-7	9	6	180	86	-457
-5	9	6	739	1129	-351
-3	9	6	1453	1207	206
-1	9	6	222	697	-561
1	9	6	406	330	-375
3	9	6	824	922	-317
5	9	6	1806	1883	174
7	9	6	1980	1963	206
9	9	6	917	888	-341
11	9	6	257	229	-651
13	9	6	692	380	-401
15	9	6	354	791	-895
17	9	6	610	657	-646
19	9	6	311	24	-788
-16	10	6	349	128	-884
-14	10	6	355	226	-901
-12	10	6	303	814	-767
-10	10	6	1027	1514	-432
-8	10	6	387	620	-451
-6	10	6	514	828	-482
-4	10	6	1223	1288	259
-2	10	6	434	437	-505
0	10	6	899	425	-349
2	10	6	532	21	-327
4	10	6	1385	1431	264
6	10	6	2226	2028	243
8	10	6	987	985	-423
10	10	6	269	302	-681
12	10	6	613	353	-509
14	10	6	328	530	-833
-11	11	6	621	1009	-583
-9	11	6	986	1083	-376
-7	11	6	236	32	-597
-5	11	6	885	923	-370
-3	11	6	543	673	-580
-1	11	6	616	323	-418
1	11	6	294	661	-745
3	11	6	815	349	-363
5	11	6	985	1430	-390
7	11	6	574	1172	-630
9	11	6	310	61	-784
-31	1	7	573	225	-514
-29	1	7	321	30	-813
-27	1	7	988	752	-398
-25	1	7	1438	1210	282
-23	1	7	226	523	-572
-21	1	7	385	426	-303
-19	1	7	405	378	-297
-17	1	7	819	1069	-320
-15	1	7	1844	1858	138
-13	1	7	679	566	-218

H	K	L	$10F_O$	$10F_C$	10σ	H	K	L	$10F_O$	$10F_C$	10σ
-11	1	7	2020	1978	120	24	2	7	755	818	-319
-9	1	7	2220	2141	105	26	2	7	1343	1588	-458
-7	1	7	140	296	-353	28	2	7	1051	984	-417
-5	1	7	859	955	126	30	2	7	359	33	-910
-3	1	7	477	198	-165	-29	3	7	1020	150	-371
-1	1	7	3518	3557	79	-27	3	7	1108	1410	-551
1	1	7	3977	3941	78	-25	3	7	2003	2195	261
3	1	7	1546	1561	96	-23	3	7	1542	1455	202
5	1	7	969	1060	170	-21	3	7	217	249	-549
7	1	7	1386	1381	145	-19	3	7	213	382	-540
9	1	7	649	918	-264	-17	3	7	1565	1465	160
11	1	7	1548	1515	163	-15	3	7	2943	2925	124
13	1	7	229	510	-579	-13	3	7	218	693	-553
15	1	7	898	1212	-321	-11	3	7	3538	3527	106
17	1	7	1200	1144	251	-9	3	7	4812	4803	98
19	1	7	228	361	-577	-7	3	7	1864	1952	101
21	1	7	600	466	-389	-5	3	7	773	733	140
23	1	7	243	58	-615	-3	3	7	473	533	-217
25	1	7	296	796	-750	-1	3	7	5179	5233	86
27	1	7	326	857	-825	1	3	7	6803	6880	86
29	1	7	740	353	-600	3	3	7	3725	3607	91
-30	2	7	337	267	-853	5	3	7	537	959	-247
-28	2	7	303	526	-766	7	3	7	992	974	161
-26	2	7	1577	1774	331	9	3	7	1940	2061	134
-24	2	7	1305	1864	300	11	3	7	2957	2989	134
-22	2	7	358	333	-381	13	3	7	232	276	-587
-20	2	7	874	853	-255	15	3	7	2667	2589	164
-18	2	7	211	99	-536	17	3	7	2965	2854	158
-16	2	7	2427	2419	130	19	3	7	1210	1104	283
-14	2	7	2654	2592	129	21	3	7	623	203	-318
-12	2	7	855	977	199	23	3	7	654	408	-354
-10	2	7	4134	4038	99	25	3	7	2124	1540	320
-8	2	7	3395	3301	91	27	3	7	1415	1522	-506
-6	2	7	148	78	-378	29	3	7	309	574	-783
-4	2	7	955	931	131	-28	4	7	342	880	-867
-2	2	7	2487	2429	91	-26	4	7	1954	1776	319
0	2	7	6200	6138	81	-24	4	7	1049	1754	-519
2	2	7	4884	4941	84	-22	4	7	417	668	-342
4	2	7	154	88	-389	-20	4	7	221	223	-561
6	2	7	1744	1872	132	-18	4	7	208	407	-529
8	2	7	197	26	-498	-16	4	7	1886	1792	139
10	2	7	3290	3316	117	-14	4	7	1511	1350	151
12	2	7	1910	1936	148	-12	4	7	1279	1225	165
14	2	7	1286	1165	216	-10	4	7	3545	3438	105
16	2	7	2861	2701	152	-8	4	7	2838	2753	106
18	2	7	1617	1744	209	-6	4	7	799	1042	173
20	2	7	467	261	-291	-4	4	7	863	1039	199
22	2	7	414	350	-415	-2	4	7	3344	3378	96

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
0	4	7	5783	5686	94	-14	6	7	560	524	-230
2	4	7	4805	4805	95	-10	6	7	192	35	-484
4	4	7	1397	1482	128	-8	6	7	462	742	-323
6	4	7	811	640	146	-6	6	7	2079	2013	128
8	4	7	560	712	-316	-4	6	7	2588	2514	118
10	4	7	1700	1985	147	-2	6	7	1649	1584	146
12	4	7	999	1130	221	0	6	7	774	911	167
14	4	7	569	1121	-332	2	6	7	1329	1423	161
16	4	7	2617	2452	167	4	6	7	1890	2008	139
18	4	7	1579	1891	242	6	6	7	1649	1720	142
20	4	7	842	815	-285	8	6	7	718	952	-247
22	4	7	774	448	-383	10	6	7	201	534	-510
24	4	7	1110	1109	-419	12	6	7	598	903	-328
26	4	7	1515	1426	352	14	6	7	553	543	-293
28	4	7	688	935	-575	16	6	7	499	212	-274
-27	5	7	777	861	-493	18	6	7	225	553	-571
-25	5	7	930	1200	-374	20	6	7	1313	1079	326
-23	5	7	701	1140	-526	22	6	7	358	1065	-906
-21	5	7	550	757	-325	24	6	7	371	640	-939
-19	5	7	712	343	-241	-25	7	7	549	362	-541
-17	5	7	195	499	-493	-23	7	7	277	270	-700
-15	5	7	745	632	-293	-21	7	7	832	1257	-586
-13	5	7	161	77	-409	-19	7	7	1205	1304	-313
-11	5	7	963	1001	199	-17	7	7	212	111	-383
-9	5	7	1694	1778	151	-15	7	7	805	965	-286
-7	5	7	2090	2063	124	-13	7	7	549	512	-265
-5	5	7	2032	2073	115	-11	7	7	819	992	-305
-3	5	7	2710	2640	107	-9	7	7	991	1208	249
-1	5	7	2746	2802	109	-7	7	7	689	582	-236
1	5	7	3474	3422	109	-5	7	7	2688	2558	125
3	5	7	2417	2460	112	-3	7	7	2014	1964	139
5	5	7	1074	1138	205	-1	7	7	179	145	-451
7	5	7	616	788	-324	1	7	7	708	841	-235
9	5	7	1075	927	176	3	7	7	623	660	-260
11	5	7	643	531	-244	5	7	7	1636	1978	157
13	5	7	204	456	-519	7	7	7	1439	1511	220
15	5	7	1219	1186	213	9	7	7	230	472	-581
17	5	7	1876	1471	207	11	7	7	1794	1653	171
19	5	7	1242	1180	215	13	7	7	571	792	-349
21	5	7	1028	978	-275	15	7	7	662	592	-312
23	5	7	611	918	-587	17	7	7	306	611	-774
25	5	7	1020	975	-457	19	7	7	939	467	-408
27	5	7	793	781	-485	21	7	7	918	1127	-459
-26	6	7	731	213	-447	23	7	7	991	691	-465
-24	6	7	330	437	-836	-22	8	7	305	484	-772
-22	6	7	595	1057	-448	-20	8	7	777	1196	-467
-20	6	7	1163	1283	-407	-18	8	7	314	584	-794
-18	6	7	1048	767	187	-16	8	7	759	712	-320

H	K	L	$10F_o$	$10F_c$	10σ
-14	8	7	715	865	-356
-12	8	7	237	572	-599
-10	8	7	2043	1879	161
-8	8	7	276	1021	-699
-6	8	7	1277	1267	188
-4	8	7	1747	1982	167
-2	8	7	422	203	-316
0	8	7	1868	1737	163
2	8	7	1237	1262	203
4	8	7	741	604	-263
6	8	7	1590	1567	186
8	8	7	575	285	-326
10	8	7	1301	1253	207
12	8	7	1193	1301	216
14	8	7	270	275	-684
16	8	7	814	1149	-450
18	8	7	315	437	-799
20	8	7	302	641	-766
-19	9	7	330	619	-838
-17	9	7	304	135	-771
-15	9	7	303	737	-768
-13	9	7	529	158	-340
-11	9	7	956	1043	-378
-9	9	7	753	1396	-445
-7	9	7	531	277	-335
-5	9	7	659	758	-277
-3	9	7	231	125	-586
-1	9	7	1348	1325	172
1	9	7	1537	1808	207
3	9	7	674	691	-229
5	9	7	546	607	-345
7	9	7	447	510	-544
9	9	7	691	476	-389
11	9	7	942	1005	-368
13	9	7	292	248	-738
15	9	7	643	741	-515
17	9	7	387	737	-981
-14	10	7	446	329	-521
-12	10	7	276	219	-699
-10	10	7	669	821	-589
-8	10	7	596	883	-434
-6	10	7	849	481	-358
-4	10	7	272	402	-688
-2	10	7	812	882	-356
0	10	7	1046	1276	-391
2	10	7	327	1092	-828
4	10	7	305	366	-772
6	10	7	282	31	-712
8	10	7	492	155	-478
10	10	7	304	464	-772
12	10	7	331	340	-838
14	10	7	336	165	-851
-9	11	7	298	396	-754
-7	11	7	501	776	-572
-5	11	7	953	1067	-408
-3	11	7	1205	1019	270
-1	11	7	554	755	-550
1	11	7	1094	550	-382
3	11	7	634	565	-412
5	11	7	299	631	-757
7	11	7	834	534	-432
-30	0	8	325	22	-823
-28	0	8	339	706	-859
-26	0	8	879	1584	-448
-24	0	8	901	1199	-364
-22	0	8	218	535	-554
-20	0	8	2187	2090	184
-18	0	8	1415	1458	222
-16	0	8	195	279	-494
-14	0	8	532	297	-256
-12	0	8	3207	3289	118
-10	0	8	5940	6038	101
-8	0	8	5185	5162	94
-6	0	8	1762	1765	109
-4	0	8	1155	1110	131
-2	0	8	2395	2382	92
0	0	8	5274	5142	82
2	0	8	3325	3354	87
4	0	8	1129	1234	142
6	0	8	3913	3965	108
8	0	8	2194	2317	136
10	0	8	192	376	-488
12	0	8	242	173	-611
14	0	8	2461	2593	170
16	0	8	3856	3807	151
18	0	8	3109	2984	175
20	0	8	255	618	-646
22	0	8	651	145	-329
24	0	8	676	618	-364
26	0	8	692	1192	-649
28	0	8	292	650	-741
-31	1	8	317	51	-804
-29	1	8	561	164	-490
-27	1	8	314	995	-797
-25	1	8	1412	1429	-384
-23	1	8	779	584	-270

Table 71. (continued)

H	K	L	10F$_o$	10F$_c$	10σ	H	K	L	10F$_o$	10F$_c$	10σ
-19	1	8	2110	1913	149	16	2	8	2302	2237	163
-17	1	8	649	702	-314	18	2	8	1672	1522	187
-15	1	8	200	529	-505	20	2	8	663	573	-371
-13	1	8	807	804	166	22	2	8	561	203	-288
-11	1	8	4509	4417	103	24	2	8	331	506	-839
-9	1	8	5801	5666	95	26	2	8	392	499	-993
-7	1	8	3620	3478	91	28	2	8	283	154	-715
-5	1	8	980	874	118	-29	3	8	319	425	-807
-3	1	8	347	760	-215	-27	3	8	264	323	-671
-1	1	8	3133	3121	90	-25	3	8	520	120	-482
1	1	8	4707	4545	85	-23	3	8	190	271	-481
3	1	8	1385	1336	127	-21	3	8	200	486	-507
5	1	8	2689	2604	106	-19	3	8	527	234	-315
7	1	8	3359	3336	110	-17	3	8	459	515	-307
9	1	8	1293	1245	198	-13	3	8	1326	1304	216
11	1	8	217	40	-551	-11	3	8	1023	882	148
13	1	8	702	1137	-374	-9	3	8	588	442	-241
15	1	8	3088	3151	165	-7	3	8	784	735	-211
17	1	8	3405	3270	165	-5	3	8	1093	1353	170
19	1	8	1402	1441	217	-3	3	8	942	955	141
21	1	8	215	36	-542	-1	3	8	138	208	-352
23	1	8	226	182	-572	1	3	8	564	344	-197
25	1	8	815	1000	-436	3	3	8	175	154	-444
27	1	8	312	835	-791	5	3	8	467	56	-272
29	1	8	356	104	-900	7	3	8	187	27	-473
-30	2	8	311	135	-789	9	3	8	814	726	192
-28	2	8	345	479	-873	11	3	8	1141	1402	252
-26	2	8	881	856	-370	13	3	8	943	1156	210
-24	2	8	1014	852	222	15	3	8	467	647	-317
-22	2	8	186	125	-470	17	3	8	224	573	-567
-20	2	8	737	722	-297	19	3	8	657	614	-299
-18	2	8	1083	1079	241	21	3	8	440	454	-404
-16	2	8	187	319	-474	23	3	8	325	418	-825
-14	2	8	227	462	-576	25	3	8	342	25	-868
-12	2	8	1828	1860	135	27	3	8	661	191	-526
-10	2	8	3407	3361	108	-26	4	8	300	491	-758
-8	2	8	2697	2734	99	-24	4	8	536	481	-501
-6	2	8	1601	1626	107	-22	4	8	351	617	-365
-4	2	8	520	636	-194	-20	4	8	814	1170	-321
-2	2	8	1481	1453	115	-18	4	8	437	511	-398
0	2	8	2147	2153	97	-16	4	8	665	821	-221
2	2	8	1799	1859	103	-14	4	8	1230	1028	149
4	2	8	537	683	-248	-12	4	8	185	48	-467
6	2	8	1749	1761	121	-10	4	8	1612	1636	145
8	2	8	1279	1533	184	-8	4	8	835	992	189
10	2	8	795	638	-208	-6	4	8	1171	1123	151
12	2	8	698	1094	-351	-4	4	8	1763	1870	127
14	2	8	1432	1617	217	-2	4	8	331	220	-261

H	K	L	$10F_o$	$10F_c$	10σ
0	4	8	2156	2084	113
2	4	8	1717	1740	116
4	4	8	693	712	-187
6	4	8	1624	1727	150
8	4	8	670	831	-318
10	4	8	1304	1334	182
12	4	8	1585	1671	175
14	4	8	334	99	-335
16	4	8	968	1077	-297
18	4	8	547	526	-333
20	4	8	243	413	-614
22	4	8	305	721	-773
24	4	8	334	54	-847
26	4	8	821	608	-490
-27	5	8	1159	517	-344
-25	5	8	327	1016	-828
-23	5	8	280	233	-708
-21	5	8	911	1158	224
-19	5	8	1224	1197	204
-17	5	8	200	85	-506
-15	5	8	688	949	-274
-13	5	8	456	140	-288
-11	5	8	2315	2393	131
-9	5	8	3177	3046	115
-7	5	8	514	586	-329
-5	5	8	1619	1789	138
-3	5	8	1031	1048	147
-1	5	8	1647	1728	155
1	5	8	2641	2582	119
3	5	8	708	750	-208
5	5	8	1686	1628	141
7	5	8	1813	1815	139
9	5	8	187	64	-472
11	5	8	1288	1326	195
13	5	8	219	78	-555
15	5	8	1861	1851	208
17	5	8	1879	1776	205
19	5	8	236	440	-597
21	5	8	314	602	-795
23	5	8	619	330	-557
25	5	8	946	543	-405
-26	6	8	731	955	-515
-24	6	8	923	876	-355
-22	6	8	639	296	-461
-20	6	8	982	1353	-477
-18	6	8	1374	916	244
-16	6	8	333	225	-346
-14	6	8	589	447	-228

H	K	L	$10F_o$	$10F_c$	10σ
-12	6	8	1398	1379	173
-10	6	8	3103	3278	139
-8	6	8	2869	2834	126
-6	6	8	167	42	-421
-4	6	8	1232	1092	147
-2	6	8	275	556	-323
0	6	8	2409	2416	134
2	6	8	1685	1672	159
4	6	8	480	664	-318
6	6	8	2078	2225	151
8	6	8	1155	1222	242
10	6	8	229	606	-580
12	6	8	512	416	-353
14	6	8	1189	1413	233
16	6	8	2380	2372	198
18	6	8	1401	1424	-381
20	6	8	263	94	-665
22	6	8	736	217	-470
24	6	8	286	315	-724
-23	7	8	297	215	-753
-21	7	8	480	605	-597
-19	7	8	293	943	-744
-17	7	8	662	546	-353
-15	7	8	196	142	-496
-13	7	8	888	678	215
-11	7	8	1756	1985	185
-9	7	8	2712	2566	136
-7	7	8	1465	1570	189
-5	7	8	491	333	-297
-3	7	8	704	782	-242
-1	7	8	1807	1798	178
1	7	8	1386	1503	179
3	7	8	216	159	-548
5	7	8	1444	1349	211
7	7	8	1265	1551	247
9	7	8	614	559	-286
11	7	8	411	51	-389
13	7	8	654	875	-341
15	7	8	1641	1762	357
17	7	8	1652	1649	293
19	7	8	584	779	-476
21	7	8	368	281	-932
23	7	8	297	335	-753
-22	8	8	708	35	-413
-20	8	8	623	166	-357
-18	8	8	335	472	-848
-16	8	8	801	732	-390
-14	8	8	827	919	-408

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
-12	8	8	1197	1116	216	-5	11	8	1184	1262	-320
-10	8	8	1368	1467	189	-3	11	8	697	961	-468
-8	8	8	1616	1564	169	-1	11	8	693	302	-438
-6	8	8	1379	1435	183	1	11	8	510	867	-565
-4	8	8	896	1352	-343	3	11	8	282	85	-713
-2	8	8	1407	1402	246	5	11	8	355	846	-900
0	8	8	736	840	-262	-29	1	9	327	303	-828
2	8	8	370	305	-309	-27	1	9	336	32	-850
4	8	8	205	34	-520	-25	1	9	747	273	-441
6	8	8	491	519	-298	-23	1	9	200	340	-507
8	8	8	943	850	212	-21	1	9	1133	1133	229
10	8	8	811	944	-265	-19	1	9	1230	1324	184
12	8	8	334	1150	-845	-17	1	9	321	246	-354
14	8	8	968	1224	-417	-15	1	9	201	327	-510
16	8	8	839	1068	-506	-13	1	9	483	546	-307
18	8	8	820	732	-450	-11	1	9	2051	2050	131
20	8	8	889	617	-418	-9	1	9	2375	2399	114
-17	9	8	795	598	-418	-7	1	9	179	237	-451
-15	9	8	1051	1149	-344	-5	1	9	1674	1802	120
-13	9	8	1045	998	-426	-3	1	9	1988	1909	104
-11	9	8	419	570	-493	-1	1	9	159	86	-402
-9	9	8	441	669	-533	1	1	9	895	767	128
-7	9	8	599	1314	-487	3	1	9	389	278	-252
-5	9	8	1895	1925	212	5	1	9	2339	2433	110
-3	9	8	1231	1704	228	7	1	9	1930	1983	143
-1	9	8	398	520	-315	9	1	9	880	742	-240
1	9	8	430	344	-326	11	1	9	210	174	-533
3	9	8	260	28	-656	13	1	9	756	685	-294
5	9	8	679	524	-445	15	1	9	1420	1694	231
7	9	8	251	61	-636	17	1	9	1359	1642	215
9	9	8	1166	899	-385	19	1	9	455	92	-440
11	9	8	1103	1489	-371	21	1	9	854	776	-308
13	9	8	1311	1239	-478	23	1	9	862	672	-402
15	9	8	304	586	-773	25	1	9	491	62	-468
17	9	8	335	255	-847	27	1	9	362	293	-917
-14	10	8	874	1097	-392	-30	2	9	335	670	-850
-12	10	8	290	428	-734	-28	2	9	295	230	-747
-8	10	8	238	399	-602	-24	2	9	296	430	-749
-6	10	8	1276	1466	312	-22	2	9	859	1255	-383
-4	10	8	1853	1840	242	-20	2	9	2629	2836	169
-2	10	8	272	770	-688	-18	2	9	2153	2142	143
0	10	8	297	559	-753	-16	2	9	190	82	-482
2	10	8	277	575	-700	-14	2	9	415	634	-271
4	10	8	516	449	-446	-12	2	9	1631	1591	140
6	10	8	294	789	-747	-10	2	9	3502	3610	113
8	10	8	292	121	-738	-8	2	9	2887	2824	110
10	10	8	351	1172	-889	-6	2	9	1251	1223	122
12	10	8	1394	1247	-389	-4	2	9	3102	2965	98

Table 71. (continued)

H	K	L	$10F_o$	$10F_c$	10σ
-2	2	9	811	834	135
0	2	9	1884	1874	113
2	2	9	837	909	166
4	2	9	3155	3234	107
6	2	9	4867	5160	107
8	2	9	2857	2970	124
10	2	9	380	321	-375
12	2	9	604	159	-272
14	2	9	1330	1563	233
16	2	9	2760	2719	172
18	2	9	1247	1329	235
20	2	9	509	571	-387
22	2	9	1119	1121	273
24	2	9	595	252	-478
26	2	9	664	412	-465
28	2	9	297	125	-751
-29	3	9	768	524	-364
-27	3	9	320	201	-811
-25	3	9	299	593	-757
-23	3	9	519	440	-291
-21	3	9	2238	2344	184
-19	3	9	2720	2951	153
-17	3	9	1221	1351	205
-15	3	9	501	193	-312
-13	3	9	609	686	-274
-11	3	9	3211	3197	122
-9	3	9	3962	3943	109
-7	3	9	1262	1178	158
-5	3	9	2204	2151	111
-3	3	9	1825	1964	120
-1	3	9	920	877	191
1	3	9	1679	1671	115
3	3	9	1595	1714	123
5	3	9	5031	5191	108
7	3	9	4897	4842	114
9	3	9	1721	1648	155
11	3	9	512	80	-271
13	3	9	688	648	-274
15	3	9	2467	2527	170
17	3	9	2203	2335	193
19	3	9	527	375	-345
21	3	9	1118	1048	221
23	3	9	751	703	-564
25	3	9	667	203	-470
27	3	9	332	331	-842
-28	4	9	587	168	-633
-26	4	9	312	266	-791
-24	4	9	511	45	-435

H	K	L	$10F_o$	$10F_c$	10σ
-22	4	9	688	1092	-419
-20	4	9	2276	2047	165
-18	4	9	1649	1862	191
-16	4	9	689	919	-305
-14	4	9	841	1027	-249
-12	4	9	2311	2304	127
-10	4	9	3510	3436	113
-8	4	9	2307	2323	120
-6	4	9	180	39	-454
-4	4	9	1713	1675	135
-2	4	9	559	712	-260
0	4	9	186	434	-471
2	4	9	387	518	-288
4	4	9	3113	3007	113
6	4	9	3831	3825	119
8	4	9	2593	2595	129
10	4	9	464	904	-343
12	4	9	596	664	-324
14	4	9	1479	1631	186
16	4	9	2001	2113	193
18	4	9	976	1200	-322
20	4	9	269	326	-481
22	4	9	932	722	-417
24	4	9	312	230	-791
26	4	9	640	131	-478
-27	5	9	276	27	-702
-25	5	9	592	30	-459
-23	5	9	687	349	-490
-21	5	9	914	957	-379
-19	5	9	961	1323	-315
-17	5	9	1448	1438	211
-15	5	9	1280	1371	197
-13	5	9	1704	1625	159
-11	5	9	2091	1985	136
-9	5	9	1942	1859	129
-7	5	9	1044	1154	183
-5	5	9	178	82	-451
-3	5	9	546	592	-245
-1	5	9	224	495	-568
1	5	9	419	730	-334
3	5	9	1530	1636	143
5	5	9	2114	2069	134
7	5	9	1930	1962	143
9	5	9	1419	1590	196
11	5	9	878	1324	-354
13	5	9	883	1315	-347
15	5	9	1096	1183	239
17	5	9	1156	866	214

Table 71. (continued)

H	K	L	$10F_o$	$10F_c$	10σ
19	5	9	301	267	-763
21	5	9	323	201	-817
23	5	9	276	213	-699
25	5	9	275	176	-695
-24	6	9	298	554	-755
-22	6	9	303	319	-769
-18	6	9	445	698	-351
-16	6	9	1119	1545	-287
-14	6	9	1604	1720	188
-12	6	9	691	1034	-312
-10	6	9	205	265	-520
-8	6	9	192	391	-486
-6	6	9	1218	1125	201
-4	6	9	1038	1076	183
-2	6	9	204	110	-517
0	6	9	1006	1206	224
2	6	9	1707	1795	157
4	6	9	1099	1036	182
6	6	9	580	444	-251
8	6	9	823	893	-252
10	6	9	1798	1738	201
12	6	9	1767	1748	187
14	6	9	889	827	-253
16	6	9	238	22	-428
18	6	9	290	31	-734
20	6	9	314	163	-795
22	6	9	573	160	-536
24	6	9	314	127	-796
-23	7	9	333	405	-846
-21	7	9	535	395	-555
-19	7	9	297	428	-752
-17	7	9	690	745	-489
-15	7	9	1677	1799	281
-13	7	9	1109	1223	223
-11	7	9	214	406	-543
-9	7	9	1012	1097	191
-7	7	9	373	269	-313
-5	7	9	1635	1724	166
-3	7	9	1129	1212	238
-1	7	9	734	837	-276
1	7	9	2063	2008	146
3	7	9	957	1109	216
5	7	9	229	550	-579
7	7	9	370	583	-402
9	7	9	917	1037	-264
11	7	9	2082	1968	209
13	7	9	735	1106	-276
15	7	9	312	369	-791
19	7	9	327	24	-827
21	7	9	355	475	-900
-20	8	9	968	904	-389
-18	8	9	499	343	-500
-16	8	9	840	873	-375
-14	8	9	603	1140	-472
-12	8	9	287	107	-727
-10	8	9	1136	1321	203
-8	8	9	755	778	-265
-6	8	9	985	974	196
-4	8	9	1465	1604	209
-2	8	9	626	179	-304
0	8	9	1435	1532	165
2	8	9	672	1279	-379
4	8	9	211	442	-536
6	8	9	1361	1432	242
8	8	9	249	367	-446
10	8	9	1153	1237	287
12	8	9	894	1233	-454
14	8	9	290	171	-734
16	8	9	874	1017	-404
18	8	9	652	567	-385
-17	9	9	260	171	-657
-15	9	9	292	440	-740
-13	9	9	228	101	-579
-11	9	9	731	859	-381
-9	9	9	691	1056	-447
-7	9	9	409	107	-503
-5	9	9	761	1001	-371
-3	9	9	904	820	-270
-1	9	9	573	356	-361
1	9	9	276	881	-700
3	9	9	244	21	-616
5	9	9	1045	1062	-407
7	9	9	765	1108	-456
9	9	9	313	74	-792
11	9	9	705	556	-329
13	9	9	290	37	-734
15	9	9	1286	815	285
-12	10	9	282	466	-716
-10	10	9	596	731	-513
-8	10	9	616	499	-441
-6	10	9	273	93	-691
-4	10	9	278	471	-705
-2	10	9	303	209	-770
0	10	9	285	127	-720
2	10	9	321	136	-813
4	10	9	803	689	-425

Table 71. (continued)

H	K	L	$10F_O$	$10F_C$	10σ
6	10	9	672	963	-558
8	10	9	757	719	-508
10	10	9	334	306	-847
-28	0	10	546	833	-531
-26	0	10	311	81	-787
-24	0	10	540	236	-535
-22	0	10	1509	1532	274
-20	0	10	2816	2997	168
-18	0	10	1864	2098	188
-16	0	10	492	35	-274
-14	0	10	687	883	-298
-12	0	10	912	779	227
-10	0	10	1633	1594	144
-8	0	10	164	152	-417
-6	0	10	3176	3201	99
-4	0	10	5431	5398	96
-2	0	10	3299	3298	99
0	0	10	190	337	-481
2	0	10	686	539	140
4	0	10	3483	3419	109
6	0	10	5008	5005	114
8	0	10	2863	2791	131
10	0	10	517	284	-318
12	0	10	1224	1243	243
14	0	10	702	34	-274
16	0	10	870	1112	-322
18	0	10	227	103	-575
20	0	10	1758	1801	226
22	0	10	1843	2153	318
24	0	10	650	1128	-524
26	0	10	579	219	-627
-29	1	10	382	878	-968
-27	1	10	305	400	-771
-25	1	10	267	40	-675
-23	1	10	547	851	-402
-21	1	10	2541	2366	172
-19	1	10	2691	2694	160
-17	1	10	783	864	-259
-15	1	10	922	1010	209
-13	1	10	186	313	-472
-11	1	10	1036	1307	238
-9	1	10	1439	1383	129
-7	1	10	1079	1178	148
-5	1	10	4335	4155	95
-3	1	10	4486	4313	96
-1	1	10	1518	1443	131
1	1	10	187	63	-474
3	1	10	2195	2151	108

H	K	L	$10F_O$	$10F_C$	10σ
5	1	10	4327	4412	109
7	1	10	3822	3876	114
9	1	10	524	863	-328
11	1	10	994	971	221
13	1	10	692	609	-281
15	1	10	244	667	-618
17	1	10	498	714	-478
19	1	10	604	850	-342
21	1	10	1918	1884	252
23	1	10	930	1456	-576
25	1	10	340	573	-863
27	1	10	311	150	-785
-28	2	10	329	548	-835
-26	2	10	721	401	-429
-24	2	10	306	390	-775
-22	2	10	860	1105	-288
-20	2	10	1670	1675	215
-18	2	10	958	1356	-313
-16	2	10	226	91	-572
-14	2	10	348	188	-367
-12	2	10	347	351	-367
-10	2	10	806	888	190
-6	2	10	1406	1417	139
-4	2	10	2831	2796	104
-2	2	10	2202	2246	112
0	2	10	1209	1007	156
2	2	10	1085	1270	188
4	2	10	2630	2759	119
6	2	10	2817	2892	119
8	2	10	1625	1624	139
10	2	10	200	117	-507
12	2	10	450	474	-337
14	2	10	426	27	-379
16	2	10	217	436	-550
18	2	10	246	101	-625
20	2	10	840	924	-333
22	2	10	676	1055	-502
24	2	10	276	666	-699
26	2	10	274	331	-696
-27	3	10	342	493	-865
-25	3	10	942	670	-393
-23	3	10	297	399	-753
-21	3	10	408	192	-338
-19	3	10	524	194	-327
-17	3	10	222	465	-560
-15	3	10	836	979	-228
-13	3	10	714	836	-287
-11	3	10	183	128	-462

Table 71. (continued)

H	K	L	$10F_o$	$10F_c$	10σ
-9	3	10	628	621	-259
-7	3	10	175	317	-445
-5	3	10	173	136	-440
-3	3	10	676	698	-202
-1	3	10	1311	1459	137
1	3	10	1896	1789	132
3	3	10	1608	1667	128
5	3	10	692	897	-210
7	3	10	169	92	-425
9	3	10	425	482	-294
11	3	10	620	614	-259
13	3	10	446	323	-311
15	3	10	240	58	-608
17	3	10	418	366	-352
19	3	10	217	355	-549
21	3	10	345	189	-874
23	3	10	682	172	-396
25	3	10	716	299	-454
-26	4	10	729	515	-427
-24	4	10	971	565	-402
-22	4	10	306	208	-777
-20	4	10	681	771	-294
-18	4	10	440	394	-334
-16	4	10	1117	875	182
-14	4	10	1158	1374	189
-12	4	10	209	245	-527
-10	4	10	1452	1258	162
-8	4	10	394	668	-313
-6	4	10	807	892	178
-4	4	10	1613	1609	130
-2	4	10	177	180	-448
0	4	10	1298	1408	146
2	4	10	1468	1384	145
4	4	10	211	312	-535
6	4	10	1589	1578	167
8	4	10	359	590	-339
10	4	10	1184	1077	238
12	4	10	841	1065	-323
14	4	10	237	82	-601
16	4	10	744	883	-335
18	4	10	270	614	-682
20	4	10	282	299	-713
22	4	10	853	609	-447
24	4	10	530	146	-495
-25	5	10	331	429	-838
-23	5	10	350	102	-886
-21	5	10	934	1120	-388
-19	5	10	661	1210	-484
-17	5	10	346	60	-421
-15	5	10	1280	1412	210
-13	5	10	573	826	-307
-11	5	10	844	1164	-288
-9	5	10	1717	1792	155
-7	5	10	196	180	-496
-5	5	10	2358	2445	124
-3	5	10	2486	2295	127
-1	5	10	476	368	-212
1	5	10	954	945	167
3	5	10	169	111	-430
5	5	10	2077	2058	146
7	5	10	2249	2238	155
9	5	10	192	35	-483
11	5	10	796	1359	-350
13	5	10	498	550	-352
15	5	10	843	910	-335
17	5	10	1358	1162	-413
19	5	10	560	54	-467
21	5	10	344	1008	-871
23	5	10	846	863	-482
-24	6	10	330	78	-836
-22	6	10	721	821	-413
-20	6	10	1464	1620	346
-18	6	10	1057	1041	-320
-16	6	10	226	488	-405
-14	6	10	1025	1097	-271
-10	6	10	1578	1688	189
-6	6	10	1906	1922	160
-4	6	10	2928	2964	135
-2	6	10	1620	1769	154
0	6	10	368	161	-336
2	6	10	185	44	-468
4	6	10	1592	1860	196
6	6	10	3134	3019	150
8	6	10	1462	1567	203
10	6	10	476	512	-337
12	6	10	546	846	-395
14	6	10	388	339	-408
16	6	10	676	964	-469
18	6	10	318	343	-807
20	6	10	323	745	-816
22	6	10	1118	1101	-409
-21	7	10	1297	1085	-335
-19	7	10	1182	1350	-401
-17	7	10	655	707	-445
-15	7	10	255	109	-644
-13	7	10	352	189	-353

H	K	L	10F_o	10F_c	10σ
-11	7	10	231	529	-584
-9	7	10	222	446	-559
-7	7	10	589	815	-309
-5	7	10	2010	1923	171
-3	7	10	1725	1891	175
-1	7	10	250	1002	-633
1	7	10	451	513	-326
3	7	10	1382	1266	206
5	7	10	2480	2466	151
7	7	10	2324	2116	166
11	7	10	413	314	-317
13	7	10	289	41	-733
15	7	10	340	396	-861
17	7	10	306	196	-773
19	7	10	322	427	-815
-18	8	10	779	828	-440
-14	8	10	290	352	-736
-12	8	10	255	143	-644
-10	8	10	226	97	-573
-8	8	10	286	550	-723
-6	8	10	868	883	-234
-4	8	10	904	1018	-254
-2	8	10	1595	1294	202
0	8	10	1318	1401	221
2	8	10	1667	1383	176
4	8	10	1183	1481	182
6	8	10	950	1290	-371
8	8	10	298	865	-755
10	8	10	272	451	-689
12	8	10	327	338	-828
14	8	10	311	193	-786
16	8	10	750	137	-414
18	8	10	278	431	-705
-15	9	10	827	898	-489
-13	9	10	274	548	-694
-11	9	10	557	267	-389
-9	9	10	821	822	-358
-7	9	10	255	638	-645
-5	9	10	277	205	-702
-3	9	10	286	516	-723
-1	9	10	656	1379	-553
1	9	10	1338	1657	285
3	9	10	618	1151	-473
5	9	10	1041	474	-345
7	9	10	696	275	-358
9	9	10	328	538	-830
11	9	10	351	803	-889
13	9	10	318	444	-805

H	K	L	10F_o	10F_c	10σ
-10	10	10	310	841	-784
-8	10	10	513	846	-523
-6	10	10	334	52	-847
-4	10	10	291	405	-736
-2	10	10	309	425	-782
0	10	10	1534	1468	281
2	10	10	840	1391	-517
4	10	10	334	411	-845
6	10	10	307	270	-779
8	10	10	319	26	-808
-27	1	11	326	85	-825
-25	1	11	307	306	-779
-23	1	11	270	4	-683
-21	1	11	770	778	-358
-19	1	11	690	913	-288
-15	1	11	1094	1247	221
-13	1	11	1050	1284	239
-11	1	11	195	183	-493
-9	1	11	200	426	-507
-7	1	11	526	532	-282
-5	1	11	1903	2014	136
-3	1	11	2148	2116	116
-1	1	11	557	539	-210
1	1	11	634	638	-227
3	1	11	167	56	-422
5	1	11	925	1164	172
7	1	11	1265	1049	200
9	1	11	340	210	-260
11	1	11	1665	1693	170
13	1	11	775	971	-239
15	1	11	417	22	-304
17	1	11	441	476	-349
19	1	11	302	262	-765
21	1	11	596	894	-540
23	1	11	630	727	-471
25	1	11	558	102	-681
-28	2	11	336	644	-852
-26	2	11	322	234	-815
-24	2	11	491	402	-568
-22	2	11	290	603	-733
-20	2	11	1369	1564	257
-18	2	11	822	789	-275
-16	2	11	1400	1333	216
-14	2	11	2296	2409	140
-12	2	11	950	1021	238
-10	2	11	921	899	171
-8	2	11	192	92	-487
-6	2	11	2996	3044	121

H	K	L	$10F_o$	$10F_c$	10σ
-4	2	11	4660	4580	106
-2	2	11	2583	2509	115
0	2	11	617	956	-277
2	2	11	1202	1080	146
4	2	11	890	920	178
6	2	11	2473	2461	130
8	2	11	871	920	-234
10	2	11	1767	1797	176
12	2	11	2580	2523	162
14	2	11	727	829	-326
16	2	11	495	501	-353
18	2	11	237	46	-599
20	2	11	1126	1233	-371
22	2	11	1897	1624	302
24	2	11	568	688	-537
26	2	11	319	143	-806
-25	3	11	306	302	-775
-23	3	11	289	93	-731
-21	3	11	1163	1262	-316
-19	3	11	1527	1429	208
-17	3	11	366	317	-340
-15	3	11	2313	2388	146
-13	3	11	2452	2401	130
-11	3	11	427	345	-311
-9	3	11	301	337	-333
-7	3	11	1707	1701	142
-5	3	11	4745	4515	112
-3	3	11	4232	4114	111
-1	3	11	1119	1221	145
1	3	11	995	1017	210
3	3	11	194	218	-490
5	3	11	1888	2015	148
7	3	11	1982	1957	150
9	3	11	612	654	-293
11	3	11	2602	2666	148
13	3	11	2047	2040	192
15	3	11	436	280	-356
17	3	11	228	57	-577
19	3	11	991	1019	-407
21	3	11	1978	1904	289
23	3	11	1374	1350	-467
25	3	11	315	252	-797
-26	4	11	508	290	-603
-24	4	11	261	80	-662
-22	4	11	561	577	-477
-20	4	11	698	1034	-517
-18	4	11	238	437	-602
-16	4	11	649	1154	-336
-14	4	11	2273	2147	140
-12	4	11	1474	1569	200
-10	4	11	545	560	-254
-8	4	11	783	1001	-203
-6	4	11	2760	2791	120
-4	4	11	3688	3737	117
-2	4	11	2601	2464	121
0	4	11	377	635	-328
2	4	11	407	72	-266
4	4	11	769	1155	-261
6	4	11	1578	1675	142
8	4	11	518	519	-249
10	4	11	1214	1459	206
12	4	11	2147	2209	245
14	4	11	1166	1326	223
16	4	11	281	509	-711
18	4	11	510	823	-590
20	4	11	1074	1538	-437
22	4	11	1218	1446	-421
24	4	11	635	707	-587
-25	5	11	293	438	-743
-23	5	11	823	408	-411
-21	5	11	312	435	-792
-19	5	11	287	303	-726
-17	5	11	423	266	-351
-15	5	11	759	923	-289
-13	5	11	1116	1105	269
-11	5	11	989	1110	221
-9	5	11	1132	1181	228
-7	5	11	2233	1966	135
-5	5	11	2332	2347	146
-3	5	11	1999	2188	136
-1	5	11	1635	1330	158
1	5	11	889	995	-231
3	5	11	498	742	-254
5	5	11	871	872	-248
7	5	11	180	338	-455
9	5	11	506	460	-274
11	5	11	763	1113	-375
13	5	11	1141	1301	229
15	5	11	1098	1016	220
17	5	11	770	968	-405
19	5	11	385	1139	-977
21	5	11	894	981	-476
23	5	11	281	687	-712
-22	6	11	309	225	-781
-20	6	11	499	116	-550
-18	6	11	302	103	-765

Table 71. (continued)

H	K	L	$10F_O$	$10F_C$	10σ
-16	6	11	246	102	-622
-14	6	11	393	45	-298
-12	6	11	482	670	-388
-10	6	11	1496	1496	207
-8	6	11	1438	1541	211
-6	6	11	958	1108	242
-4	6	11	615	680	-260
-2	6	11	790	1051	-300
0	6	11	1658	1762	168
2	6	11	1453	1455	219
4	6	11	370	386	-415
6	6	11	550	635	-297
8	6	11	624	673	-336
10	6	11	241	229	-611
12	6	11	514	179	-289
14	6	11	301	708	-762
16	6	11	865	1044	-429
18	6	11	1347	1027	293
20	6	11	333	536	-844
-21	7	11	926	303	-417
-19	7	11	327	488	-827
-17	7	11	315	209	-797
-15	7	11	761	937	-382
-13	7	11	265	469	-671
-11	7	11	912	937	-353
-9	7	11	1631	1723	333
-7	7	11	728	776	-276
-5	7	11	590	475	-258
-3	7	11	485	373	-303
-1	7	11	1551	1176	201
1	7	11	1900	1895	159
3	7	11	586	781	-286
5	7	11	841	967	-338
7	7	11	1046	1268	256
9	7	11	557	176	-452
11	7	11	605	713	-477
13	7	11	288	188	-729
15	7	11	363	752	-921
17	7	11	913	1033	-510
19	7	11	565	400	-431
-18	8	11	616	154	-464
-16	8	11	558	770	-433
-14	8	11	725	1138	-437
-12	8	11	657	158	-434
-10	8	11	665	1067	-494
-8	8	11	747	980	-421
-6	8	11	864	485	-294
-4	8	11	1069	1241	-289
-2	8	11	281	301	-712
0	8	11	878	1018	-369
2	8	11	811	1013	-394
4	8	11	292	405	-741
6	8	11	1463	1245	233
8	8	11	305	530	-772
10	8	11	721	735	-444
12	8	11	294	844	-745
14	8	11	514	59	-498
16	8	11	329	787	-836
-13	9	11	312	749	-790
-11	9	11	320	109	-810
-9	9	11	302	551	-767
-7	9	11	267	220	-675
-5	9	11	754	1235	-486
-3	9	11	971	1097	-300
-1	9	11	282	87	-715
1	9	11	501	544	-421
3	9	11	269	79	-679
5	9	11	280	782	-711
7	9	11	559	709	-602
9	9	11	664	279	-483
11	9	11	681	851	-454
-6	10	11	335	896	-849
-4	10	11	515	998	-553
-2	10	11	285	562	-722
0	10	11	537	159	-477
2	10	11	287	89	-727
4	10	11	327	325	-826
-26	0	12	542	712	-521
-24	0	12	837	1168	-455
-22	0	12	309	404	-782
-20	0	12	391	474	-336
-18	0	12	571	460	-335
-16	0	12	2440	2409	149
-14	0	12	3426	3446	135
-12	0	12	2265	2399	152
-10	0	12	436	553	-278
-8	0	12	687	413	-227
-6	0	12	2697	2709	124
-4	0	12	3704	3533	107
-2	0	12	1270	1303	154
0	0	12	2267	2071	126
2	0	12	2554	2628	120
4	0	12	674	687	-268
6	0	12	177	178	-447
8	0	12	756	738	-279
10	0	12	2768	2982	156

Table 71. (continued)

H	K	L	$10F_o$	$10F_c$	10σ
12	0	12	3317	3360	154
14	0	12	1700	1765	225
16	0	12	232	6	-588
20	0	12	736	1083	-497
22	0	12	345	1173	-874
24	0	12	311	236	-786
-25	1	12	709	888	-522
-23	1	12	281	710	-713
-21	1	12	483	154	-433
-19	1	12	336	85	-409
-17	1	12	1359	1430	203
-15	1	12	2638	2815	149
-13	1	12	2671	2690	135
-11	1	12	1204	1153	201
-9	1	12	353	193	-234
-7	1	12	1266	1403	176
-5	1	12	3130	3139	115
-3	1	12	2573	2377	112
-1	1	12	584	557	-233
1	1	12	2413	2231	124
3	1	12	1708	1510	131
5	1	12	369	119	-270
7	1	12	320	452	-359
9	1	12	2030	1838	173
11	1	12	3186	3126	145
13	1	12	2144	2388	186
15	1	12	401	577	-476
17	1	12	233	51	-591
19	1	12	329	640	-833
21	1	12	778	1111	-517
23	1	12	562	666	-571
25	1	12	305	189	-773
-26	2	12	315	99	-798
-24	2	12	533	426	-524
-22	2	12	557	187	-368
-20	2	12	255	102	-457
-18	2	12	480	635	-339
-16	2	12	1713	1561	160
-14	2	12	1909	1855	161
-12	2	12	1291	1409	202
-10	2	12	371	549	-335
-8	2	12	322	523	-340
-6	2	12	1078	1468	167
-4	2	12	1913	1897	125
-2	2	12	175	533	-442
0	2	12	864	970	185
2	2	12	1123	1097	199
4	2	12	856	708	188
6	2	12	585	507	-257
8	2	12	1132	1165	183
10	2	12	1698	1801	179
12	2	12	2013	1952	159
14	2	12	570	951	-431
16	2	12	649	329	-332
18	2	12	262	334	-473
20	2	12	862	656	-363
22	2	12	276	461	-699
24	2	12	845	76	-438
-25	3	12	320	312	-810
-23	3	12	256	68	-648
-21	3	12	508	309	-404
-19	3	12	705	576	-399
-17	3	12	532	444	-295
-15	3	12	409	333	-305
-13	3	12	527	646	-232
-11	3	12	1011	1230	204
-9	3	12	936	1050	213
-7	3	12	182	260	-462
-3	3	12	174	263	-442
-1	3	12	158	88	-400
1	3	12	188	320	-477
3	3	12	171	64	-432
5	3	12	1049	1050	191
7	3	12	832	903	204
9	3	12	470	625	-349
11	3	12	188	400	-478
13	3	12	617	576	-310
15	3	12	874	771	-288
17	3	12	755	598	-296
19	3	12	285	326	-724
21	3	12	290	120	-733
23	3	12	334	207	-845
-24	4	12	329	650	-835
-22	4	12	291	26	-737
-20	4	12	722	625	-398
-18	4	12	807	393	-321
-16	4	12	638	654	-318
-14	4	12	864	925	-252
-12	4	12	207	138	-525
-10	4	12	1336	1305	187
-8	4	12	888	848	-253
-6	4	12	632	737	-282
-4	4	12	1351	1388	176
-2	4	12	379	732	-377
0	4	12	994	940	184
2	4	12	931	1196	-268

Table 71. (continued)

H	K	L	$10F_o$	$10F_c$	10σ	H	K	L	$10F_o$	$10F_c$	10σ
4	4	12	296	213	-375	8	6	12	243	289	-615
6	4	12	1092	1202	250	10	6	12	1814	1750	244
8	4	12	578	524	-306	12	6	12	897	1903	-582
10	4	12	226	545	-572	14	6	12	657	845	-538
12	4	12	733	784	-259	16	6	12	585	145	-525
14	4	12	528	44	-298	18	6	12	290	53	-736
16	4	12	307	704	-777	20	6	12	524	660	-590
18	4	12	316	466	-801	-19	7	12	615	187	-469
20	4	12	329	285	-833	-17	7	12	662	795	-434
22	4	12	324	635	-820	-15	7	12	1520	1490	330
-23	5	12	623	445	-503	-13	7	12	537	1361	-607
-21	5	12	905	472	-408	-11	7	12	304	621	-773
-19	5	12	316	647	-800	-9	7	12	261	224	-662
-17	5	12	615	539	-417	-7	7	12	519	705	-391
-15	5	12	1831	1889	188	-5	7	12	1467	1389	366
-13	5	12	1196	1584	282	-3	7	12	1255	1111	-342
-11	5	12	197	127	-498	-1	7	12	360	243	-303
-9	5	12	757	1024	-300	1	7	12	1025	1205	223
-7	5	12	187	18	-473	3	7	12	733	937	-280
-5	5	12	1616	1504	162	5	7	12	282	303	-714
-3	5	12	1293	1323	179	7	7	12	278	390	-704
-1	5	12	660	501	-219	9	7	12	972	1225	-477
1	5	12	1901	1908	164	11	7	12	938	1519	-437
3	5	12	824	800	-260	13	7	12	1005	1114	-391
5	5	12	930	1083	-289	15	7	12	296	493	-747
7	5	12	906	1043	222	17	7	12	310	222	-787
9	5	12	198	686	-503	-16	8	12	506	697	-541
11	5	12	1883	1887	184	-14	8	12	627	849	-465
13	5	12	1314	1319	231	-12	8	12	560	991	-558
15	5	12	320	69	-812	-10	8	12	870	1081	-472
17	5	12	834	597	-396	-8	8	12	599	938	-434
19	5	12	294	82	-746	-6	8	12	889	738	-374
21	5	12	388	792	-984	-4	8	12	516	584	-490
-22	6	12	286	101	-725	-2	8	12	266	289	-674
-20	6	12	318	427	-805	0	8	12	233	117	-592
-18	6	12	442	179	-444	2	8	12	269	412	-683
-16	6	12	1050	1549	-395	4	8	12	772	680	-485
-14	6	12	1719	2094	309	6	8	12	743	872	-459
-12	6	12	896	1007	213	8	8	12	1272	1058	322
-10	6	12	215	329	-545	10	8	12	1072	1006	-473
-8	6	12	190	166	-481	12	8	12	994	848	-407
-6	6	12	1216	1088	229	14	8	12	792	762	-486
-4	6	12	1707	1726	178	-11	9	12	720	1117	-481
-2	6	12	224	366	-568	-9	9	12	1107	1368	-360
0	6	12	1479	1411	168	-7	9	12	1074	835	-275
2	6	12	1498	1603	210	-5	9	12	278	142	-705
4	6	12	230	81	-582	-3	9	12	439	58	-523
6	6	12	235	751	-594	-1	9	12	254	219	-644

H	K	L	10F$_o$	10F$_c$	10σ	H	K	L	10F$_o$	10F$_c$	10σ
1	9	12	283	373	-717	12	2	13	2169	2183	190
3	9	12	631	96	-577	14	2	13	678	633	-341
5	9	12	632	874	-559	16	2	13	731	892	-263
7	9	12	1090	1229	-391	18	2	13	615	839	-490
9	9	12	316	862	-801	20	2	13	827	109	-423
-25	1	13	360	833	-912	22	2	13	308	376	-779
-23	1	13	323	698	-818	-25	3	13	1200	1418	-315
-21	1	13	310	28	-788	-23	3	13	1221	1307	-373
-19	1	13	264	277	-671	-21	3	13	264	329	-669
-17	1	13	699	371	-250	-19	3	13	879	61	-341
-15	1	13	1198	1292	273	-17	3	13	912	1078	215
-13	1	13	909	1120	213	-15	3	13	2254	2324	158
-11	1	13	182	41	-462	-13	3	13	1614	1812	186
-9	1	13	864	1067	-271	-11	3	13	195	261	-493
-7	1	13	404	662	-335	-9	3	13	1426	1492	171
-5	1	13	192	348	-486	-7	3	13	208	598	-526
-3	1	13	377	384	-303	-5	3	13	1121	1067	159
-1	1	13	857	915	189	-3	3	13	224	573	-565
1	1	13	1935	1886	134	-1	3	13	1967	1929	144
3	1	13	1508	1430	146	1	3	13	3665	3742	123
5	1	13	417	14	-263	3	3	13	2925	2875	126
7	1	13	209	362	-529	5	3	13	584	632	-249
9	1	13	230	775	-584	7	3	13	185	73	-470
11	1	13	1453	1481	230	9	3	13	1218	1443	194
13	1	13	1363	1237	262	11	3	13	2486	2382	161
15	1	13	252	61	-638	13	3	13	1641	1482	231
17	1	13	501	622	-542	15	3	13	253	286	-640
19	1	13	684	340	-465	17	3	13	881	1018	-513
21	1	13	347	142	-878	19	3	13	315	303	-798
23	1	13	301	86	-762	21	3	13	452	369	-556
-24	2	13	1324	1333	-341	-22	4	13	317	772	-804
-22	2	13	303	714	-766	-20	4	13	296	253	-749
-20	2	13	252	121	-640	-16	4	13	1511	1653	241
-18	2	13	243	261	-441	-14	4	13	1780	2020	186
-16	2	13	1882	1670	171	-12	4	13	591	1038	-403
-14	2	13	2067	2088	150	-10	4	13	213	401	-540
-12	2	13	225	561	-568	-8	4	13	226	746	-573
-10	2	13	1221	1338	219	-6	4	13	180	19	-457
-8	2	13	1293	1465	159	-4	4	13	203	367	-512
-6	2	13	191	325	-484	-2	4	13	617	819	-333
-4	2	13	1213	1259	168	0	4	13	2620	2695	135
-2	2	13	428	403	-233	2	4	13	2885	2954	137
0	2	13	2800	2681	125	4	4	13	1655	1665	181
2	2	13	3236	3242	127	6	4	13	348	407	-350
4	2	13	1404	1261	191	8	4	13	782	768	-246
6	2	13	435	248	-234	10	4	13	1474	1695	219
8	2	13	585	508	-281	12	4	13	1545	1654	237
10	2	13	2289	2110	161	14	4	13	250	458	-633

H	K	L	10F_O	10F_C	10σ	H	K	L	10F_O	10F_C	10σ
16	4	13	302	522	-767	-7	7	13	253	236	-641
18	4	13	844	486	-416	-5	7	13	588	1021	-366
20	4	13	301	20	-761	-3	7	13	827	1112	-384
-21	5	13	322	629	-816	-1	7	13	223	142	-565
-19	5	13	719	780	-430	1	7	13	287	569	-728
-17	5	13	658	1109	-463	3	7	13	600	17	-325
-15	5	13	808	1272	-388	5	7	13	1027	1184	-346
-13	5	13	497	963	-445	7	7	13	1095	1405	-312
-11	5	13	656	438	-247	9	7	13	314	458	-794
-7	5	13	280	84	-354	11	7	13	294	437	-746
-5	5	13	223	285	-564	13	7	13	318	349	-806
-3	5	13	811	720	-244	15	7	13	519	323	-492
-1	5	13	1231	1423	175	-12	8	13	303	113	-768
1	5	13	1481	1752	181	-10	8	13	902	1007	-432
3	5	13	1289	1396	192	-8	8	13	886	885	-451
5	5	13	826	1048	-323	-6	8	13	275	317	-696
7	5	13	737	1039	-331	-4	8	13	754	1055	-458
9	5	13	1017	1183	202	-2	8	13	296	439	-749
11	5	13	711	1141	-509	0	8	13	267	753	-676
13	5	13	710	491	-445	2	8	13	311	900	-786
15	5	13	275	19	-697	4	8	13	293	195	-740
17	5	13	280	156	-709	6	8	13	924	1098	-463
19	5	13	310	149	-785	8	8	13	498	660	-468
-20	6	13	706	857	-431	10	8	13	703	447	-480
-18	6	13	320	939	-809	-7	9	13	274	219	-697
-16	6	13	314	559	-793	-5	9	13	294	447	-746
-14	6	13	226	235	-571	-3	9	13	489	377	-486
-12	6	13	247	374	-625	-1	9	13	323	461	-818
-10	6	13	532	748	-420	1	9	13	672	1039	-476
-8	6	13	562	550	-315	3	9	13	318	554	-804
-6	6	13	671	360	-280	5	9	13	274	322	-695
-4	6	13	605	1053	-394	-24	0	14	830	1497	-479
-2	6	13	981	992	219	-22	0	14	311	709	-787
0	6	13	510	544	-360	-20	0	14	321	298	-812
2	6	13	384	351	-319	-18	0	14	450	202	-492
4	6	13	813	846	-262	-16	0	14	705	868	-325
6	6	13	1777	1457	214	-14	0	14	1006	1234	254
8	6	13	1296	1244	256	-12	0	14	611	562	-299
10	6	13	535	586	-450	-10	0	14	2927	2932	146
12	6	13	282	45	-715	-8	0	14	3293	3163	131
14	6	13	290	46	-736	-6	0	14	1166	1143	181
16	6	13	293	302	-744	-4	0	14	342	233	-362
18	6	13	268	155	-678	-2	0	14	1228	1098	171
-17	7	13	294	406	-745	0	0	14	3295	3079	118
-15	7	13	308	443	-779	2	0	14	3357	3266	131
-13	7	13	480	353	-529	4	0	14	1315	1382	222
-11	7	13	644	654	-451	6	0	14	808	729	-269
-9	7	13	945	1133	-471	8	0	14	791	680	-257

H	K	L	$10F_O$	$10F_C$	10σ
10	0	14	946	827	230
12	0	14	876	858	-349
14	0	14	426	691	-407
16	0	14	2080	1900	311
18	0	14	1796	1720	297
20	0	14	383	632	-970
22	0	14	298	99	-754
-23	1	14	910	1113	-409
-21	1	14	292	169	-740
-19	1	14	737	371	-406
-17	1	14	253	182	-639
-15	1	14	933	999	-290
-13	1	14	850	506	-259
-11	1	14	1594	1474	156
-9	1	14	2828	2751	151
-7	1	14	1907	1921	160
-5	1	14	376	383	-342
-3	1	14	314	558	-345
-1	1	14	2394	2214	142
1	1	14	3298	3073	126
3	1	14	2126	2089	160
5	1	14	214	107	-541
7	1	14	938	888	-247
9	1	14	199	137	-505
11	1	14	1210	993	178
13	1	14	222	149	-562
15	1	14	1378	1238	-418
17	1	14	1505	1698	-385
19	1	14	349	1028	-885
21	1	14	319	288	-807
-24	2	14	512	820	-581
-20	2	14	286	18	-724
-18	2	14	250	26	-634
-16	2	14	277	384	-699
-14	2	14	240	505	-609
-12	2	14	359	187	-374
-10	2	14	1242	1221	176
-8	2	14	1532	1447	170
-6	2	14	582	873	-316
-4	2	14	508	834	-352
-2	2	14	1544	1435	166
0	2	14	1795	1958	156
2	2	14	1993	1682	147
4	2	14	859	805	-257
6	2	14	204	128	-516
8	2	14	202	163	-512
10	2	14	223	338	-566
12	2	14	246	301	-624
16	2	14	619	881	-545
18	2	14	661	803	-443
20	2	14	728	518	-464
-23	3	14	769	169	-442
-21	3	14	282	325	-713
-19	3	14	585	381	-425
-17	3	14	535	131	-381
-15	3	14	252	121	-640
-13	3	14	335	88	-366
-11	3	14	345	51	-322
-9	3	14	196	158	-498
-7	3	14	220	461	-559
-5	3	14	573	909	-307
-3	3	14	1249	1073	197
-1	3	14	768	731	-230
1	3	14	446	512	-287
3	3	14	704	668	-271
5	3	14	759	615	-239
7	3	14	211	353	-535
9	3	14	323	86	-385
11	3	14	208	211	-527
13	3	14	272	255	-689
15	3	14	290	205	-733
17	3	14	300	76	-759
19	3	14	342	243	-868
21	3	14	932	406	-421
-22	4	14	652	155	-430
-20	4	14	630	736	-356
-18	4	14	579	560	-484
-14	4	14	300	808	-759
-12	4	14	246	29	-447
-10	4	14	802	957	-234
-8	4	14	743	933	-303
-4	4	14	729	1218	-386
-2	4	14	370	596	-316
0	4	14	504	813	-378
2	4	14	628	888	-303
4	4	14	364	159	-390
6	4	14	1001	1070	-287
8	4	14	661	582	-273
10	4	14	661	457	-227
12	4	14	721	818	-390
14	4	14	249	227	-630
16	4	14	306	484	-773
18	4	14	490	503	-607
-19	5	14	303	868	-769
-17	5	14	673	181	-401
-15	5	14	797	837	-410

Table 71. (continued)

H	K	L	$10F_o$	$10F_c$	10σ
-13	5	14	761	661	-406
-11	5	14	308	728	-781
-9	5	14	1551	1601	164
-7	5	14	848	867	189
-5	5	14	594	565	-259
-3	5	14	478	645	-333
-1	5	14	804	974	-266
1	5	14	1869	2007	182
3	5	14	1148	1131	211
5	5	14	650	581	-258
7	5	14	915	1035	-353
9	5	14	241	35	-613
11	5	14	1363	955	292
13	5	14	930	623	-362
15	5	14	742	444	-494
-18	6	14	504	412	-608
-16	6	14	302	431	-766
-14	6	14	375	818	-950
-12	6	14	733	93	-389
-10	6	14	1033	1419	-404
-8	6	14	1577	1576	298
-6	6	14	283	482	-715
-4	6	14	241	254	-610
-2	6	14	278	550	-705
0	6	14	1700	1873	243
2	6	14	1475	1929	319
4	6	14	298	499	-755
6	6	14	451	563	-562
8	6	14	303	346	-769
10	6	14	302	582	-764
12	6	14	336	724	-851
14	6	14	292	132	-742
16	6	14	836	1003	-467
-15	7	14	556	492	-485
-13	7	14	293	185	-742
-11	7	14	1094	750	-339
-9	7	14	845	1410	-376
-7	7	14	344	1089	-872
-5	7	14	409	479	-488
-3	7	14	324	520	-820
-1	7	14	1378	1204	244
1	7	14	1432	1663	-364
3	7	14	719	1147	-465
5	7	14	282	275	-716
7	7	14	273	69	-694
9	7	14	246	152	-625
11	7	14	680	352	-394
-10	8	14	301	595	-761
-8	8	14	640	799	-508
-6	8	14	839	885	-472
-4	8	14	329	954	-836
0	8	14	875	971	-387
2	8	14	671	880	-550
4	8	14	617	645	-456
6	8	14	562	413	-478
8	8	14	304	217	-771
-23	1	15	304	332	-772
-21	1	15	855	232	-405
-19	1	15	845	605	-410
-17	1	15	274	350	-694
-15	1	15	215	134	-544
-13	1	15	433	19	-249
-11	1	15	707	855	-332
-9	1	15	1424	1459	222
-7	1	15	984	878	-250
-5	1	15	187	206	-475
-3	1	15	536	527	-307
-1	1	15	176	356	-447
1	1	15	930	1146	-244
3	1	15	432	516	-293
5	1	15	652	615	-291
7	1	15	1349	1208	188
9	1	15	477	607	-374
11	1	15	417	166	-294
13	1	15	319	145	-810
15	1	15	300	510	-759
17	1	15	320	720	-810
19	1	15	880	427	-480
-22	2	15	327	42	-829
-20	2	15	303	988	-766
-18	2	15	323	963	-819
-16	2	15	235	94	-595
-12	2	15	250	562	-448
-10	2	15	2158	2091	156
-8	2	15	2289	2288	158
-6	2	15	575	843	-287
-4	2	15	490	452	-246
-2	2	15	181	50	-459
0	2	15	1297	1271	223
2	2	15	1095	1258	240
4	2	15	760	349	-223
6	2	15	1239	1641	281
8	2	15	1569	1501	186
10	2	15	267	227	-480
12	2	15	294	322	-746
14	2	15	298	471	-755

Table 71. (continued)

H	K	L	$10F_o$	$10F_c$	10σ
16	2	15	1234	1244	-437
18	2	15	981	1120	-474
20	2	15	322	296	-816
-21	3	15	327	653	-828
-19	3	15	1236	1286	291
-17	3	15	508	762	-560
-15	3	15	795	64	-359
-13	3	15	245	171	-620
-11	3	15	1980	1667	144
-9	3	15	2959	2725	153
-7	3	15	1876	1866	165
-5	3	15	199	167	-503
-3	3	15	390	365	-337
-1	3	15	631	854	-325
1	3	15	1420	1628	188
3	3	15	673	607	-294
5	3	15	1537	1244	210
7	3	15	1965	1882	173
9	3	15	311	1035	-790
11	3	15	418	63	-498
13	3	15	277	254	-702
15	3	15	1076	1261	-430
17	3	15	1790	1638	340
19	3	15	920	921	-506
-20	4	15	537	831	-584
-18	4	15	327	1012	-829
-16	4	15	443	568	-453
-14	4	15	270	372	-683
-12	4	15	317	1032	-804
-10	4	15	1728	2094	246
-8	4	15	2279	2186	132
-6	4	15	768	978	-220
-4	4	15	346	84	-343
-2	4	15	204	262	-516
0	4	15	1280	1154	200
2	4	15	706	1081	-345
4	4	15	228	165	-410
6	4	15	1025	1296	-427
8	4	15	638	1294	-608
10	4	15	290	610	-733
12	4	15	270	436	-686
14	4	15	309	1022	-780
16	4	15	1077	1551	-448
-17	5	15	318	628	-804
-15	5	15	555	676	-424
-13	5	15	349	838	-885
-11	5	15	1150	1154	-354
-9	5	15	1428	1406	236
-7	5	15	1279	1237	271
-5	5	15	613	720	-397
-3	5	15	532	631	-430
-1	5	15	259	669	-655
1	5	15	259	522	-656
3	5	15	260	56	-658
5	5	15	468	444	-513
7	5	15	301	748	-762
9	5	15	1034	728	-361
11	5	15	750	838	-395
13	5	15	341	924	-863
15	5	15	869	1042	-457
-16	6	15	699	561	-443
-14	6	15	353	905	-894
-12	6	15	328	731	-831
-10	6	15	269	432	-681
-8	6	15	267	496	-678
-6	6	15	538	860	-510
-4	6	15	1071	1174	-314
-2	6	15	891	958	-345
0	6	15	261	148	-660
2	6	15	417	406	-523
4	6	15	270	294	-683
6	6	15	573	142	-383
8	6	15	760	285	-434
10	6	15	656	775	-548
12	6	15	857	951	-531
-11	7	15	305	67	-773
-9	7	15	498	267	-412
-7	7	15	502	229	-516
-5	7	15	722	1020	-465
-3	7	15	1181	1115	298
-1	7	15	517	191	-483
1	7	15	299	755	-757
3	7	15	277	565	-700
5	7	15	548	193	-408
7	7	15	618	418	-398
9	7	15	312	214	-791
-4	8	15	685	872	-442
-2	8	15	619	369	-465
0	8	15	235	673	-596
-20	0	16	1051	1602	-535
-18	0	16	1051	1590	-362
-16	0	16	346	569	-877
-14	0	16	262	89	-664
-12	0	16	610	742	-381
-10	0	16	2031	2094	148
-8	0	16	1752	1900	164

H	K	L	$10F_O$	$10F_C$	10σ
-6	0	16	367	40	-368
-4	0	16	1124	1508	255
-2	0	16	1238	1300	230
0	0	16	212	27	-536
2	0	16	227	252	-574
4	0	16	1643	1365	201
6	0	16	2720	2758	195
8	0	16	1917	2047	265
10	0	16	309	588	-782
12	0	16	288	123	-728
14	0	16	611	617	-458
16	0	16	924	1234	-507
18	0	16	833	903	-518
-21	1	16	774	1026	-466
-19	1	16	862	1573	-560
-17	1	16	672	1076	-450
-15	1	16	269	192	-679
-13	1	16	499	250	-396
-11	1	16	1059	1297	-352
-9	1	16	1857	1861	142
-7	1	16	484	822	-326
-5	1	16	712	762	-251
-3	1	16	1490	1282	207
-1	1	16	420	567	-342
1	1	16	193	218	-489
3	1	16	359	522	-438
5	1	16	1880	2023	172
7	1	16	2317	2316	130
9	1	16	315	1191	-798
11	1	16	303	198	-767
13	1	16	320	238	-809
17	1	16	1016	930	-470
-20	2	16	278	889	-705
-18	2	16	824	991	-419
-16	2	16	280	626	-708
-14	2	16	594	363	-364
-12	2	16	516	588	-479
-10	2	16	480	930	-464
-8	2	16	547	713	-258
-6	2	16	457	24	-285
-4	2	16	440	554	-304
-2	2	16	483	589	-324
0	2	16	519	296	-245
2	2	16	209	289	-528
4	2	16	1045	961	192
6	2	16	939	1490	-392
8	2	16	1215	1266	307
10	2	16	528	590	-529
12	2	16	535	374	-527
14	2	16	273	410	-690
16	2	16	298	506	-755
-19	3	16	632	192	-410
-17	3	16	304	451	-769
-15	3	16	309	683	-781
-13	3	16	740	617	-412
-11	3	16	283	304	-719
-9	3	16	253	77	-642
-7	3	16	295	96	-748
-5	3	16	233	90	-589
-3	3	16	251	28	-452
-1	3	16	525	285	-206
1	3	16	520	600	-259
3	3	16	248	537	-630
5	3	16	285	398	-723
7	3	16	537	319	-470
9	3	16	242	378	-611
11	3	16	923	562	-353
13	3	16	338	563	-856
15	3	16	749	162	-372
-18	4	16	523	367	-420
-16	4	16	305	407	-772
-14	4	16	885	806	-366
-12	4	16	762	283	-380
-10	4	16	582	657	-419
-8	4	16	1042	749	-347
-6	4	16	239	149	-606
-4	4	16	581	840	-501
-2	4	16	492	339	-424
0	4	16	804	616	-329
2	4	16	613	843	-365
4	4	16	267	63	-674
6	4	16	547	730	-644
8	4	16	273	485	-694
10	4	16	313	315	-792
12	4	16	578	720	-502
14	4	16	831	184	-420
-15	5	16	546	375	-556
-13	5	16	453	383	-523
-11	5	16	700	554	-405
-9	5	16	627	1175	-481
-7	5	16	425	399	-473
-5	5	16	291	976	-738
-3	5	16	820	1253	-414
-1	5	16	268	116	-678
1	5	16	1001	891	-343
3	5	16	880	409	-354

H	K	L	$10F_o$	$10F_c$	10σ
5	5	16	736	902	-427
7	5	16	1293	1349	-366
9	5	16	303	565	-769
11	5	16	307	384	-779
13	5	16	475	330	-560
-12	6	16	238	266	-604
-10	6	16	374	973	-948
-8	6	16	301	836	-764
-6	6	16	595	292	-410
-4	6	16	1109	1150	-383
-2	6	16	315	775	-799
0	6	16	269	235	-680
2	6	16	672	344	-367
4	6	16	456	588	-537
6	6	16	923	1441	-415
8	6	16	564	1175	-564
10	6	16	489	258	-520
-7	7	16	287	339	-729
-5	7	16	518	365	-407
-3	7	16	656	670	-497
-1	7	16	291	355	-738
1	7	16	288	158	-729
3	7	16	855	516	-305
-17	1	17	643	302	-420
-15	1	17	339	348	-859
-13	1	17	310	505	-784
-11	1	17	250	21	-633
-9	1	17	290	372	-734
-7	1	17	261	35	-659
-5	1	17	564	930	-418
-3	1	17	638	1091	-459
-1	1	17	294	464	-745
1	1	17	242	153	-615
3	1	17	255	12	-648
5	1	17	939	784	-420
7	1	17	726	1058	-365
9	1	17	292	473	-741
11	1	17	620	222	-504
13	1	17	629	317	-544
15	1	17	654	10	-380
-18	2	17	531	955	-581
-16	2	17	617	58	-461
-14	2	17	624	847	-477
-12	2	17	270	471	-684
-10	2	17	253	445	-644
-8	2	17	790	441	-310
-6	2	17	453	829	-441
-4	2	17	2071	1869	244
-2	2	17	1356	1474	274
0	2	17	418	313	-520
4	2	17	321	653	-812
6	2	17	1608	1672	311
8	2	17	802	1289	-551
10	2	17	696	106	-413
12	2	17	779	608	-342
14	2	17	897	340	-406
-15	3	17	740	450	-386
-13	3	17	307	671	-775
-11	3	17	224	153	-569
-9	3	17	519	669	-489
-7	3	17	554	212	-418
-5	3	17	1009	1718	-454