SYNTHESIS AND CHARACTERIZATION OF

TRIORGANOPHOSPHINEGOLD(I)

THIOLATES

by

PETER D. COOKSON B.Sc. (Hons)

Thesis submitted for the degree of
Master of Science
in
The Department of Chemistry
of the
University of Adelaide

June, 1993

Awarded 1994

Additional References for Chapter 1.

B.M. Sutton, *Gold Bull.*, **19**, 15 (1986).

R.V. Parish and S.M. Cottrill, *Gold Bull.*, **20**, 3 (1987).

A.J. Lewis and D.T. Walz, *Prog. Med. Chem.*, **19**, 1 (1982).

R. Koch, *Deut. Med. Wochenschr.*, **16**, 756 (1890).

C. Bruck and A. Glück, *Muenchen. Med. Wochenschr.*, **60**, 57 (1913).

F. Junker, *Muenchen. Med. Wochenschr.*, **60**, 1376 (1913).

K. Landé, *Muenchen. Med. Wochenschr.*, **74**, 1132 (1927).

I. Haiduc and C. Silvestru, *Coord. Chem. Rev.*, **99**, 253 (1990).

B.M. Sutton, E. McGusty, D.T. Walz and M.J. DiMartino, *J. Med. Chem.*, **15**, 1095 (1972).

G.G. Graham, J.R. Bales, M.C. Grootveld and P.J. Sadler, *J. Inorg. Biochem.*, **25**, 163 (1985).

G.G. Graham, T.M. Haavisto, H.M. Jones and G.D. Champion, *Biochem. Pharmacol.*, **33**, 1257 (1984).

T. Stelmaszynska and J.M. Zgliczynski, in *Cyanide in Biology*, Academic Press, pg 371 (1981).

D.R. Haynes and M.W. Whitehouse, in *New Developments in Antirheumatic Therapy*, K.D. Rainsford and G.P. Velo (Eds.), *Inflammation and Drug Therapy Series*, Vol. III, pg 207 (1989).

Amended version of Table 4.4.2.

Complex	H^2	H^9	H^8	Phenyl Protons	H_a	H_b
6-MPH	8.45(s)	13.62(br,s)	8.26(s)	-	-	-
[dppm(Au(6-MP))$_2$]	8.36(s)	13.12(br,s)	8.17(s)	7.95 - 7.37(br,m)	4.64(m)	-
[dppe(AuCl)(Au(6-MP))]	8.36(s)	13.25(br,s)	8.09(s)	7.87 - 7.47(br,m)	3.02(m)	-
[dppe(Au(6-MP))$_2$]	8.37(s)	13.13(br,s)	8.24(s)	7.89 - 7.49(br,m)	3.04(m)	-
[dppp(AuCl)(Au(6-MP))]	8.40(s)	13.22(br,s)	8.20(s)	7.74 - 7.50(br,m)	3.07(m)	1.73(m)
[dppp(Au(6-MP))$_2$]	8.38(s)	13.18(br,s)	8.19(s)	7.83 - 7.42(br,m)	3.16(m)	1.89(m)

Note: Coupling constants, in parentheses, are in units of Hertz: a: $^3J_{H-H}$, b: $^3J_{P-H}$ and c: $^2J_{P-H}$.

DECLARATION

This work contains no material which has been accepted for the award of any other degree or diploma in any university or other institution and, to the best of my knowledge and belief, contains no material previously published or written by another person, except where due reference has been made in the text.

I give consent to this copy of my thesis, when deposited in the University Library, being available for photocopying and loan.

SIGNED: DATE: 15/8/93

ACKNOWLEDGEMENTS

ABSTRACT

The aim of this work was to synthesize a range of novel triorganophosphinegold(I) 6-mercaptopurinate complexes and to evaluate their potential anti-arthritic activity. The resultant complexes are based on the P–Au–S moiety, structurally related to the widely available pharmaceutical Auranofin, where the phosphorus atom is part of a triethylphosphine ligand and the sulphur atom derived from a tetraacetylated thioglucose anion.

Via alteration of the identity of the triorganophosphine group, a variety of complexes were synthesized from triorganophosphinegold(I) chloride precursors, falling into three main types: 1) triorganophosphinegold(I) 6-mercaptopurinate complexes with the general formula [R_3PAu(6-MP)], where R_3P = Et_3P, $Cycl_3P$, $PhMe_2P$, Ph_3P, (o-Tol)$_3$P, (m-Tol)$_3$P or (p-Tol)$_3$P; 2) [μ-1,n-bis(diphenylphosphino)alkane]gold(I) chloride gold(I) 6-mercaptopurinate complexes with the general formula [($Ph_2P(CH_2)_nPPh_2$)(AuCl)(Au(6-MP))] where n = 2 or 3; and 3) [μ-1,n-bis(diphenylphosphino)alkane]bis(gold(I) 6-mercaptopurinate) complexes with the general formula [($Ph_2P(CH_2)_nPPh_2$)(Au(6-MP))$_2$] where n = 1, 2 or 3. These complexes and the triorganophosphinegold(I) chloride precursors were characterized using multinuclear magnetic resonance, infrared and Fast Atom Bombardment mass spectroscopic techniques. Unambiguous structure determinations of a selection of the complexes were achieved by single crystal X-ray crystallographic methods. Unit cell dimensions were: [$PhMe_2PAuCl$], orthorhombic space group $P2_12_12_1$, a = 12.639(4), b = 16.931(6), c = 9.458(3) Å, V = 2024(1) Å^3 and Z = 4; [Ph_3PAu(6-MP)].C_2H_5OH, triclinic space group $P\bar{1}$, a = 11.066(3), b = 13.552(3), c = 8.705(2) Å, α = 91.51(2), β = 113.06(2), γ = 89.69(2)°, V = 1200.8(5) Å^3 and Z = 2; and [(o-Tol)$_3$PAu(6-MP)].C_2H_5OH, monoclinic space group $P2_1/n$, a = 10.067(2), b = 10.518(2), c = 25.416(4) Å, β = 98.42(2)°, V = 2662.1(9) Å^3 and Z = 4. The structures were refined to final R values of 0.035, 0.034 and 0.040, respectively, for reflections satisfying the $I \geq 3.0\sigma(I)$ criterion: 1608, 3978 and 4183, respectively. The results for [$PhMe_2PAuCl$] were utilized, in part, for a cone-angle to bond length correlation

study on triorganophosphinegold(I) chloride complexes. The structures of [Ph$_3$PAu(6-MP)] and [(o-Tol)$_3$PAu(6-MP)] revealed a near linear P–Au–S chromophore, with angles of 173.71(6) and 177.03(8)°, respectively. A crystal structure analysis of a closely related triorganophosphinegold(I) thiolate complex, [Cycl$_3$PAu(6p2-TU)], revealed a similar P–Au–S chromophore with an angle of 177.6(1)°. Unit cell dimensions were: monoclinic space group $P2_1/c$, a = 9.539(2), b = 16.452(4), c = 16.880(2) Å, β = 95.37(2)°, V = 2637.4(8) Å^3 and Z = 4. The final refinement value was R = 0.043, for 3695 reflections with $I \geq 3.0\sigma(I)$. The results for the three thiolate complexes were utilized in a correlation study of cone-angles to intramolecular parameters for triorganophosphinegold(I) thiolate complexes in general.

The combined microanalytical, spectroscopic and crystallographic studies verified the formation of all the thionucleobase complexes mentioned above and demonstrated that the gold centre is linearly bound to both the phosphorus and sulphur atoms.

A number of the triorganophosphinegold(I) 6-mercaptopurinate complexes were tested for their anti-arthritic activity in Dark Agouti rats with promising results.

ABBREVIATIONS

Å	Angström
br	broad
°C	degree Celsius
^{13}C NMR	carbon-13 nuclear magnetic resonance
Cycl	cyclohexyl
d	doublet
dd, dm, dt	doublet of doublets, multiplets, triplets
dec.	decomposition point
dppe	μ-1,2-bis(diphenylphosphino)ethane
dppm	μ-bis(diphenylphosphino)methane
dppp	μ-1,3-bis(diphenylphosphino)propane
Et	ethyl
FAB-MS	Fast Atom Bombardment - mass spectroscopy
g	gram
^{1}H NMR	proton nuclear magnetic resonance
Hz	hertz
IR, ir	infrared spectroscopy
$^{x}J_{AB}$	coupling constant between nuclei A and B over x bonds
m	multiplet (nmr)
m	medium (ir)
M	molar (mol dm^{-3})
[M]$^{+}$	molecular ion
2mbaH	2-mercpatobenzoic acid
6m2-TUH	6-methyl-2-thiouracil
Me	methyl
MHz	mega-hertz

ml	millilitre
mmol	millimole
m.p.	melting point
6-MPH	6-mercaptopurine
MW	molecular weight
m/z	mass to charge ratio
6p2-TUH	6-n-propyl-2-thiouracil
NMR, nmr	nuclear magnetic resonance (Fourier Transform)
N.O.	not observed
Obs.	obscured
^{31}P NMR	phosphorus-31 nuclear magnetic resonance
Ph	phenyl
PhO	phenoxy
ppm	parts per million
q	quartet
s	singlet (nmr)
s	strong (ir)
sh	shoulder
t	triplet
TMS	tetramethylsilane
m-Tol	*meta*-tolyl
o-Tol	*ortho*-tolyl
p-Tol	*para*-tolyl
2-TUH	2-thiouracil
vs	very strong
w	weak
%Y	percentage yield
δ(A–B)	bending frequency of A–B bond
λ	wavelength
ν(A–B)	stretching frequency of A–B bond

TABLE OF CONTENTS

CHAPTER 1

Introduction

1.1 *Introduction*

Interest in gold(I) compounds has increased in recent years due to the growing importance of certain gold(I) complexes in the treatment of a variety of common ailments. The most well known use of gold compounds in medicine is in the treatment of rheumatoid arthritis, where commercially available drugs are now utilized widely. The compound known as Myochrysine, shown in Figure 1.1, is the lead compound for the treatment of rheumatoid arthritis. Another gold(I) thiolate compound, Auranofin, has been found to be effective in the treatment of both rheumatoid arthritis and cancerous tumours[1,2], while other less well known compounds, such as Solganal, Allochrysine and Sanocrisin (Figure 1.1), are also in current use against rheumatoid arthritis. Whereas Auranofin displays some anti-tumour activity[1,2], the compound bis[μ-1,2-bis(diphenylphosphino)ethane]gold(I) chloride has shown more promising results in the treatment of cancer[3]. However, these are only a few examples of how gold plays a useful role in medicine. In fact, gold has a long history of medicinal applications. This chapter will discuss the history of gold compounds in medicine, and the use of modern day gold compounds, especially the class of compounds known as phosphinegold(I) thiolates, in the treatment of rheumatoid arthritis. The chemistry of gold and the triorganophosphinegold(I) thiolate complexes will be introduced, and how the spectroscopic and crystallographic characterizations of a selection of new triorganophosphinegold(I) thiolates is of interest to this field will be discussed.
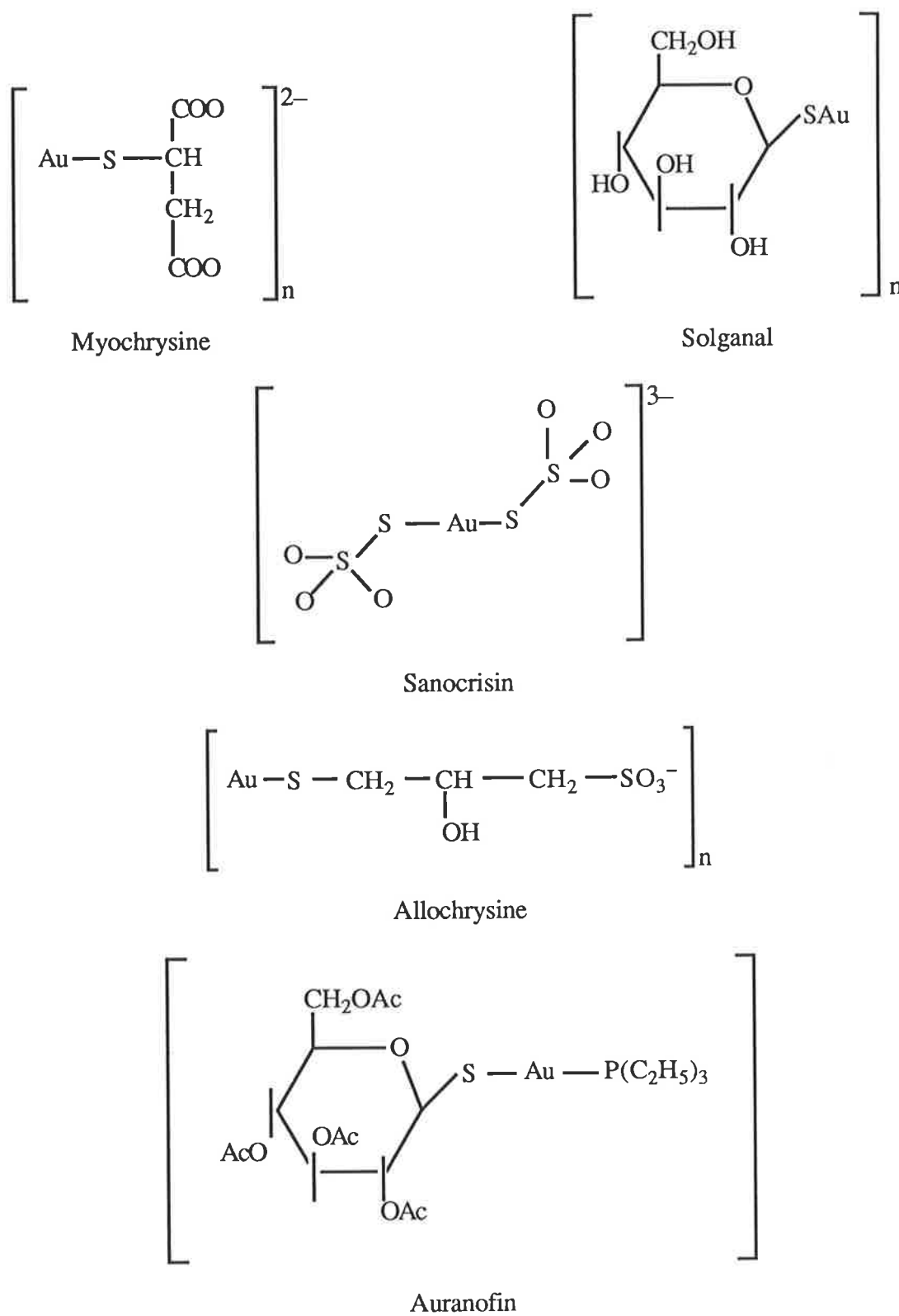
Figure 1.1: *Structures Of Some Biologically Active Gold(I) Thiolates.*

1.2 *History of gold in medicine*

The use of gold in medicine dates back to ancient times. As early as 2500 B.C., Chinese and Arabic physicians were reported to have used gold preparations, whilst Pliny in the 1st century recorded that gold could be used successfully in the cures of such ailments as haemorrhoids, warts and fistulas[4,5]. These early remedies were based on concoctions using metallic gold, and usually associated with ceremonial incantations. Gold was considered a substance of the gods, a holy metal that possessed magical properties: meso-American Indians saw gold as the 'sweat of the sun'; and the Egyptian pharaohs and priests considered it a giver of life, a connection between this world and the next[4,5]. The rarity of gold and its consequent availability to only the rich and the religious only promoted the superstitious aura surrounding the metal. In reality, the chemical inertness of metallic gold meant that it was probably quite inactive in the internal biochemistry of those who used it. Hence any cures that might have resulted could in a large part have been of a purely psychological nature.

In the Middle Ages, gold began to be utilized in a less superstitious manner. While metallic gold was still being used to gild medicinal tablets, and royalty drank wine from gold coated vessels as a tasteful way of consuming the metal, the 'science' of alchemy was coming to the fore. In the 13th century, Geber reported the preparation of the substance *aqua regia* from a combination of mineral acids, now known to be nitric and hydrochloric acids, having the ability to dissolve gold[5]. This was an important discovery, as actual compounds of gold could at last be prepared. However, physicians of the Renaissance expressed little interest in doing so, since the purity of metallic gold was still considered to be the most important factor in the curative properties of the metal[5].

The first significant compound to be prepared after this time was the 'muriate of gold and soda', $Na[AuCl_4]$[5]. The French physician Chrestien in 1811 described this compound as being an effective treatment for syphilis and chronic alcoholism: it is still recognized today as having legitimate effect against at least the former[5]. The advances in medical and scientific knowledge

around this period mark the beginning of modern medicine, and serious investigations into the medicinal applications of gold compounds began.

1.3 *Modern applications of gold in medicine*

The beginning of the role of gold in modern medicine began with the discovery early this century of the effectiveness of aurothioglucose in treating rheumatic fever[5]. Tuberculosis and rheumatoid arthritis were also found to be combatted to some extent by gold compounds[5]. Despite the promising results that emerged, concerns about the toxicity and side-effects of these compounds, which were usually manifested as kidney and liver problems, to a large extent discouraged further investigations in this context[5]. It was the almost accidental discovery of the *in vitro* anti-cancer activity of the platinum based drug cisplatin[6] (a square planar Pt(II) complex: *cis*-diaminodichloroplatinum), shown in Figure 1.3, that renewed interest in the possible medicinal usefulness of platinum group metals, and hence research into gold based drugs gained new momentum.
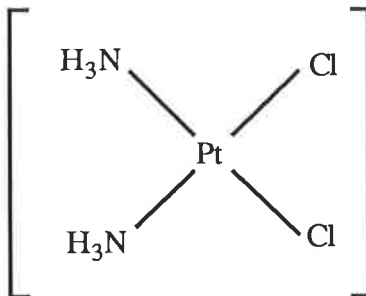
Figure 1.3: *Cisplatin.*

Perhaps the most significant gold compound found to date is Auranofin, discovered in 1972, which is useful in the treatment of rheumatoid arthritis[2]. Recent unpublished results from research conducted in the Department of Chemistry at Adelaide, concentrating on the effect of triorganophosphinegold(I) thionucleobase complexes on rheumatoid arthritis, stems from the success of Auranofin. The project embodied in this thesis is concerned with the characterization of certain triorganophosphinegold(I) thiolate complexes which may also prove to be active against this ailment.

1.4 *Arthritis and treatment with gold complexes*

The debilitating disease of rheumatoid arthritis is characterized by the chronic inflammation of joint tissue about the skeletal connections in the body, and usually leads with time to the disintegration of bone structure in these regions, crippling the sufferer. The biochemical cause for the onset of the disease is still unclear, but the effects can be neutralized in part by the suppression of the inflammatory action. One physical answer is to apply pressure to the region, especially during periods of rest, when swelling of the synovial fluid due to inflammation is at its greatest. The biochemical approach is by application of certain drugs, although the precise biochemical reactions that make such drugs effective are not known.

The field known as chrysotherapy has hence developed, which is generally defined as the treatment of rheumatoid arthritis with gold-based drugs[4]. Of these drugs, the gold compounds depicted in Figure 1.1 have dominated the treatment of this disease. Two classes of compounds are represented: the polymeric type, such as Solganal (gold sodium thiosulphate), Myochrysine (sodium aurothiomalate), Allochrysine (gold sodium thiopropanol sulphonate) and Sanocrisin (gold sodium thiosulphate), and the monomeric type, such as Auranofin (*S*-2,3,4,5-tetraacetyl-1-β-D-thioglucose(triethylphosphine)gold(I)). The administration of these two classes of compounds is determined by their solubilities in bodily fluids: the polymeric compounds are hydrophilic and are thus injected intravenously, while the monomeric species Auranofin is lipophilic, and can be administered orally[1]. In terms of ease and expense of application, the orally administered Auranofin has been found to be the popular compound for routine use.

The difference in solubility and application method might suggest different modes of action for the two classes of compounds. As has been mentioned above, the exact biochemical reactions involved to combat the symptoms of rheumatoid arthritis are not known. A few hypotheses exist, however, as to how the compounds are delivered to the site of inflammation. The polymeric complexes all feature Au–S bonds, and studies on the activity of Myochrysine have revealed that this bond is cleaved in the blood stream in order to create another Au–S bond between the gold and the thiol group of cysteine-34 of a plasma protein albumin[1,7]. The

resultant auroalbumin complex may then undergo ligand exchange to form a dimeric species, which is then ingested by certain immunological macrophages to be transported to the site of disease. Reactive leukocytes at the sites of inflammation have the ability to produce cyanide from glycine, which reacts with gold(I) to form a $[Au(CN)_2]^-$ species, thus concentrating gold in this region. The $[Au(CN)_2]^-$ anion can permeate many types of cell membrane, possibly then interfering with DNA-based functions which lead to the production of inflammatory fluids.

A dose of Auranofin, however, consists of discrete molecules, and the interaction of Auranofin with the albumin protein is likely to be different. Auranofin can be classed as a triorganophosphinegold(I) thiolate: while clinical trials on gold(I) thiolates have proven to be ineffective via oral administration[7], a phosphine group bound to the gold imparts lipid solubility to the complexes, allowing this mode of administration. It is possible for either the phosphine or thiolate group to be cleaved from Auranofin on reaction with albumin. However, the thiolate group seems to be the more labile, and initial binding to the albumin appears to occur via loss of thiolate[1]. The phosphine group can be substituted for another thiol molecule accompanied by oxidation of the phosphine, and the gold centre then becomes doubly coordinated by sulphur atoms, and is thus carried to the site of inflammation. The final fate of the gold is hence the same for both polymeric and monomeric compounds, the main differences in activity being due to the initial mode of transportation in the body. This is possibly related to the solubilities of the molecules[8].

In finding other compounds that might be useful in this field, it is necessary to alter the structure of the present compounds in order to obtain complexes of differing solubilities (if we wish to work on the same hypothesis concerning their initial metabolism). The polymeric molecules are restricted in their chemical composition by the ability to form a polymer. Monomeric compounds, however, are neutral and discrete, and the structures of the phosphine and thiolate moieties can potentially be altered to achieve a desired measure of solubility for an orally ingested drug.

1.5 *Recent advances in the treatment of rheumatoid arthritis by triorganophosphinegold(1) thiolates*

Previous work, published and unpublished, has been performed on other compounds analogous to those appearing in this thesis. The utilization of thionucleobases as the thiolate component is a choice that can be based on toxicity; the biological system contains many examples of nucleobases, the most well known being those associated with the macromolecules RNA and DNA. 2-thiouracil (2TUH), the thio analogue of uracil, bound to gold in the complex 2-thiouracilato(triphenylphosphine)gold(I), Figure 1.5.1, has been tested for anti-arthritic activity in a model rat strain and found to be comparable with Auranofin[9]. Other pyrimidine- and purine-based gold(I) phosphines have also been tested in a study[10] which yielded an interesting general result. The best phosphine found in terms of the activity of the resultant gold(I) complex was triphenylphosphine; the triethylphosphine analogues, e.g. Figure 1.5.2, were found to be ineffective and even toxic in some cases. This contrasts with Auranofin, which is active and contains a Et_3P group. Such an anomalous result goes against any structure-activity correlation that might have been forthcoming from the study.
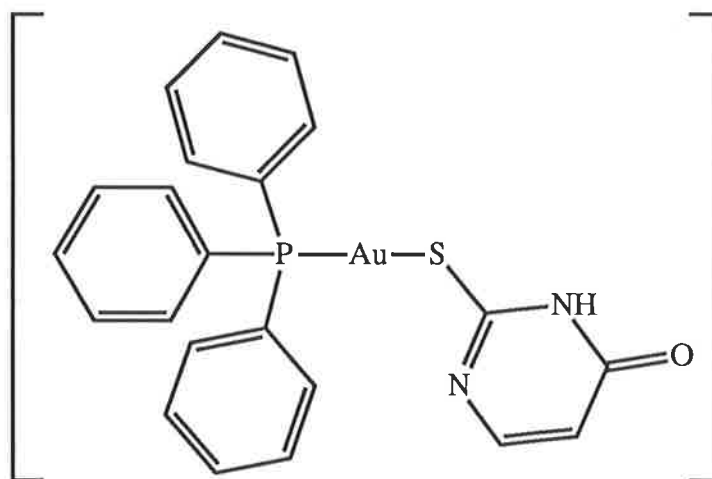
Figure 1.5.1: *2-thiouracilato(triphenylphosphine)gold(I).*

The most effective thionucleobase of those tested was found to be 6-mercaptopurine, with the complex 6-mercaptopurinato(triphenylphosphine)gold(I), [Ph₃PAu(6-MP)], shown in Figure 1.5.3, being even more active against the disease than Auranofin. This compound has already been noted in the literature as having significant antineoplastic activity against leukemia in

8
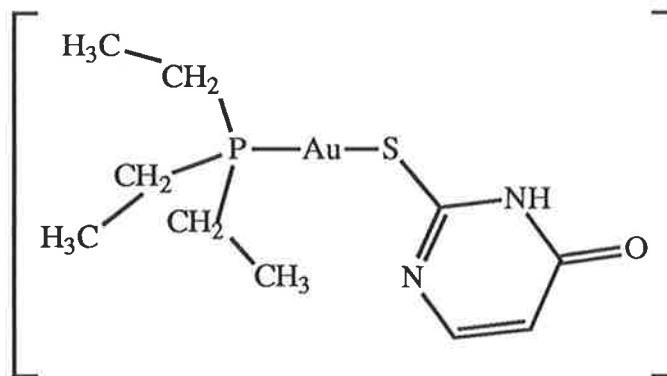
Figure 1.5.2: *2-thiouracilato(triethylphosphine)gold(I)*.

mice[11]. 6-mercaptopurine (6-MPH) itself has been reported as possessing chemotherapeutic activity, notably in the treatment of leukemia[12], and its complexes have shown anti-tumor activity e.g. $Cu(I)(6\text{-}MPH)Cl_2$ and $Cd(6\text{-}MPH)_4Cl_2$[13]. Other uses found have been for the inhibitory action by ribonucleoside analogues on *de novo* purine biosynthesis[14], and against such conditions as urate microcrystal arthritis in poultry[15]. The compound (8-thiotheophyllinato)(triphenylphosphine)gold(I), a structural variant of [Ph₃PAu(6-MP)], has also been effective in the treatment of arthritis, leukemia and cancerous tumours[16,17].
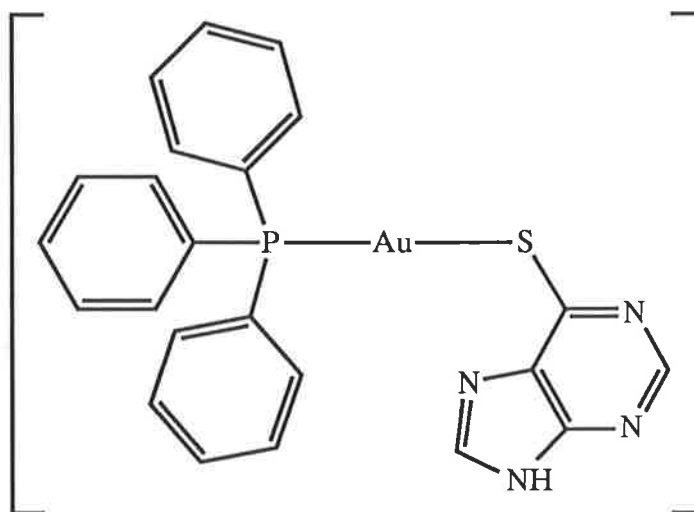
Figure 1.5.3: *6-mercaptopurinato(triphenylphosphine)gold(I)*.

The choice of thiolate for all the complexes prepared in this thesis was thus chosen to be 6-mercaptopurine, and the phosphines chosen were: Et₃P, Cycl₃P, PhMe₂P, Ph₃P, (*o*-Tol)₃P, (*m*-Tol)₃P and (*p*-Tol)₃P, to give complexes of the type [R₃PAu(6-MP)]; and [μ-bis(diphenylphosphino)methane], [μ-1,2-bis(diphenylphosphino)ethane] and [μ-1,3-bis(di-

phenylphosphino)propane], to give mono- and di-substituted compounds of the type shown schematically in Figure 1.5.4.
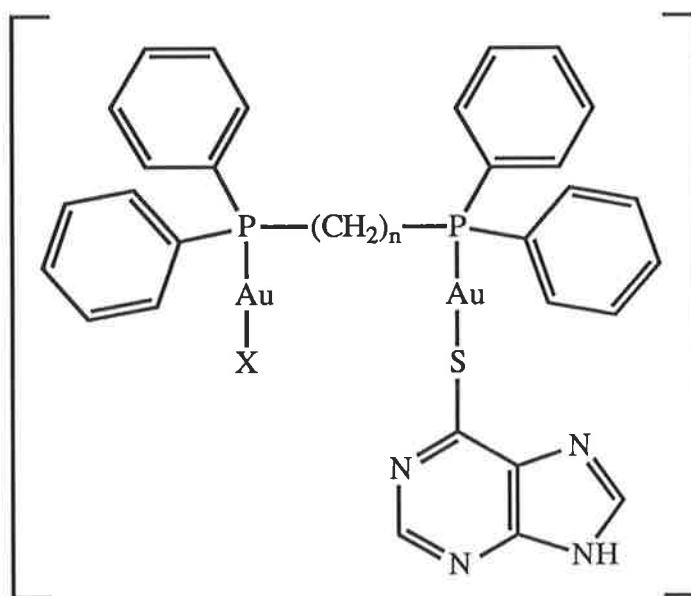
Figure 1.5.4: *Diagram For Mono- And Di-substituted Complexes.*
n = 1, 2 or 3; X = Cl For Mono-substituted, X = 6-MP For Di-substituted.

1.6 *The chemistry of gold and triorganophosphinegold(I) thiolates*

Gold can exist in a variety of oxidation states, but it is dominated in its chemistry by the two most stable states, I and III[18]. Gold(III) has the electronic configuration $[Xe]4f^{14}5d^8$, and is thus isoelectronic with platinum(II). This would suggest that gold(III) complexes analogous to cisplatin might have comparable anti-tumour activity. Some complexes have proven active[1], but the reducing mammalian environment tends to reduce the gold(III) complexes, and so they have not been found to be generally effective. Gold(I), with the stable 'filled shell' electronic configuration of $[Xe]4f^{14}5d^{10}$, is thus better suited to the body's biochemistry, a fact which is illustrated by the variety of anti-arthritic gold(I) compounds already mentioned.

Both gold(III) and gold(I) are soft metal ions, with gold(I) more so, and these ions prefer to bind to soft donor atoms such as sulphur and phosphorus. Whereas a 'naked' gold(I) ion would be transmuted to gold(0) and gold(III) in the body, a gold(I) atom stabilized by sulphur will be less susceptible to oxidation and reduction. The phosphorus of the phosphine ligand is a σ-electron donor, and is also thought to be a π-electron acceptor from the $5d^{10}$ orbital of the gold(I) atom. Thus, both sulphur and phosphorus help to stabilize the gold(I) species.

Triorganophosphinegold(I) thiolates possess certain structural characteristics. Thiolate groups containing one exocyclic sulphur tend to coordinate in a monodentate mode via the sulphur atom to the gold centre. Other possible coordinating atoms or functional groups of the thiolate can associate with the gold but only through secondary interactions. One common feature is the tendency of nitrogen-containing thiolates to orient themselves in the crystal lattice such that the nitrogen is in close proximity to the gold centre. The intramolecular distance is invariably less than the sum of the van der Waals radii. The main feature of these complexes is the presence of a P–Au–S chromophore, found from crystallographic studies to be near linear in most examples regardless as to the identity of the phosphine or thiolate. These structural characteristics were looked for in the crystal structures reported in this thesis, and how they compare to other gold(I) thiolate complexes.

The compounds studied in this thesis were prepared via an established method, involving first the synthesis of a triorganophosphinegold(I) chloride precursor. This is detailed in Chapter 2; briefly, the procedure involved the reduction of an aqueous gold(III) chloride solution, by using thiodiglycol, to give an aqueous gold(I) species, which was then reacted *in situ* with the stoichiometric amount of the desired phosphine. The resultant air-stable triorgano-phosphinegold(I) chloride was then reacted in an equimolar, metathetical reaction with 6-mercaptopurine in the presence of a base.

1.7 *Discussion of results*

The focus of this thesis is on the preparation, spectroscopic characterization and, where appropriate, X-ray crystal structure determination, of series of complexes with the general formulae of [R_3PAu(6-MP)] (where R_3P = Et$_3$P, Cycl$_3$P, PhMe$_2$P, Ph$_3$P, (*o*-Tol)$_3$P, (*m*-Tol)$_3$P or (*p*-Tol)$_3$P), [(Ph$_2$P(CH$_2$)$_n$PPh$_2$)(AuCl)(Au(6-MP))] (where n = 2 or 3), and [(Ph$_2$P(CH$_2$)$_n$PPh$_2$)(Au(6-MP))$_2$] (where n = 1, 2 or 3).

The thesis is divided into three main sections. The first is the experimental section, in which the preparative methods employed will be detailed, along with the instrumentation used. The next two sections are devoted to the spectral characterization of the complexes prepared and of

the triorganophosphinegold(I) chloride precursors that were involved. As little information exists in the literature regarding the characterizations of triorganophosphinegold(I) chlorides, this data has been collected here. The X-ray crystal structure of [PhMe$_2$PAuCl] is presented, followed by a study to find a possible correlation between the phosphine cone-angle and the Au-Cl bond length in triorganophosphinegold(I) chloride complexes. The effects on the 6-mercaptopurine moiety upon complexation to gold are deduced from spectroscopic and crystallographic analyses. The methods utilized were Fast Atom Bombardment mass spectrometry, ^{1}H, ^{13}C and ^{31}P nuclear magnetic resonance spectroscopy and Fourier Transform infrared spectroscopy. X-ray crystallographic techniques were performed on two complexes, [Ph$_3$PAu(6-MP)].C$_2$H$_5$OH and [(o-Tol)$_3$PAu(6-MP)].C$_2$H$_5$OH, in order to confirm the precise nature of the products and to determine what effect the Au–S coordination has on the electronic structure of the 6-mercaptopurinate moiety.

The X-ray crystal structure determination of the complex 6-n-propyl-2-thiouracilato(tricyclohexylphosphine)gold(I), [Cycl$_3$PAu(6p2-TU)], is given, which, along with data from a variety of other triorganophosphinegold(I) thiolates, is utilized in a cone-angle correlation to determine the effect of the phosphine ligand on the P–Au–S chromophore.

A selection of the complexes prepared were assessed for their anti-arthritic activity using the commercially available drugs as standards. The results of these tests are given, where available, with comments on the possible structure / activity correlations. The conclusion summarizes what the characterizations and crystallographic analyses have revealed about the new complexes.

CHAPTER 2

Experimental

2.1 *Introduction*

This chapter comprises three main sections: 1) a description of the experimental methods used in the preparations of the triorganophosphinegold(I) chloride and 6-mercaptopurinate complexes, including the melting points, yields and microanalytical data - examples for the preparation of [Ph₃PAuCl] and [Ph₃PAu(6-MP)] are given; 2) brief notes on the reagents and the instrumentation used for the characterizations; and 3) a general discussion of the instrumentation used and the methods employed in solving the crystal structures detailed in later chapters via an example, namely [(*o*-Tol)₃PAu(6-MP)].C₂H₅OH.

2.2 *Preparation of the complexes*

The preparation of all the complexes was based on a procedure adapted from ref. [19] for the preparation of the compound 2-thiouracilato(triphenylphosphine)gold(I). The procedure involved the equimolar metathetical reaction between triphenylphosphinegold(I) chloride and 2-thiouracil in the presence of a base in an ethanolic solution. This reaction has since been found to be generally applicable for the preparation of analogous complexes containing a variety of phosphines and thionucleobases[10], and so was utilized to prepare the complexes reported in this thesis. General reaction schemes for the preparation of the complexes with the general formulae of [R₃PAu(6-MP)] (where R₃P = Et₃P, Cycl₃P, PhMe₂P, Ph₃P, (*o*-Tol)₃P,

(m-Tol)$_3$P or (p-Tol)$_3$P), [(Ph$_2$P(CH$_2$)$_n$PPh$_2$)(AuCl)(Au(6-MP))] (where n = 2 or 3) and

[(Ph$_2$P(CH$_2$)$_n$PPh$_2$)(Au(6-MP))$_2$] (where n = 1, 2 or 3) are shown in Figure 2.2.1.

$$R_3PAuCl + 6\text{-MPH} + KOH \longrightarrow R_3PAu(6\text{-MP}) + KCl + H_2O$$

Ph$_2$P(CH$_2$)$_n$PPh$_2$(AuCl)$_2$

1) $\longrightarrow$ Ph$_2$P(CH$_2$)$_n$PPh$_2$(AuCl)(Au(6-MP))

2) $\longrightarrow$ Ph$_2$P(CH$_2$)$_n$PPh$_2$(Au(6-MP))$_2$

1) + 6-MPH + KOH

2) + 2(6-MPH) + 2KOH
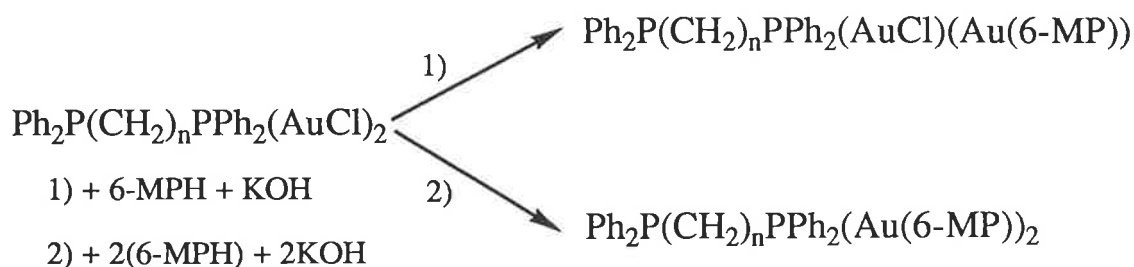
Figure 2.2.1: *General Reaction Schemes For The Preparation Of The Complexes.*

In this thesis, for reasons of brevity those compounds of the general formulae [(Ph$_2$P(CH$_2$)$_n$PPh$_2$)(AuCl)(Au(6-MP))] and [(Ph$_2$P(CH$_2$)$_n$PPh$_2$)(Au(6-MP))$_2$] will be given the abbreviations for the Ph$_2$P(CH$_2$)$_n$PPh$_2$ phosphine ligand of dppm, dppe and dppp for n = 1, 2 or 3, respectively. A detailed example of a preparation is given later.

The triorganophosphinegold(I) chloride complexes of the general formulae [R$_3$PAuCl] (where R$_3$P is as defined previously) and [Ph$_2$P(CH$_2$)$_n$PPh$_2$(AuCl)$_2$] were prepared by a procedure based on an example found in the literature[20,21]. This method basically involves the reduction of tetrachloroauric acid ([HAuCl$_4$].3H$_2$O)[22] by thiodiglycol followed by the addition of the desired phosphine species in molar quantities. What follows is an example of one such preparation.

Example: *Preparation of [Ph$_3$PAuCl].*

$$HAuCl_4.3H_2O \xrightarrow[\text{2) Ph}_3\text{P}]{\text{1) 3(HOCH}_2\text{CH}_2)_2\text{S}} Ph_3PAuCl$$
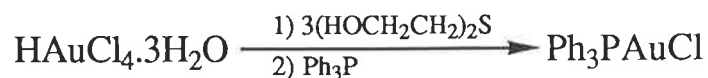
Figure 2.2.2: *Reaction Scheme For The Preparation Of [Ph$_3$PAuCl].*

To a stirred solution of acetone (1 cm^3) and H$_2$O (3 cm^3) held in an ice bath under a nitrogen atmosphere was added HAuCl$_4$.3H$_2$O (0.600 g, 1.52 mmol). Thiodiglycol (0.56 g, 4.57

mmol) was then added dropwise to the yellow-orange solution over a period of 2 h. Extra drops were added until a clear solution was obtained. The solution was then filtered under nitrogen to remove undissolved solids. Ph_3P (0.417 g, 1.52 mmol) dissolved in hot acetone (*ca* 5 cm^3) was added dropwise over a period of 10 min to the stirred solution. The resultant white solid that formed immediately was collected via vacuum filtration and washed with a small quantity of acetone. The solid product was air-dried for 5 min and recrystallized from hot ethanol. The resultant crystalline material was dried for 12 h over anhydrous phosphorus pentoxide under vacuum. Yield = 0.678 g; % yield = 90.0%; m.p. (dec.) = 233 - 234° C.

All the other compounds were prepared in an analogous manner using the appropriate molar quantities. The only variation to this procedure was for the preparation of [Et$_3$PAuCl]; Et$_3$P is a liquid at room temperature, and so was added as such via a syringe over a 5 min period.

The transparent crystalline products are all air stable at room temperature. For the most part, this procedure gave good yields: percentage yields based on 0.500 g HAuCl$_4$.3H$_2$O used are shown in Table 2.2.1, along with melting points and the corresponding literature values where available.

Example: *Preparation of [Ph$_3$PAu(6-MP)].*

$$Ph_3PAuCl + 6\text{-}MPH + KOH \longrightarrow Ph_3PAu(6\text{-}MP) + KCl + H_2O$$

Figure 2.2.3: *Reaction Scheme For The Preparation Of [Ph$_3$PAu(6-MP)].*

To a stirred ethanolic solution (*ca* 30 cm^3) of [Ph$_3$PAuCl] (0.200 g, 0.405 mmol) and 6-mercaptopurine (0.062 g, 0.405 mmol) aqueous potassium hydroxide (0.200 mol dm^{-3}, 0.405 mmol) was added dropwise over a few minutes. After 15 min of stirring, a pale yellow solid started to form in the clear solution. The solution was left to stir for a further 1 h, then left in a fumehood until the solvent evaporated. The solid residue was dissolved with stirring into boiling acetone (*ca* 100 cm^3), then vacuum filtered to remove undissolved solids. The filtrate was left to stand until the acetone evaporated, and the off-white product was

Table 2.2.1: *Melting Points And Yields For Triorganophosphinegold(I) Chloride*

Complexes.

Compound	m.p. (°C)	yield (g)	% yield	literature values	(°C)
[Et$_3$PAuCl]	68 - 69	0.405	91.0	84 - 86	[23]
[Cycl$_3$PAuCl]	117 - 118	0.379	58.2	-	
[PhMe$_2$PAuCl]	132 - 133	0.308	65.4	-	
[Ph$_3$PAuCl]	242 - 243	0.590	94.0	242	[24]
[(o-Tol)$_3$PAuCl]	(274 - 275)	0.619	90.8	283 - 285	[25]
[(m-Tol)$_3$PAuCl]	152 - 153	0.590	86.6	-	
[(p-Tol)$_3$PAuCl]	(186 - 187)	0.578	84.7	-	
[dppm(AuCl)$_2$]	270 - 271	0.407	75.5	273	[26]
[dppe(AuCl)$_2$]	(288 - 289)	0.565	96.4	290 - 292	[27]
[dppp(AuCl)$_2$]	(255 - 256)	0.358	64.3	256 - 257	[28]

Note: Brackets around the melting point value indicates decomposition point.

recrystallized twice from a small quantity of 1:1 ethanol / dichloromethane to give a pale yellow microcrystalline product. Yield = 0.231 g; % yield = 93.7%; m.p. (dec.) = 254 - 255° C.

This procedure was adapted to prepare all the complexes for this project. They are all air-stable solids, and vary in colour from very pale to bright yellow. The melting points, % yields (based on 0.200 g of [R$_3$PAuCl] or [Ph$_2$P(CH$_2$)$_n$PPh$_2$(AuCl)$_2$] used), colour and microanalytical results are shown in Tables 2.2.2 and 2.2.3.

2.3 *Instrumentation*

All melting points were determined using a Gallemkamp melting point apparatus calibrated with benzil.

Infrared spectra for all complexes were recorded on a Perkin-Elmer 1720X FT spectrometer calibrated with the polystyrene absorption at 1601 cm^{-1}, as KBr discs in the range of 400 - 4000 cm^{-1}.

Proton and carbon-13 NMR spectra were recorded on a Bruker ACP-300 NMR spectrometer with d$_6$-dimethylsulphoxide as the solvent. The recording frequencies used were 300.13 MHz for ^{1}H NMR and 75.47 MHz for ^{13}C NMR. The internal reference used was SiMe$_4$ (TMS). Phosphorus-31 NMR spectra were recorded on a Bruker CXP-300 NMR spectrometer at 121.5 MHz, also as d$_6$-dimethylsulphoxide solutions, with the ~~internal~~ external reference being 85% H$_3$PO$_4$ in D$_2$O.

FAB mass spectra were obtained using a VG ZAB-2HF spectrometer. The excitation gas was argon at a source pressure of typically 10^{-6} mbar. The FAB voltage was 7 kV with a current of 1 mA, the ion accelerating potential being 8 kV. A drop of a *ca* 0.5 mol dm^{-3} solution of the complex in dichloromethane was added to a drop of 3-nitrobenzyl alcohol matrix and applied to the probe tip. The spectra were recorded as a mass to charge ratio, m/z. Relative abundance was

Table 2.2.2: *Melting Points, Yields And Colours For The Triorganophosphinegold(I)*
6-mercaptopurinate Complexes.

Compound	m.p. (°C)	yield (g)	% yield	colour
[Et$_3$PAu(6-MP)]	102-103	0.264	99.2	pale yellow
[Cycl$_3$PAu(6-MP)]	139-140	0.228	93.2	light yellow
[PhMe$_2$PAu(6-MP)]	173-175	0.212	80.6	yellow-green
[Ph$_3$PAu(6-MP)]	254-255	0.231	93.7	off white
[(*o*-Tol)$_3$PAu(6-MP)]	(253-254)	0.235	96.7	pale yellow
[(*m*-Tol)$_3$PAu(6-MP)]	108-109	0.238	97.9	pale yellow
[(*p*-Tol)$_3$PAu(6-MP)]	105-106	0.238	98.1	pale yellow
[dppe(AuCl)(Au(6-MP))]	(183-185)	0.215	94.8	pale yellow
[dppp(AuCl)(Au(6-MP))]	(203-204)	0.212	93.6	pale yellow
[dppm(Au(6-MP))$_2$]	179-180	0.189	74.3	off white
[dppe(Au(6-MP))$_2$]	150-151	0.209	82.4	off white
[dppp(Au(6-MP))$_2$]	161-162	0.211	83.5	off white

Note: Brackets around the melting point value indicates decomposition point.

Table 2.2.3: *Microanalytical Data For The Triorganophosphinegold(I) 6-mercaptopurinate Complexes.*

Compound	$\%C_{calc}$	$\%C_{found}$	$\%H_{calc}$	$\%H_{found}$
[Et$_3$PAu(6-MP)]	28.33	28.19	3.89	4.06
[Cycl$_3$PAu(6-MP)]	43.95	44.02	5.77	6.03
[PhMe$_2$PAu(6-MP)].0.5EtOH	33.02	33.15	3.36	3.11
[Ph$_3$PAu(6-MP)]	45.26	45.19	2.97	2.98
[(o-Tol)$_3$PAu(6-MP)]	47.86	47.71	3.71	3.90
[(m-Tol)$_3$PAu(6-MP)]	47.86	47.82	3.71	3.94
[(p-Tol)$_3$PAu(6-MP)].H$_2$O	46.86	46.85	3.71	3.81
[dppe(AuCl)(Au(6-MP))]	38.03	38.12	2.78	2.75
[dppp(AuCl)(Au(6-MP))].H$_2$O	38.02	37.87	3.09	3.08
[dppm(Au(6-MP))$_2$].2H$_2$O	37.63	37.72	2.87	2.46
[dppe(Au(6-MP))$_2$].2H$_2$O	38.24	38.15	3.03	2.60
[dppp(Au(6-MP))$_2$].CH$_2$Cl$_2$	38.24	38.07	2.87	2.63

Note: Microanalysis performed by Chemical And Microanalytical Services Pty. Ltd.

calculated by designating the most abundant peak as 100% and determining the abundance of the other peaks based on their relative heights in the spectra to this peak.

2.4 *Chemicals*

The chemicals utilized in the synthesis of the complexes and their sources were: triphenylphosphine (B.D.H.), triethylphosphine (Fluka), tricyclohexylphosphine (Strem), tri(o-tolyl)phosphine (Aldrich), tri(m-tolyl)phosphine (Aldrich), tri(p-tolyl)phosphine (Aldrich), [μ-bis-(diphenylphosphino)methane] (Strem), [μ-1,2-bis(diphenylphosphino)ethane] (Strem), [μ-1,3-bis(diphenylphosphino)propane] (Strem), thiodiglycol (Aldrich) and 6-mercaptopurine (Sigma). All the solvents employed were of analytical grade.

2.5 *Crystallography: Instrumentation and methods*

All the crystals were grown from the vapour diffusion of diethyl ether into an ethanolic solution of the compound. The colourless crystals were collected and their identities confirmed by spectral and melting point comparisons with the bulk material. The dimensions and crystallographic parameters are given in later chapters where the results are presented. The following description concerns the data collection and structure solution for [(o-Tol)$_3$PAu(6-MP)].C_2H_5OH; the methods utilized for the other crystal structure determinations were similar.

The crystal was mounted on a glass fibre using cyanoacrylate glue, and then placed on the goniometer of a Rigaku AFC6R diffractometer fitted with graphite-monochromatized MoKα radiation, λ = 0.71073 Å. The unit cell dimensions were determined from the least squares refinement of 25 well-centred reflections in the range of 7.7 < θ < 12.8°, and, with the aid of Delauney reduction and a Laue symmetry check, was found to be monoclinic primitive with the Laue class of 2/m. Intensity data was then collected at 23° C in the ranges of 0 < h < 12, 0 < k < 13 and 0 < l < 33, to a maximum Bragg angle of 2θ = 55.8°. The intensities of 6280 reflections were measured using the ω:2θ scan technique, of which 5913 were unique. The

value for R_{amal} was 0.025, where

$$R_{amal} = \frac{\sum_{i=1}^{n} \sum_{j=1}^{m} |<F^2_i> - F^2_{ij}|}{\sum_{i=1}^{n} m \times <F^2_i>}$$

n = the number of unique reflections that were observed more than once

m = the number of times a given reflection is observed

$<F^2_i>$ = the average value of F^2 for the unique reflection i

No significant decomposition of the crystal occurred during the data acquisition. The data set was processed and corrected for Lorentz and polarization effects, and the space group determined to be $P2_1/n$, based on the analysis of systematic absences. A total of 4183 reflections satisfied the criterion of observability of $I \geq 3.0\sigma(I)$ and were used in the subsequent analysis.

The structure was solved by direct methods using the SHELXS86[29] program and refined by a full matrix least-squares procedure based on F[30]. The function minimized was

$$\sum_{i=1}^{n} w_i (|F_{obs}|_i - |F_{calc}|_i)^2$$

where n is the number of reflections, and

$$w = \frac{1}{\sigma^2(F_{obs})}$$

The non-hydrogen atoms were refined with anisotropic thermal parameters, and the hydrogen atoms were included in the model in calculated positions of C–H = 0.97 Å and N–H = 0.95 Å. The absorption correction used was DIFABS[31]. A weighting scheme was introduced based on sigma weights. At convergence, the values of R and R_w were 0.040 and 0.041 respectively,

where

$$R = \frac{\sum\limits_{i=1}^{n} (|F_{obs}|_i - |F_{calc}|_i)}{\sum\limits_{i=1}^{n} |F_{obs}|_i}$$

and

$$R_w = \left\{ \frac{\sum\limits_{i=1}^{n} w_i(|F_{obs}|_i - |F_{calc}|_i)^2}{\sum\limits_{i=1}^{n} w_i |F_{obs}|^2} \right\}^{1/2}$$

The maximum and minimum residual electron density peaks in the final difference map were 1.25 and -1.46 e $\mathring{A}^{-3}$. Scattering factors for all the atoms were those incorporated in the teXsan software package[30] which was installed on a Silicon Graphics Indigo computer system. Tables of bond distances and bond angles, fractional atomic coordinates, anisotropic thermal and hydrogen atom parameters and mean plane data are found in Chapter 3 for [PhMe$_2$PAuCl], Chapter 5 for [Ph$_3$PAu(6-MP)].C$_2$H$_5$OH and [(o-Tol)$_3$PAu(6-MP)].C$_2$H$_5$OH and Chapter 6 for [Cycl$_3$PAu(6p2-TU)]. Structure factors for all determinations are located in the Appendix. The expression for the anisotropic thermal parameter of the non-hydrogen atoms is

$$T_{aniso} = \exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2hka^*b^*U_{12} + 2hla^*c^*U_{13} + 2klb^*c^*U_{23})]$$

and the expression for B(eq) for the hydrogen atoms is

$$B(eq) = 8\pi^2(U_{11} + U_{22} + U_{33})/3.$$

CHAPTER 3

Characterization of Triorganophosphinegold(I) Chloride and [µ-1,n-bis(diphenylphosphino)alkane]bis(gold(I) chloride) Complexes

3.1 *Introduction*

This chapter discusses the characterization of the complexes of the general formula [R_3PAuCl] (where R_3P = Et_3P, $Cycl_3$P, $PhMe_2$P, Ph_3P, (o-Tol)$_3$P, (m-Tol)$_3$P or (p-Tol)$_3$P) and those of the general formula [(Ph_2P(CH_2)$_n$$PPh_2$)(AuCl)$_2$] (where n = 1, 2 or 3). While complexes of this type are well known, documentation of their spectroscopic characteristics is not readily available and hence this Chapter. The discussion consists of three main parts: 1) the spectral characterization via infrared and multinuclear nmr techniques, 2) the crystal structure determination of the [$PhMe_2$PAuCl] complex, and 3) a comparative study of triorganophosphinegold(I) chlorides found in the literature with respect to phosphine cone-angles and the P–Au and Au–Cl bond lengths. The last study will aim to determine whether a correlation exists between the cone angles of the triorganophosphine ligands and the lengths of the P–Au and Au–Cl bonds. The spectral characterization will be discussed in terms of how the data relate to analogous information found in the literature, what it describes about the chemical nature of these complexes, and how the information is useful for the characterization of the triorganophosphinegold(I) 6-mercaptopurinate complexes discussed in Chapter 4.

3.2 *Spectral characterization of the triorganophosphinegold(I) chloride complexes*

3.2.1 *Infrared spectroscopy*

The spectra were recorded as described in Chapter 2. The appearance of all the spectra were fairly simple, containing a few strong absorptions with a number of very weak ones. These absorptions are due to the vibrational modes associated with the phosphine ligands, since the modes involving the gold(I) and chloride atoms, such as ν(P–Au) and ν(Au–Cl), occur below 400 cm^{-1} and were not recorded owing to the limitations of the instrumentation. Table 3.2.1 lists the major absorptions found in each spectrum and the functional group vibrations to which they have been assigned. Infrared studies of these compounds in the literature are usually concerned with the P–Au and Au–Cl stretching modes[32,33], so the assignments are based on comparisons with the spectra of free phosphines. Figures 3.2.1 a) - d) show the infrared spectra of some selected compounds, and it is clear that by comparing, for example, the spectra of [Et$_3$PAuCl] and [Ph$_3$PAuCl], the absorption peaks found at 1586 cm^{-1} and at 1480 cm^{-1} for [Ph$_3$PAuCl] and not found for [Et$_3$PAuCl] must be due to aromatic ring vibrations. The main peaks found below *ca* 1450 cm^{-1} are due to ν(C–C), ν(P–C) and δ(C–H) vibrations. These latter absorptions are listed together, as it is not possible to assign them unambiguously due to their overlapping absorption ranges[34,35]. Comparison with the infrared spectra of the free phosphines[36] shows that, for Ph$_3$P, the ν(P–C) vibration occurs at 1430 cm^{-1}, but it is unclear how the stretching frequency of this bond is affected when the phosphorus atom binds to the gold(I) atom. The aromatic absorptions for Ph$_3$P[36] occur at *ca* 1580 cm^{-1} and 1480 cm^{-1}, indicating a slight change upon coordination, related to the change in electron density about the gold centre. The ν(C–H) absorptions for alkyl C–H groups are more intense than those for aryl C–H groups in the complexes, an observation that has been made before[34], which is due to the hydrogen atoms being more tightly bound to the aromatic rings than to alkyl carbon atoms. This is also the reason why the aryl C–H absorptions occur between 50 and 100 wavenumbers higher than alkyl C–H absorptions. The alkyl absorptions are most intense in the spectrum of

Table 3.2.1: *Infrared Data For The Triorganophosphinegold(I) Chloride Complexes.*

Complex	v(C–H)	v(C=C)	v(C–C), v(P–C), δ(C–H)
[Et₃PAuCl]	2962s, 2932m, 2905m, 2874m	-	1456s, 1413m, 1384m, 1259w,br,sh, 1044vs
[Cycl₃PAuCl]	2922vs, 2852s	-	1447s, 1176m, 1040w
[Ph₃PAuCl]	3071w, 3058w,br	1586w, 1480m	1435s, 1180w, 1103s
[(o-Tol)₃PAuCl]	3054w, 2971m, 3023w, 2930m	1589m, 1565w, 1468s	1448s, 1376m, 1163m, 1133s, 1070w
[(m-Tol)₃PAuCl]	3050w,br, 2911w	1593m, 1578w, 1478s	1447s, 1404m, 1383m, 1309w, 1108s, 1045w
[(p-Tol)₃PAuCl]	3014w, 2963w, 2917w	1598m, 1559w, 1498m	1447w,br, 1397m, 1384w, 1310w, 1188m, 1103vs
[PhMe₂PAuCl]	3056w, 3041w, 3023w, 2990m,sh, 2850m,br	1587w, 1573w, 1507w, 1490w, 1473w	1437s, 1426m, 1413s, 1384m, 1190m, 1161m, 1112s, 1073m
[dppm(AuCl)₂]	3050w,br, 2916m, 2853w	1483w	1436vs, 1385m, 1185w, 1160w, 1103s, 1069m
[dppe(AuCl)₂]	3053m,br, 2906m	1587w, 1573w, 1482m	1435s, 1411m, 1173s, 1106vs, 1071m
[dppp(AuCl)₂]	3049m,br, 2917m, 2901m, 2851m	1586m, 1571w, 1481s	1434vs, 1405s, 1385s, 1184m, 1158m, 1104vs, 1069m

Note: Units are wavenumbers (cm⁻¹).

a)

v(C–H)

4000   3200   2400 2000   1600   1200   600   400
                          CM–1

b)

v(C–H)

1586

1480

4000   3200   2400 2000   1600   1200   800   400
                          CM–1
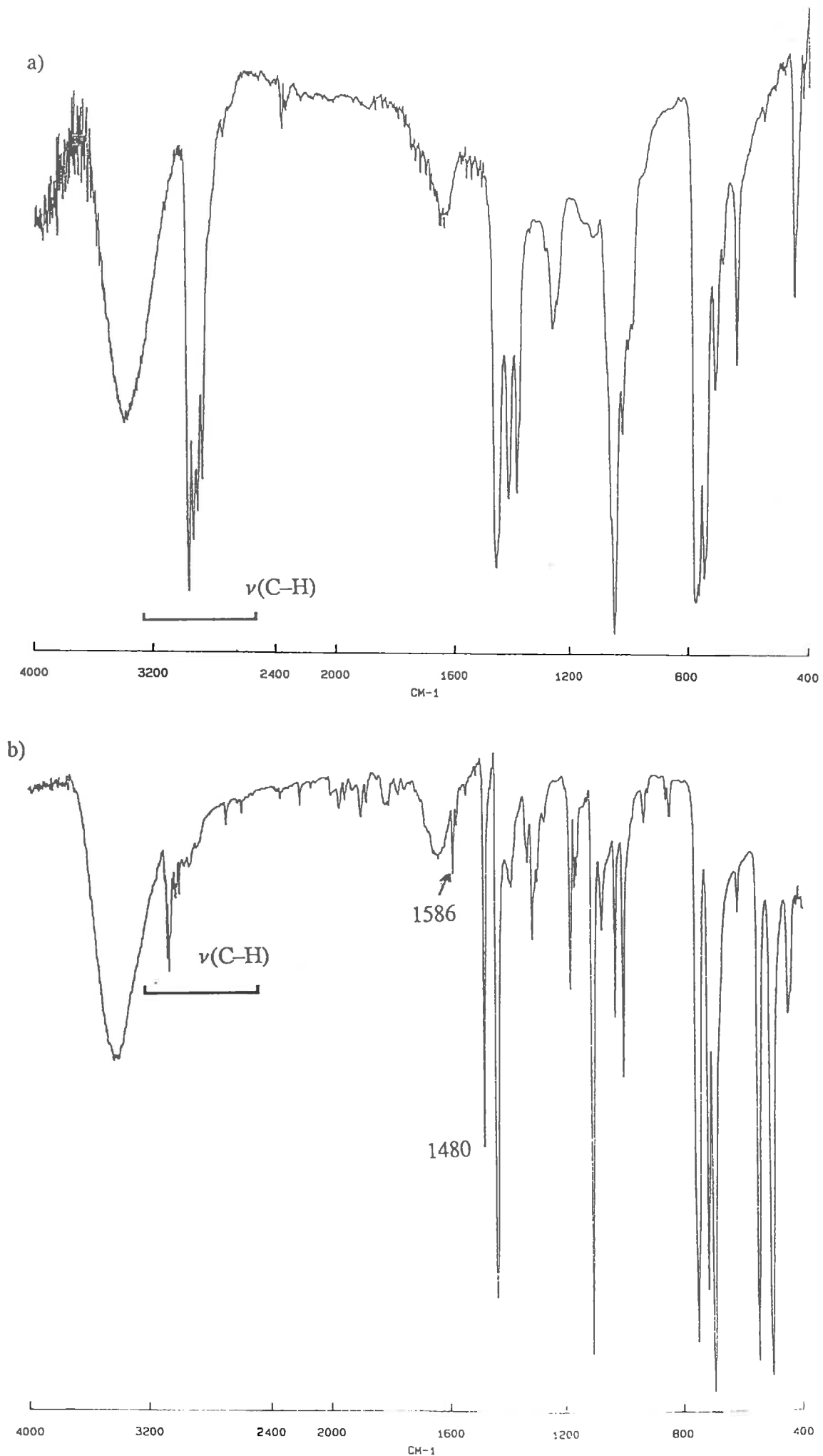
Figure 3.2.1: *IR Spectra Of a) Triethylphosphinegold(I) Chloride, [Et₃PAuCl],*

b) Triphenylphosphinegold(I) Chloride, [Ph₃PAuCl].

c)

ν(C–H)

4000   3200   2400   2000   1600   1200   800   400

CM-1

d)

aryl ν(C–H)

alkyl ν(C–H)

1483

4000   3200   2400   2000   1600   1200   800   400

CM-1
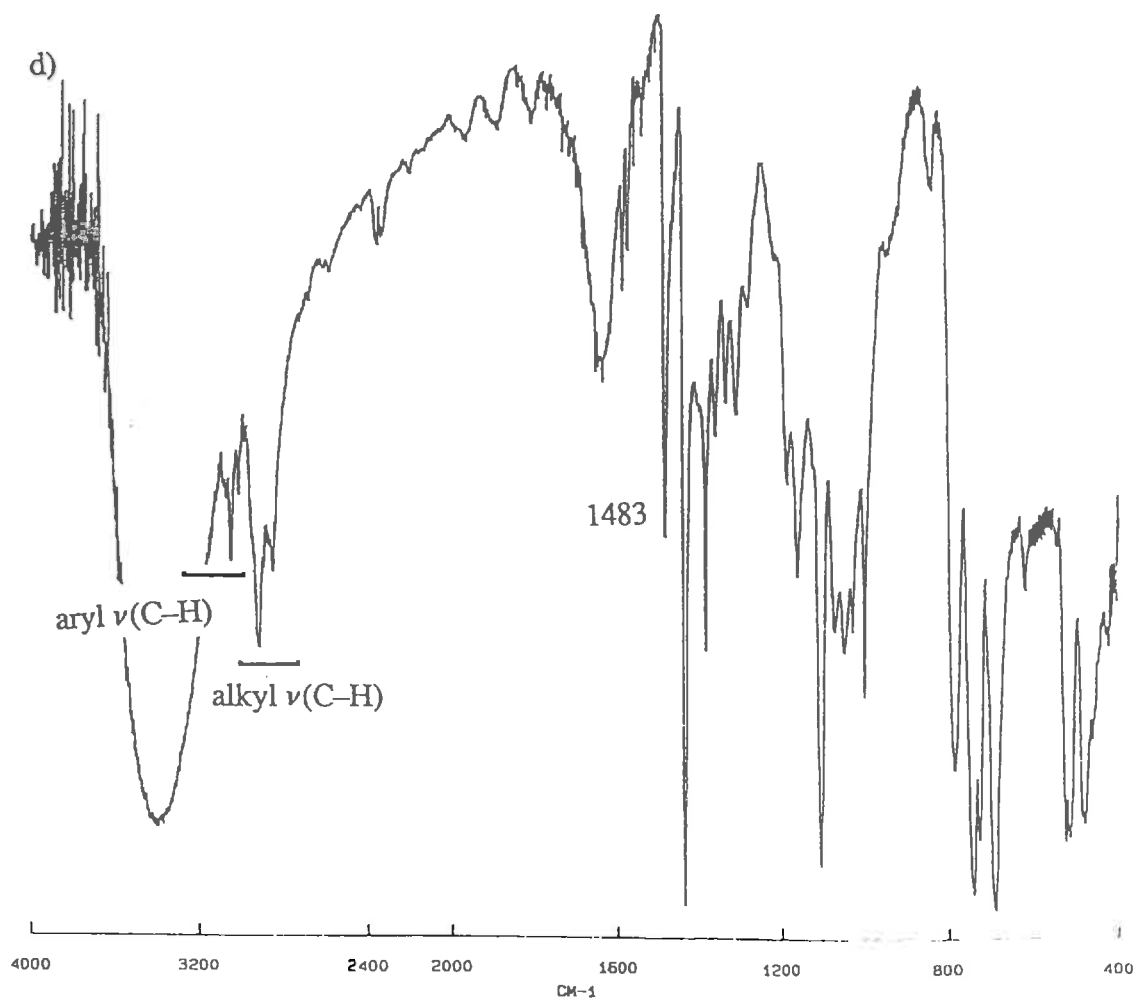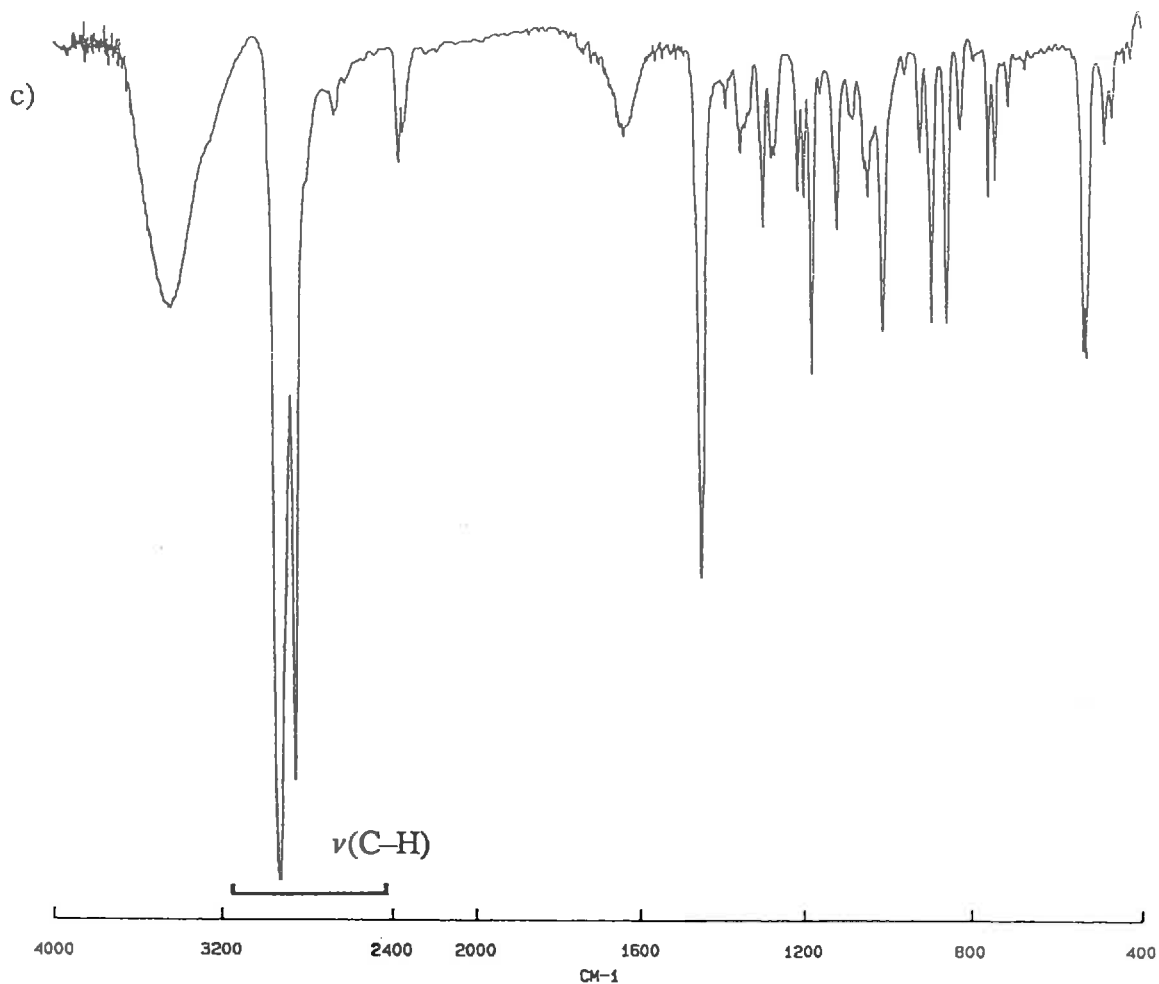
Figure 3.2.1: *IR Spectra Of c) Tricyclohexylphosphinegold(I) Chloride, [Cycl₃PAuCl],*
d)[μ-bis(diphenylphosphino)methane]bis(gold(I)chloride), [(Ph₂PCH₂PPh₂)(AuCl)₂].
d) [μ-bis(diphenylphosphino)methane]bis(gold(I) chloride), [(Ph₂PCH₂PPh₂)](AuCl)₂]

25

[Cycl3PAuCl], in Figure 3.2.3. Figure 3.2.1 d) shows the relative intensities of aryl to alkyl absorptions in the [dppm(AuCl)2] complex.

The data listed here will be useful in Chapter 4 as it can help assign those absorptions due to the phosphine group in the spectra of the complexes, simplifying the analysis. There are significant differences between the spectra of the triorganophosphinegold(I) chloride complexes and the free phosphines to suggest product formation. However, the respective absorptions between the gold(I) complexes are similar, indicating that the constituent absorptions are largely independent of the nature of the rest of the molecule, as expected.

3.2.2 ^1H NMR spectroscopy

The proton NMR spectra were obtained as described in Chapter 2. Although soluble in chloroform, for reasons of consistency the solvent used for these complexes was d_6-dimethylsulphoxide, as this was the solvent utilized for the 6-mercaptopurinate complexes in Chapter 4. Figure 3.2.2 a) shows the labeling scheme adopted for the carbon atoms and the protons bound to them.
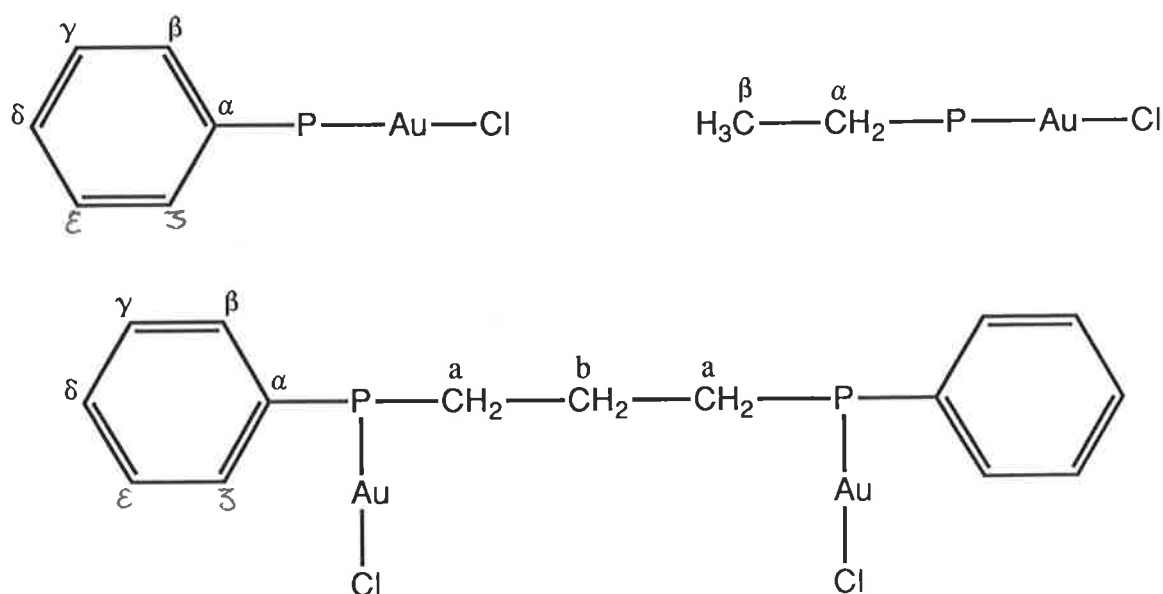
Figure 3.2.2 a): *Labeling Scheme Adopted For NMR Assignments.*

Table 3.2.2 lists the assignments for the protons in each complex, including the multiplicity and coupling constants. The methyl group of the tolyl phosphine complexes and of [PhMe$_2$PAuCl] are designated by a CH$_3$ subscript. The resonances for aromatic protons occur as complex multiplets due to the complicated proton-proton and phosphorus-proton coupling combinations, so are given as a range. This range is typical of triphenylphosphine absorptions e.g. as found in [Ru(6-MP)$_2$(PPh$_3$)$_2$]$^{2+}$ and Ph$_3$P[37,38]. These resonances occur downfield at *ca* 7.5 ppm because of the deshielding effect of the delocalized electrons in the aromatic moiety. As expected, there is little difference between these regions in the spectra of all the complexes containing this type of group. A similar but broader complex multiplet occurs for the cyclohexyl protons of [Cycl$_3$PAuCl], also due to complex coupling patterns, but upfield due to their alkyl nature. Broad multiplets have been assigned to each proton type, but no coupling could be resolved.

Two-bond indirect spin-spin coupling between the phosphorus atom and the protons was observed for the resonance of the alpha protons in [Et$_3$PAuCl], giving rise to two overlapping quartets, where $^3J_{HH}$ = 7.71Hz, but $^2J_{PH}$ was unresolved. The value of $^3J_{PH}$ = 18.89Hz for the beta protons results in a doublet of triplets, which is shown in Figure 3.2.2 b). The uniformity of the shapes of these resonances suggests free rotation about the C–C and P–C bonds in the phosphine groups. Phosphorus to proton coupling was manifested in the resonance of H$_a$ for [dppm(AuCl)$_2$], appearing as a triplet due to coupling with the two magnetically equivalent phosphorus nuclei. It was not, however, distinguished for the H$_a$ and H$_b$ protons in the spectra of the [dppe(AuCl)$_2$] and [dppp(AuCl)$_2$] complexes, the resonances being broad and featureless. The reason for this is that the protons involved couple to two phosphorus atoms, and, in the case of H$_a$, the signs of the coupling constants are opposite, hence giving a net coupling which is unresolved in the spectra, and further complicated by proton–proton coupling. This corresponds with the resonance in the free phosphines, e.g. H$_a$ in dppe is just resolved as a triplet centred at δ 2.10 ppm[38], compared to δ 2.97 ppm in [dppe(AuCl)$_2$]. The latter observation is consistent with the deshielding effect expected at these nuclei upon complexation to the gold centre.

Table 3.2.2: *^1H NMR Chemical Shift Values (ppm) For Triorganophosphinegold(I) Chloride Complexes.*

Complex	H_α	H_β	H_γ	H_δ	H_{-CH3}	H_a	H_b
[Et₃PAuCl]	1.94(m) (7.71)	1.10(dt) (7.39) (18.89)	-	-	-	-	-
[Cycl₃PAuCl]	2.13(m)	1.79(m)	1.35(m)	1.26(m)	-	-	-
[Ph₃PAuCl]		7.63 - 7.51(m)			-	-	-
[(o-Tol)₃PAuCl]		7.64 - 6.87(m)			2.59(s)	-	-
[(m-Tol)₃PAuCl]		7.52 - 7.23(m)			2.34(s)	-	-
[(p-Tol)₃PAuCl]		7.42 - 7.39(m)			2.38(s)	-	-
[PhMe₂PAuCl]		7.86 - 7.56(m)			1.94(d) (11.35)ᶜ	-	-
[dppm(AuCl)₂]		7.77 - 7.44(m)			-	4.70(t) (12.58)ᶜ	-
[dppe(AuCl)₂]		7.79 - 7.59(m)			-	2.97(m)	-
[dppp(AuCl)₂]		7.76 - 7.51(m)			-	3.05(m)	1.71(m)

Note: All coupling constants, in parentheses, are in units of hertz: a = $^3J_{HH}$, b = $^3J_{PH}$, c = $^2J_{PH}$.

Figure 3.2.2 b): ^1H *NMR Spectrum Of Triethylphosphinegold(I) Chloride, [Et₃PAuCl].*

H_α (m)

H_β (dt)

Ref.

2.0   1.8   1.6   1.4   1.2   1.0   .8   .6   .4   .2   0.0
PPM
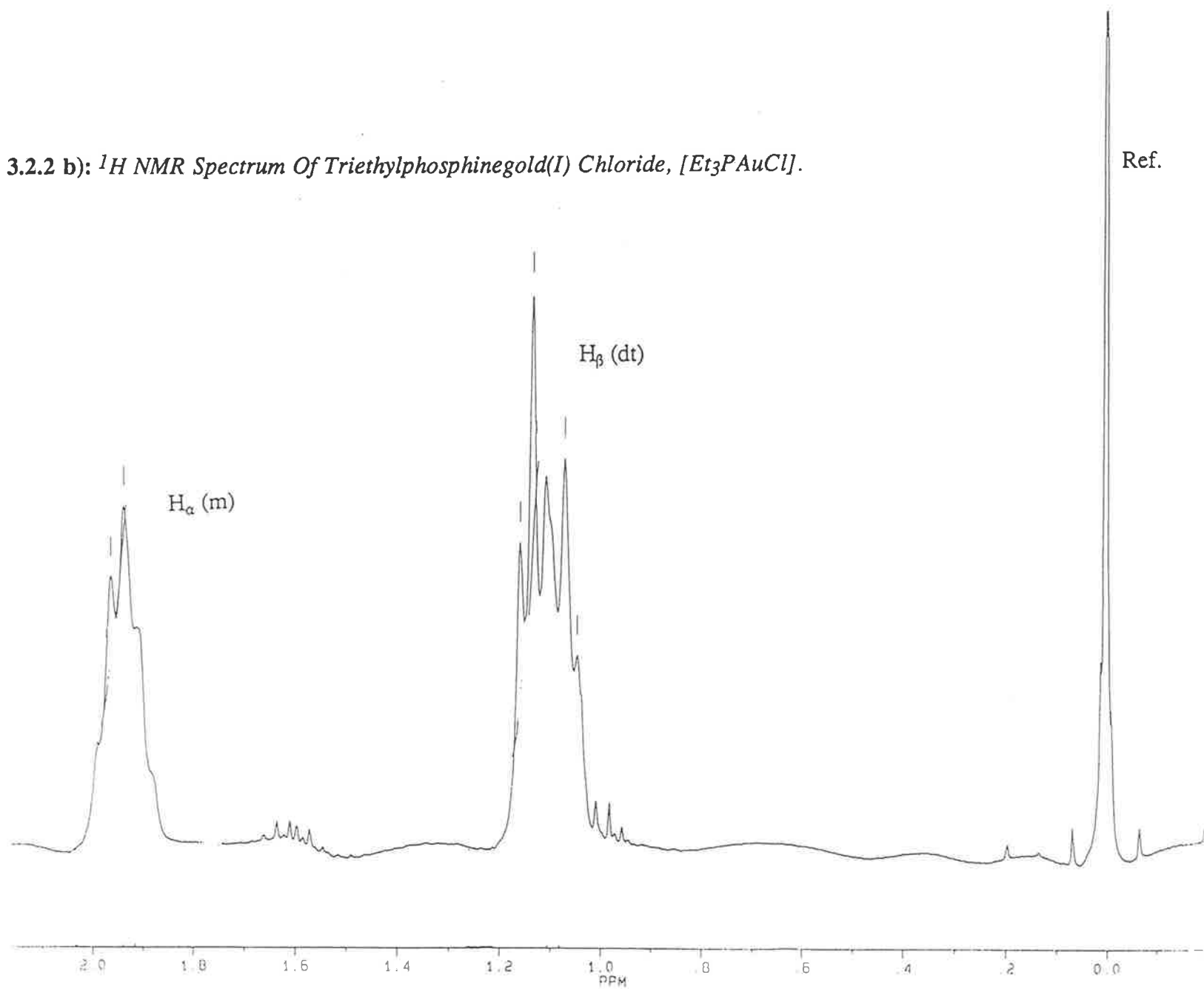
The data for the proton nmr studies on the complexes is consistent with literature values for the free phosphines and analogous complexes, and are useful for comparison with the 6-mercaptopurinate complexes in the next chapter.

3.2.3 ^{13}C $\{^1H\}$ NMR spectroscopy

The carbon-13 chemical shifts and phosphorus to carbon coupling constants are listed in Table 3.2.3. The phenyl-type carbon atoms are seen to resonate downfield, owing to the deshielding effect of the delocalized electron density in the ring. Of particular interest is the observation that the beta and gamma carbons in the [dppm(AuCl)$_2$] and [dppe(AuCl)$_2$] compounds appear as multiplets, where they would normally be expected to appear as doublets due to coupling with one phosphorus atom. This phenomenon has been noted before in the literature, the explanation being based on the fact that the two phosphorus atoms in the complexes are chemically equivalent but magnetically inequivalent due to the isotope effect (where a single ^{13}C atom in the molecule creates isotopic asymmetry)[39]. Indeed, in the spectrum of [dppe(AuCl)$_2$], the beta and gamma carbon resonances resemble triplets, where the coupling value given represents the separation between the peaks. This structure can clearly be seen in Figure 3.2.3. As with the proton spectra, the C$_a$ resonances are seen only as multiplets, but for the spectra of [dppp(AuCl)$_2$] a doublet of multiplets can be resolved. The problems with the resolution are more than likely due to the isotope effect.

As expected, the phenyl-region chemical shifts for the [(μ-1,n-(diphenyl-phosphino)alkane)bis(gold(I) chloride)] complexes are similar to those found for [Ph$_3$PAuCl] and the tolyl compounds, the assignments of which were based on analogous complexes found in the literature. The alpha, beta, gamma and delta resonances for Ph$_3$P are 137.2, 133.6, 128.5 and 128.4 respectively[40], so it is apparent that coordination to the gold results in a major shift in the C$_\alpha$ shift value but only minor shifts in the others[41]. The former shift is likely to be a reflection of the change in electron density about the phosphorus atom when the P–Au bond is formed: the $^1J_{PC}$ value increases from 11.3 Hz in Ph$_3$P to 61.03 Hz in the [Ph$_3$PAuCl] complex. Similar trends can be observed for the alpha carbon in all phenyl containing

Table 3.2.3: ^{13}C *Chemical Shifts Values (ppm) For The Triorganophosphinegold(I) Chloride Complexes.*

Complex	C_α	C_β	C_γ	C_δ	C_ϵ	C_ζ	-CH3	C_a	C_b
[Et3PAuCl]	16.9(d) (36.23)[a]	9.05	-	-	-	-	-	-	-
[Cycl3PAuCl]	32.3(d) (31.55)[a]	26.2(d) (12.08)[b]	30.3	25.7	30.3	26.2(d) (12.08)[b]	-	-	-
[Ph3PAuCl]	128.3(d) (61.03)[a]	133.9(d) (13.36)[b]	129.8(d) (10.49)[c]	132.4	129.8(d) (10.49)[c]	133.9(d) (13.36)[b]	-	-	-
[(o-Tol)3PAuCl]	124.2(d) (64.70)[a]	141.9 (11.93)[b]	132.6(d) (8.91)[c]	132.4	127.2(d) (10.57)[c]	133.0(d) (9.66)[b]	22.3(d) (11.02)[c]	-	-
[(m-Tol)3PAuCl]	128.2(d) (61.36)[a]	139.2(d) (12.15)[b]	130.9(d) (12.83)[c]	133.1	129.6(d) (12.08)[c]	134.1(d) (14.87)[b]	21.0	-	-
[(p-Tol)3PAuCl]	125.3(d) (64.53)[a]	133.7(d) (14.27)[b]	130.2(d) (12.15)[c]	142.5(d) (2.19)	130.2(d) (12.15)[c]	133.7(d) (14.27)[b]	21.0	-	-
[PhMe2PAuCl]	Obs.	131.8(d) (12.19)[b]	129.1(d) (11.10)[c]	131.6(d)	129.1(d) (11.10)[c]	131.8(d) (12.19)[b]	14.4(d) (39.78)[a]	-	-
[dppm(AuCl)2]	128.7(m)	133.4(m)	129.3(m)	132.3	129.3(m)	133.4(m)	-	24.6(m)	-
[dppe(AuCl)2]	128.7(d) (58.60)[a]	133.3(t) (6.42)	129.5(t) (5.29)	132.2	129.5(t) (5.29)	133.3(t) (6.42)	-	22.4(m)	-
[dppp(AuCl)2]	128.8(d) (59.85)[a]	133.1(d) (13.36)[b]	129.5(d) (11.85)[c]	132.2	129.5(d) (11.85)[c]	133.1(d) (13.36)[b]	-	26.5(d) (52.49)[a]	20.3(m)

Note: ^{31}P-^{13}C coupling constants, in parentheses, are in units of hertz: a = $^{1}J_{PC}$, b = $^{2}J_{PC}$ and c = $^{3}J_{PC}$.

Figure 3.2.3 : *^{13}C NMR Spectrum Of [µ-1,2-bis(diphenylphosphino)ethane]bis(gold(I) chloride), [(Ph$_2$P(CH$_2$)$_2$PPh$_2$)(AuCl)$_2$].*
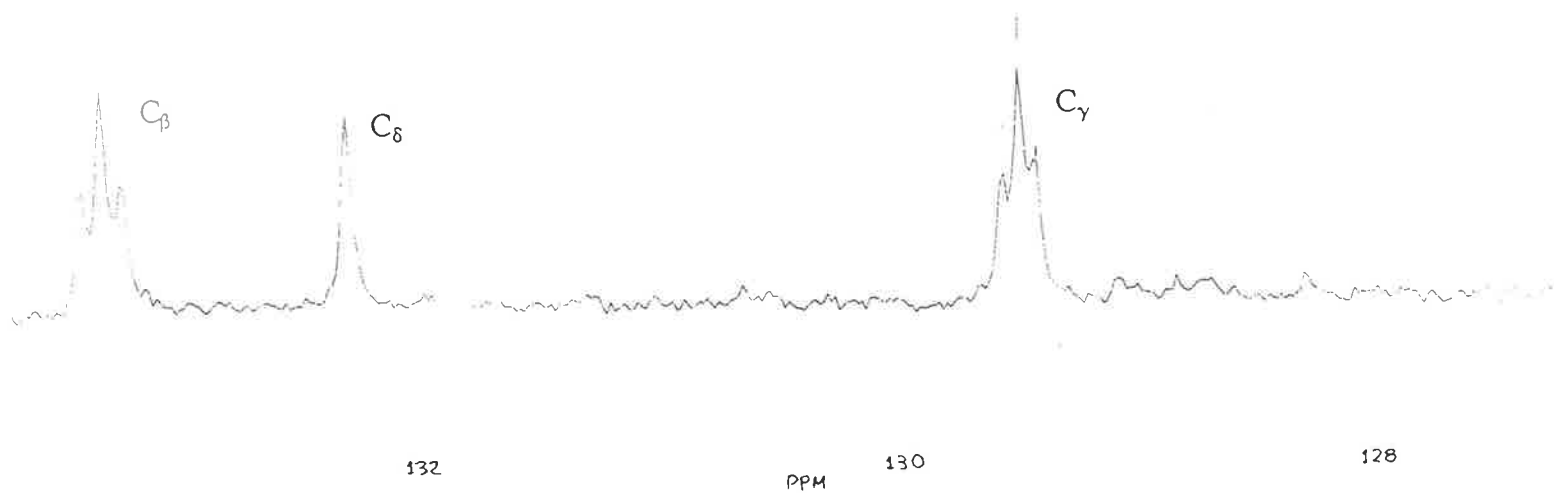
phosphines in going from the free phosphine to the complex, although the same was not necessarily true for the proton resonances. It should be noted that for [(o-Tol)₃PAuCl] and [(m-Tolyl)₃PAuCl] the assignments made for the six aromatic carbons are tentative due to the closeness of the resonance values[40]. Assignments in the spectrum of [Cycl₃PAuCl] are based on the data for the free phosphine[42,43]; the C_α chemical shift remains static, but the $^1J_{PC}$ value increases from 18.6 Hz to 31.55 Hz in the complex. The other ring carbons altered very little in terms of chemical shifts and coupling constants. A similar result is observed for Et₃P and [Et₃PAuCl][42]. This suggests that the chemical shifts of phosphorus-bound carbons in an aromatic environment are more sensitive to coordination effects at the phosphorus atom than are alkyl-type carbons.

The spectroscopic data confirm the stoichiometries of the triorganophosphinegold(I) chlorides and provide an essential reference for the interpretation of the spectra for the triorganophosphinegold(I) 6-mercaptopurinate complexes.

3.3 *Crystal structure determination of the [PhMe₂PAuCl] complex*

The general details concerning the data collection procedure used in the crystal structure determination of this complex have already been given in Chapter 2. What follows here is a discussion of the unit cell and the molecular structure obtained by refinement of this data.

Crystals of the complex were grown from the slow evaporation of a concentrated ethanolic solution of the compound. The [PhMe₂PAuCl] complex crystallizes in the achiral space group $P2_12_12_1$ (D_2^4, No. 19)[44] and the absolute configuration was determined on the basis of the differences between high-angle Friedel pairs included in the data set. Crystal and refinement data are listed in Table 3.3.1 and crystallographic results are summarized in Tables 3.3.2 to 3.3.7. A list of the observed and calculated structure factors is given in the Appendix. The crystallographic numbering scheme drawn with the ORTEP[45] program is shown in Figure 3.3.1.

Table 3.3.1: *Crystallographic Parameters for the [PhMe₂PAuCl] Complex.*

Data	[PhMe₂PAuCl]
Formula	$C_8H_{11}AuClP$
Formula weight	370.6
Crystal shape	block
Crystal dimensions (mm)	0.27 x 0.14 x 0.14
Crystal system	orthorhombic
Space group	$P2_12_12_1$ (D_2^4, No. 19)
a (Å)	12.639(4)
b (Å)	16.931(6)
c (Å)	9.458(3)
α (°)	90
β (°)	90
γ (°)	90
V (Å³)	2024(1)
Z	8
ρ_{calc} (g cm⁻³)	2.432
F(000)	1360
μ (cm⁻¹)	148.55
θ limits, cell (°)	8.0 to 12.8
θ limits, data (°)	1.5 to 25.4
hkl range	0 to 15, 0 to 20, 0 to 11
Range of transmission factors	0.945 to 1.058
Scan technique	ω:2θ
No. of data measured	3015
No. of unique data	2143
R_{amal}	0.046
No. of unique data used	1608
Criterion of observability	$I \geq 3.0\sigma(I)$
No. of parameters	199
R	0.035
R_w	0.039
Residual electron density (e Å⁻³)	-0.99 to 0.94

Table 3.3.2: *Fractional Atomic Coordinates For The [PhMe₂PAuCl] Complex.*

Atom	x	y	z
Au(1)	0.54801(7)	0.35615(5)	0.52508(10)
Au(2)	0.46393(7)	0.32211(5)	0.21977(10)
Cl(1)	0.6889(5)	0.2949(4)	0.4228(8)
Cl(2)	0.4269(5)	0.4549(3)	0.1866(7)
P(1)	0.4152(5)	0.4157(4)	0.6343(6)
P(2)	0.4450(5)	0.1923(3)	0.2333(6)
C(12)	0.3771(17)	0.3718(15)	0.8006(27)
C(13)	0.2956(18)	0.4149(14)	0.5424(32)
C(22)	0.4590(19)	0.1540(13)	0.4053(21)
C(23)	0.5613(18)	0.1549(14)	0.1520(23)
C(111)	0.4417(18)	0.5158(11)	0.6767(18)
C(112)	0.3623(18)	0.5682(14)	0.7121(28)
C(113)	0.3843(22)	0.6416(17)	0.7472(31)
C(114)	0.4867(23)	0.6699(15)	0.7451(24)
C(115)	0.5677(20)	0.6198(15)	0.7089(27)
C(116)	0.5450(17)	0.5445(13)	0.6746(21)
C(211)	0.3342(18)	0.1439(15)	0.1591(25)
C(212)	0.3288(18)	0.0602(14)	0.1650(26)
C(213)	0.2458(20)	0.0246(12)	0.0926(34)
C(214)	0.1736(20)	0.0645(15)	0.0269(37)
C(215)	0.1819(19)	0.1470(17)	0.0182(33)
C(216)	0.2618(17)	0.1840(13)	0.0777(35)

Table 3.3.3: *Anisotropic Thermal Parameters For The [PhMe$_2$PAuCl] Complex.*

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Au(1)	0.0389(5)	0.0414(5)	0.0407(5)	0.0026(5)	0.0041(6)	-0.0044(5)
Au(2)	0.0344(5)	0.0331(4)	0.0337(5)	0.0000(5)	-0.0012(5)	-0.0029(4)
Cl(1)	0.044(4)	0.054(4)	0.090(6)	0.007(3)	0.012(4)	-0.019(4)
Cl(2)	0.038(3)	0.031(3)	0.082(5)	0.001(3)	-0.004(4)	0.001(3)
P(1)	0.039(4)	0.049(4)	0.025(4)	-0.003(3)	0.005(3)	-0.001(3)
P(2)	0.032(3)	0.035(3)	0.027(3)	0.003(3)	-0.006(4)	-0.001(3)
C(12)	0.05(2)	0.07(2)	0.05(2)	-0.00(1)	0.01(2)	0.02(2)
C(13)	0.05(2)	0.07(2)	0.09(2)	0.00(1)	-0.00(2)	-0.06(2)
C(22)	0.07(2)	0.05(1)	0.02(1)	0.01(2)	0.02(1)	0.01(1)
C(23)	0.04(1)	0.05(2)	0.03(1)	0.00(2)	0.03(1)	0.00(1)
C(111)	0.04(1)	0.04(1)	0.003(9)	-0.01(1)	0.00(1)	0.007(9)
C(112)	0.05(2)	0.05(2)	0.03(2)	0.00(1)	0.02(2)	-0.00(2)
C(113)	0.08(2)	0.06(2)	0.06(2)	0.02(2)	0.04(2)	0.04(2)
C(114)	0.10(2)	0.06(2)	~~0.00(1)~~ 0.01(1)	-0.02(2)	0.00(1)	0.02(1)
C(115)	0.05(2)	0.08(2)	0.04(2)	-0.03(2)	-0.01(2)	-0.01(2)
C(116)	0.03(1)	0.05(1)	0.02(1)	-0.00(1)	-0.02(1)	-0.01(1)
C(211)	0.04(1)	0.04(1)	0.05(2)	-0.01(1)	-0.02(1)	0.01(1)
C(212)	0.05(2)	0.05(2)	0.05(2)	-0.00(1)	-0.02(2)	0.01(1)
C(213)	0.04(1)	0.03(1)	0.12(3)	-0.01(1)	-0.01(2)	-0.01(2)
C(214)	0.06(2)	0.05(2)	0.12(3)	-0.00(2)	-0.05(2)	-0.03(2)
C(215)	0.06(2)	0.08(2)	0.09(2)	0.00(2)	-0.05(2)	0.02(2)
C(216)	0.04(1)	0.03(1)	0.15(3)	0.01(1)	-0.06(2)	0.02(2)

Table 3.3.4: *Hydrogen Atom Parameters For The [PhMe₂PAuCl] Complex.*

Atom	x	y	z	B(eq)
H(12a)	0.3231	0.4041	0.8451	4.6
H(12b)	0.3493	0.3192	0.7840	4.6
H(12c)	0.4383	0.3685	0.8622	4.6
H(13a)	0.2435	0.4456	0.5940	5.8
H(13c)	0.2709	0.3609	0.5326	5.8
H(15b)	0.3059	0.4378	0.4494	5.8
H(22a)	0.3998	0.1709	0.4630	4.0
H(22b)	0.4605	0.0967	0.4013	4.0
H(22c)	0.5245	0.1731	0.4465	4.4
H(23a)	0.5604	0.0976	0.1553	3.8
H(23b)	0.5639	0.1722	0.0543	3.8
H(23c)	0.6230	0.1744	0.2019	3.8
H(112)	0.2892	0.5507	0.7112	4.3
H(113)	0.3272	0.6766	0.7751	5.7
H(114)	0.5012	0.7246	0.7689	5.1
H(115)	0.6403	0.6384	0.7081	5.1
H(116)	0.6021	0.5093	0.6478	3.6
H(212)	0.3804	0.0293	0.2170	4.6
H(213)	0.2419	-0.0326	0.0912	5.3
H(214)	0.1140	0.0376	-0.0160	7.1
H(215)	0.1283	0.1769	-0.0321	6.8
H(216)	0.2698	0.2404	0.0639	7.0

Table 3.3.5: *Bond Distances (Å) For The [PhMe₂PAuCl] Complex.*

Atom		Atom	Distance	Atom		Atom	Distance
Au(1)	–	Cl(1)	2.277(6)	C(111)	–	C(116)	1.39(3)
Au(1)	–	P(1)	2.214(6)	C(112)	–	C(113)	1.32(4)
Au(2)	–	Cl(2)	2.273(5)	C(113)	–	C(114)	1.38(3)
Au(2)	–	P(2)	2.205(5)	C(114)	–	C(115)	1.37(3)
P(1)	–	C(12)	1.81(2)	C(115)	–	C(116)	1.35(3)
P(1)	–	C(13)	1.74(2)	C(211)	–	C(212)	1.42(3)
P(1)	–	C(111)	1.77(2)	C(211)	–	C(216)	1.38(3)
P(2)	–	C(22)	1.76(2)	C(212)	–	C(213)	1.39(3)
P(2)	–	C(23)	1.77(2)	C(213)	–	C(214)	1.30(3)
P(2)	–	C(211)	1.77(2)	C(214)	–	C(215)	1.40(3)
C(111)	–	C(112)	1.38(3)	C(215)	–	C(216)	1.31(3)

Table 3.3.6: *Bond Angles ( ) For The [PhMe₂PAuCl] Complex.*

Atom		Atom		Atom	Angle	Atom		Atom		Atom	Angle
Cl(1)	–	Au(1)	–	P(1)	177.2(3)	P(1)	–	C(111)	–	C(116)	120(2)
Cl(2)	–	Au(2)	–	P(2)	175.4(2)	C(112)	–	C(111)	–	C(116)	117(2)
Au(1)	–	P(1)	–	C(12)	114.9(9)	C(111)	–	C(112)	–	C(113)	121(2)
Au(1)	–	P(1)	–	C(13)	114.9(9)	C(112)	–	C(113)	–	C(114)	122(3)
Au(1)	–	P(1)	–	C(111)	113.4(8)	C(113)	–	C(114)	–	C(115)	119(2)
C(12)	–	P(1)	–	C(13)	102(1)	C(114)	–	C(115)	–	C(116)	119(2)
C(12)	–	P(1)	–	C(111)	104(1)	C(111)	–	C(116)	–	C(115)	122(2)
C(13)	–	P(1)	–	C(111)	106(1)	P(2)	–	C(211)	–	C(212)	119(2)
Au(2)	–	P(2)	–	C(22)	115.2(7)	P(2)	–	C(211)	–	C(216)	121(2)
Au(2)	–	P(2)	–	C(23)	111.6(8)	C(212)	–	C(211)	–	C(216)	119(2)
Au(2)	–	P(2)	–	C(211)	113.7(8)	C(211)	–	C(212)	–	C(213)	117(2)
C(22)	–	P(2)	–	C(23)	101(1)	C(212)	–	C(213)	–	C(214)	123(2)
C(22)	–	P(2)	–	C(211)	106(1)	C(213)	–	C(214)	–	C(215)	120(2)
C(23)	–	P(2)	–	C(211)	109(1)	C(214)	–	C(215)	–	C(216)	120(2)
P(1)	–	C(111)	–	C(112)	122(2)	C(211)	–	C(216)	–	C(215)	121(2)

Table 3.3.7: *Mean Plane Data For The [PhMe₂PAuCl] Complex.*

Plane number 1: Least-squares plane through the phenyl ring defined by atoms C(111) to C(116).

Atoms Defining Plane	Distance (Å)	esd (Å)
C(111)	0.0057	0.0171
C(112)	-0.0124	0.0263
C(113)	0.0081	0.0274
C(114)	-0.0008	0.0222
C(115)	0.0006	0.0255
C(116)	-0.0030	0.0200
Additional Atom	Distance (Å)	
P(1)	0.0323	

Mean deviation from plane is 0.0051 Å.

Chi-squared: 0.4.

Plane number 2: Least-squares plane through the phenyl ring defined by atoms C(211) to C(216).

Atoms Defining Plane	Distance (Å)	esd (Å)
C(211)	-0.0241	0.0246
C(212)	0.0434	0.0327
C(213)	-0.0144	0.0323
C(214)	-0.0305	0.0346
C(215)	0.0234	0.0301
C(216)	0.0022	0.0257
Additional Atom	Distance (Å)	
P(2)	0.1208	

Mean deviation from plane is 0.0230 Å.

Chi-squared: 4.3.
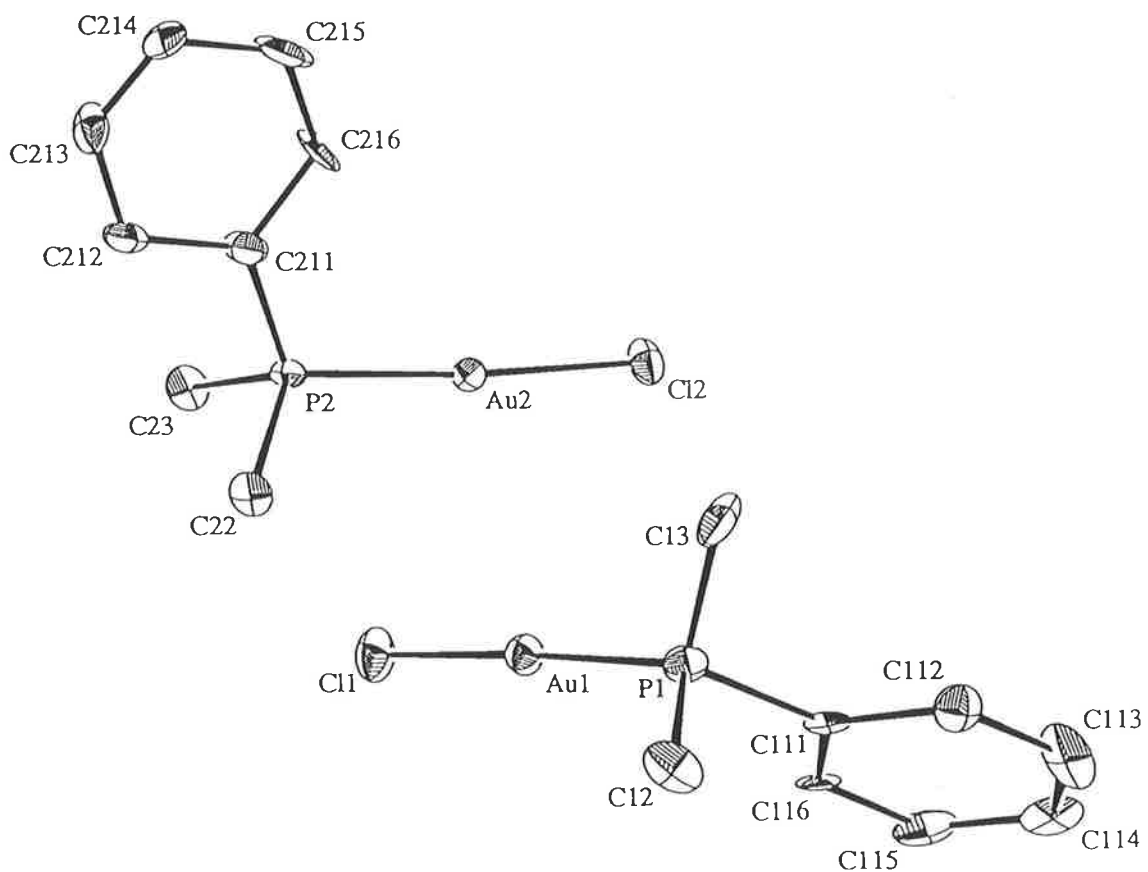
Figure 3.3.1: *Molecular Structure And Crystallographic Numbering Scheme For*

[PhMe₂PAuCl].

A diagram of the unit cell is shown in Figure 3.3.2. The unit cell is comprised of eight molecules, the asymmetric unit therefore contains two molecules, labeled molecules 1 and 2 respectively; see Figure 3.3.1. The molecules are arranged in the unit cell in what appears to be a dimeric relationship, known as head-to-tail dimers. Such interactions have been observed before for triorganophosphinegold(I) chlorides where the phosphine is relatively small in size, and are attributable to the presence of close gold to gold interactions in the lattice[46]. The Au(1)...Au(2) interaction is at a distance of 3.262(1) Å, which is less than the sum of the van der Waals radii of 3.40 Å, but is due more to relativistic effects than a significant bonding interaction[46].

Both Au(1) and Au(2) exist in the expected linear geometry, clearly demonstrated in Figure 3.3.1, with P–Au–Cl angles of 177.2(3) and 175.4(2)° respectively, comparable with 179.63(8)° for [Ph_3PAuCl][47]. The respective P–Au bond distances are 2.214(6) and 2.205(5) Å, which are equivalent within standard deviation. The Au–Cl bond distances of 2.277(6) and 2.273(5) Å, respectively are also within standard deviation range. The bond distances of P(1)–C(111) and P(2)–C(211) are both 1.77(2) Å, a value lower but consistent with those observed for [Ph_3PAuCl]. The phosphorus to methyl group bond lengths in the range of 1.76(2) to 1.81(2) Å are comparable to those found for [Et_3PAuCl][48]. Analysis of Tables 3.3.5 and 3.3.6 reveals that all the remaining corresponding intramolecular parameters between molecules 1 and 2 are identical to within standard deviation.

The phenyl rings are planar for both molecules, with mean deviations from planarity of 0.01(2) and 0.02(3) Å for molecules 1 and 2 respectively. The internal carbon to carbon bond distances range from 1.32(4) to 1.39(3) Å for molecule 1 and from 1.30(3) to 1.42(3) Å for molecule 2. These values are typical for phenyl ring systems and are indicative of electron delocalization.

The main difference between the two molecules in the asymmetric crystallographic unit is in the geometry of the gold atoms as manifested by the respective values for the P–Au–Cl angle. This difference might be attributable to the presence of the dimer in the lattice, where the Au(1)...Au(2) interaction gives rise to unequal distortions in the ideal linear geometries about
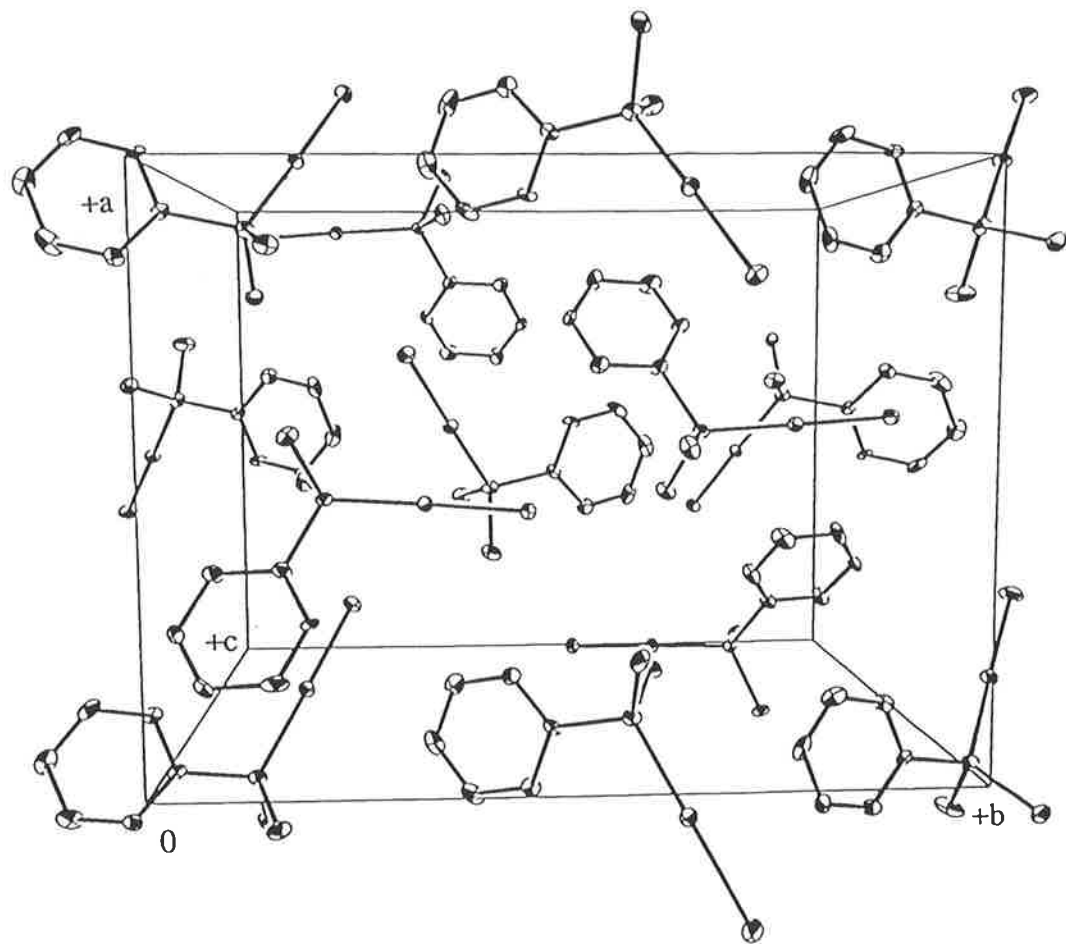
Figure 3.3.2: *Unit Cell Diagram For [PhMe2PAuCl].*

the two gold atoms[46]. The two independent molecules also differ from each other in the relative orientations of the phosphine-bound substituents, as shown in the values of the torsion angles Cl(n) / Au(n) / P(n) / C(n2), C(n3), C(n11) of -47, -165 and 72° for n = 1 and -178, 68 and -56° for n = 2, respectively. The next section investigates whether the size of the phosphine as represented by the cone-angle has any effect on the intramolecular parameters associated with the gold atom.

3.4 *Cone-angle correlation for triorganophosphinegold(I) chloride complexes*

The cone-angle of a phosphine is a structural property first introduced by Tolman[49], and is useful in defining the volume of space about a phosphine complex within which steric (van der Waals) interactions are likely to occur. Tolman's original work was centred on phosphinenickel carbonyl compounds, in which the nickel atom formed the fourth substituent on the phosphorus atom, to give this centre an approximately tetrahedral geometry. The substituents on the phosphorus can sweep out a maximum volume of space about the P–Ni axis in the shape of a cone whose apex lies on the metal centre, and the angle between the edge of this cone and a line extended from the P–Ni bond axis (the apical axis) is defined as half of the cone-angle[50]. Cone-angles can usually be determined from crystallographic data, although for phosphines containing mixed substituents, further mathematical treatment is required, resulting in a weighted cone-angle. The Tolman cone-angles are hence dependent on the spatial size of the substituents and on the lengths of the P–Ni bonds. Tolman's analysis assumed this bond length to be of a constant value, but in reality the bulkiness of the substituents and the P–Ni bond length is likely to be interdependent[49].

A recent publication by Brown[51] introduced a new parameter that complements the cone-angle concept. Known as the *ligand repulsive energy*, E_R, this quantity results from energy-minimization studies on phosphinechromium carbonyls, and represents the van der Waals interactions between the phosphine substituents and moieties along the P–Cr bond axis. The main advantage of the E_R quantity is that it distinguishes steric effects from electronic effects, and is more easily applied to phosphines bound to other elements. Using Tolman's calculated

cone-angles (θ) for the nickel compounds, Brown found that the E_R parameter correlated surprisingly well with the cone-angle; i.e. the relationship between E_R and θ was found to be linear for analogous Cr and Ni compounds to within a small margin of error[51].

This study is concerned with the application of θ and E_R to triorganophosphinegold(I) chloride complexes of the general formula [R_3PAuCl]. Complexes of this type invariably possess a gold atom of linear geometry i.e. the P–Au–Cl bond angle is close to 180°. Hence the purely steric effects on the chlorine atom that arise from the size of the phosphine are likely to be minimized. Since the cone-angle parameter encompasses electronic effects also[49,50] (the electronic nature of the groups bound to the phosphorus atom will influence the length of the phosphorus to metal bond and thus the magnitude of the derived or calculated cone-angle), then variations in the P–Au and Au–Cl bonds with a change in θ are likely to be attributable to electronic rather than steric effects. Therefore, a correlation may be drawn between these parameters. The quantity of E_R, which should describe only van der Waal or purely steric effects, should thus correlate less well with the intramolecular parameters if electronic effects are significant. The parameters for a range of triorganophosphinegold(I) chlorides have been collated from literature reports and are shown, together with calculated θ and E_R values, in Table 3.4.

Both θ and E_R have been plotted against the P–Au and Au–Cl bonds; the results are shown in Figure 3.4. At first inspection there seem to be no linear relationships present between the parameters and bond lengths. However, closer analysis of some of the plots reveals that a common trend does exist, albeit with some exceptions. The plot of P–Au versus cone-angle contains points that appear to form a linear distribution, with the anomalous points representing [(PhO)$_3$PAuCl] and [PhMe$_2$PAuCl]. The analogous plot against E_R demonstrates the same linear appearance, with the same two exceptions. The values of P–Au for those complexes on the linear progression are in fact all equivalent within experimental error. Hence, there is no noticeable electronic effect due to the phosphine ligand on the length of P–Au. The values for θ can thus be regarded as absolute, similarly to Tolman's assumption of a constant P–Ni bond for various phosphine ligands. The plot of P–Au versus E_R displays a similar appearance to the

Table 3.4: *Cone Angles (θ), Ligand Repulsive Energies (E$_R$) And Intramolecular Parameters Of The [R$_3$PAuCl] Complexes.*

R$_3$P	θ (°)	E$_R$ (kcal mol^{-1})	P–Au–Cl (°)	P–Au (Å)	Au–Cl (Å)	Ref.
Et$_3$P	132	61	178.5(3)	2.232(9)	2.305(8)	[48]
			178.9(3)	2.231(8)	2.306(8)	
Cycl$_3$P	170	116	177.0(2)	2.242(4)	2.279(5)	[52]
Ph$_3$P	145	75	179.63(8)	2.235(3)	2.279(3)	[47]
Cycl$_2$PhP	162	105	178.3(1)	2.234(2)	2.281(3)	[53]
(PhO)$_3$P	128	65	178.5(2)	2.192(5)	2.273(5)	[54]
(o-Tol)$_3$P	194	113	179.4(1)	2.243(2)	2.281(3)	[55]
(m-Tol)$_3$P	145	79	175.1(1)	2.235(2)	2.288(2)	[56]
PhMe$_2$P	122	44	177.2(3)	2.214(6)	2.277(6)	This work
			175.4(2)	2.205(5)	2.273(5)	

Note: Their are two molecules in the asymmetric crystallographic units for each of [Et$_3$PAuCl] and [PhMe$_2$PAuCl].
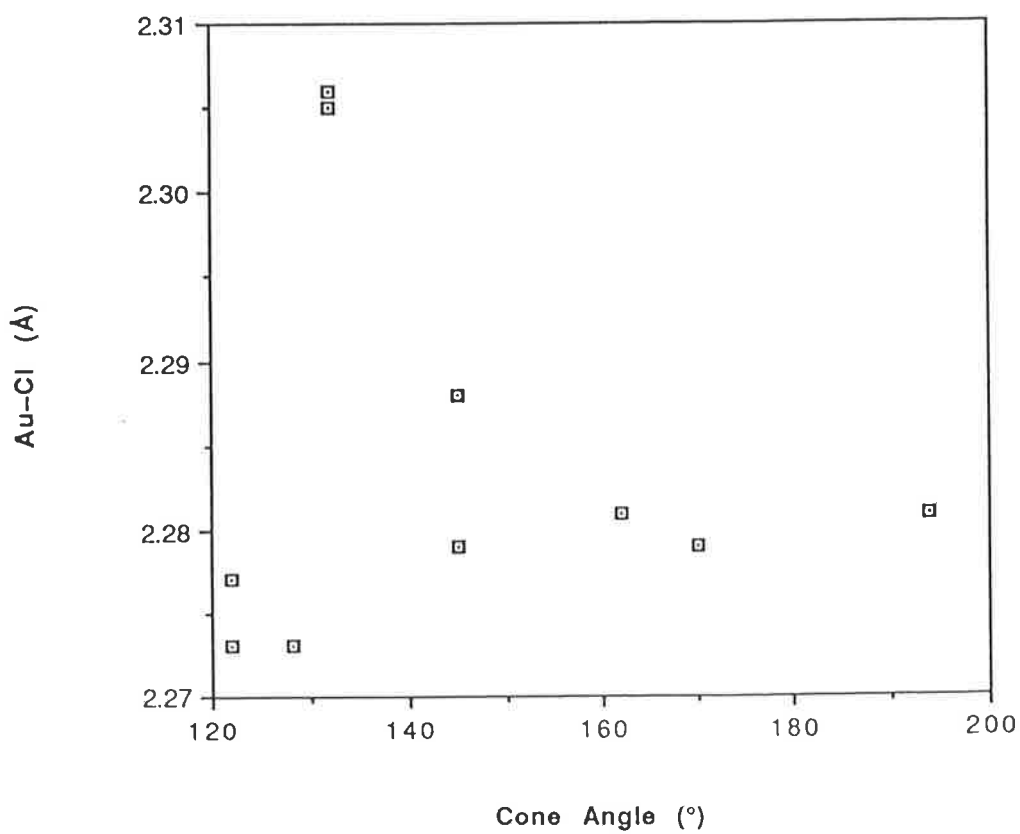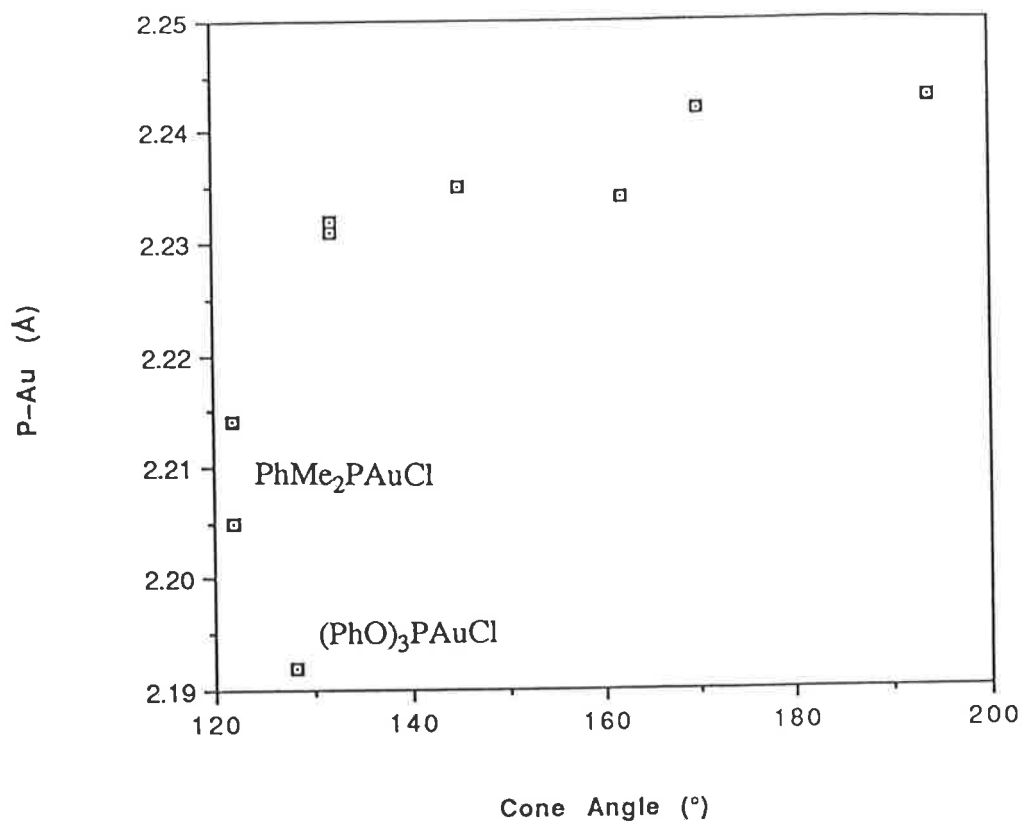
Figure 3.4: *Plots Of The Parameters* θ, *And* E_R *Versus P–Au, Au–Cl And P–Au–Cl..*
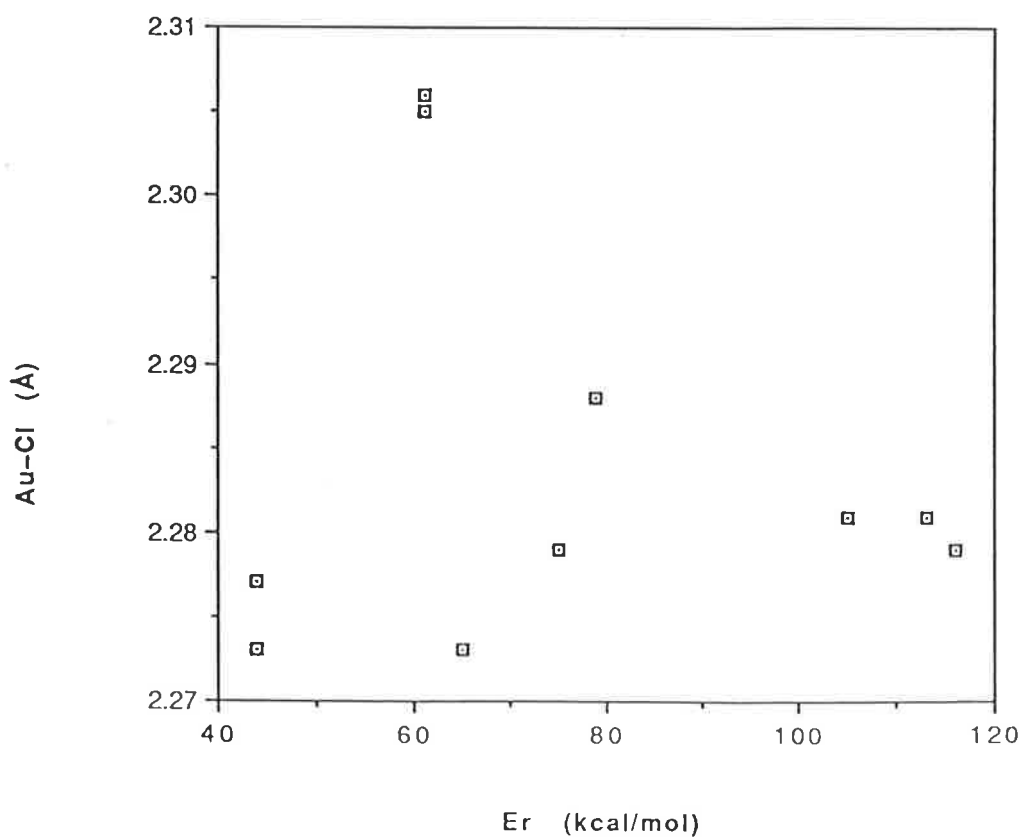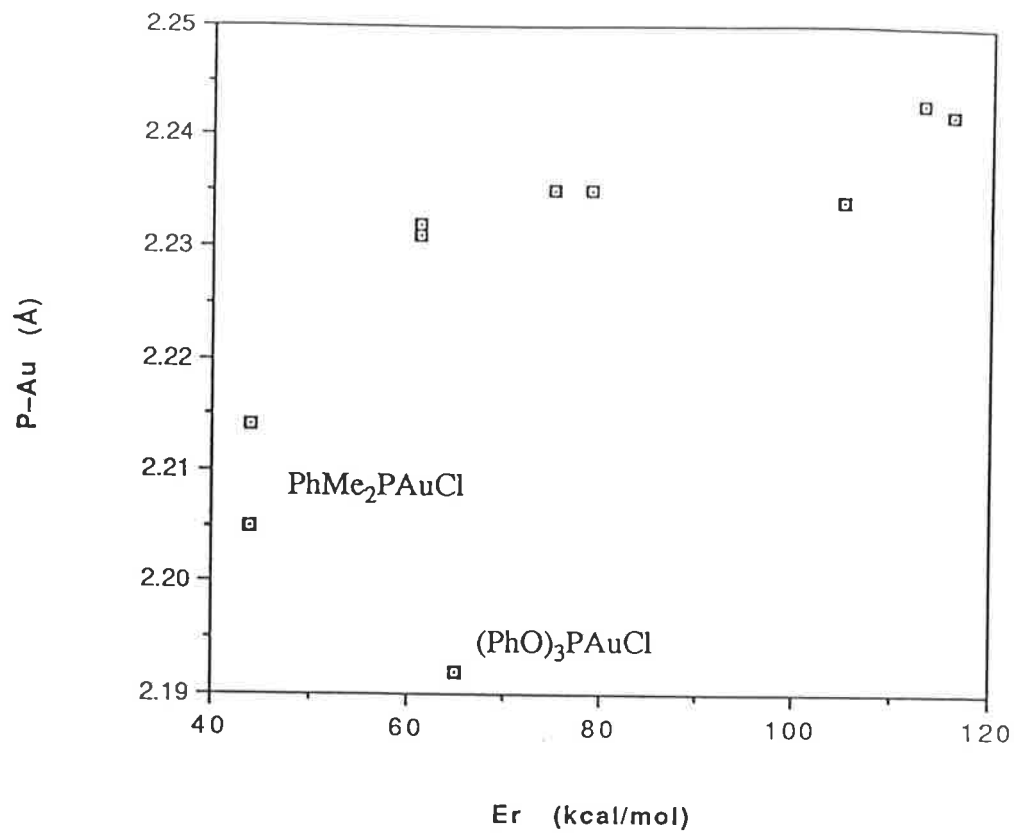
Figure 3.4 *(continued)*
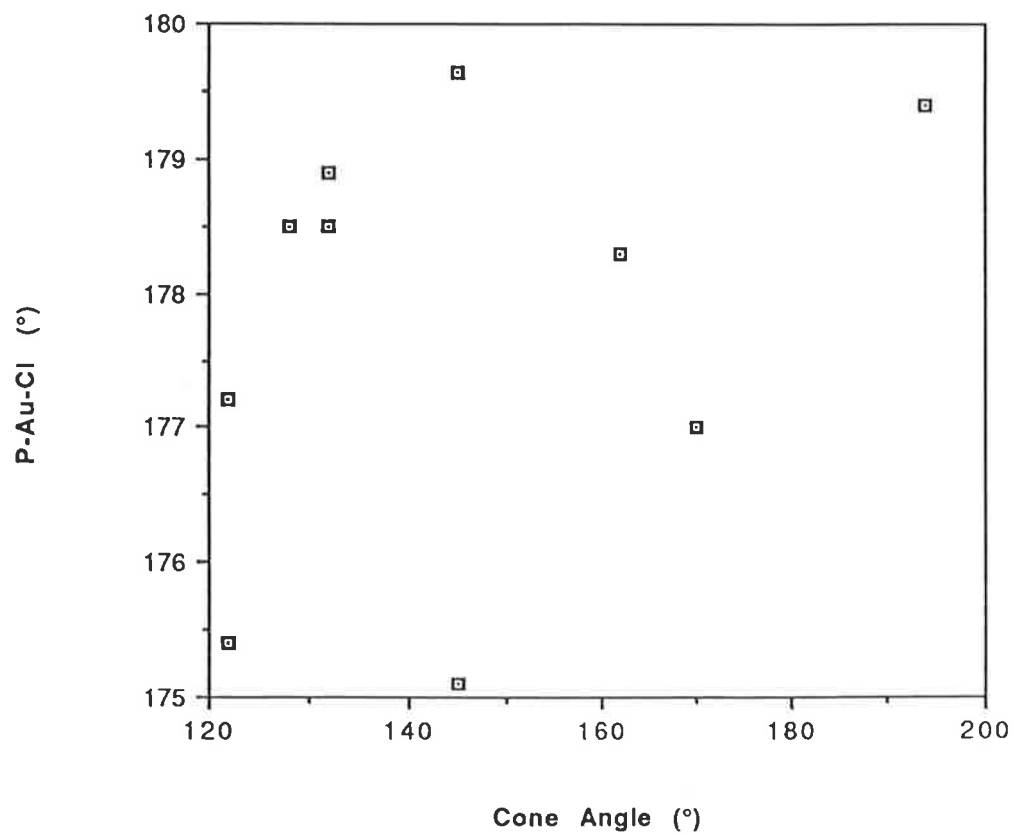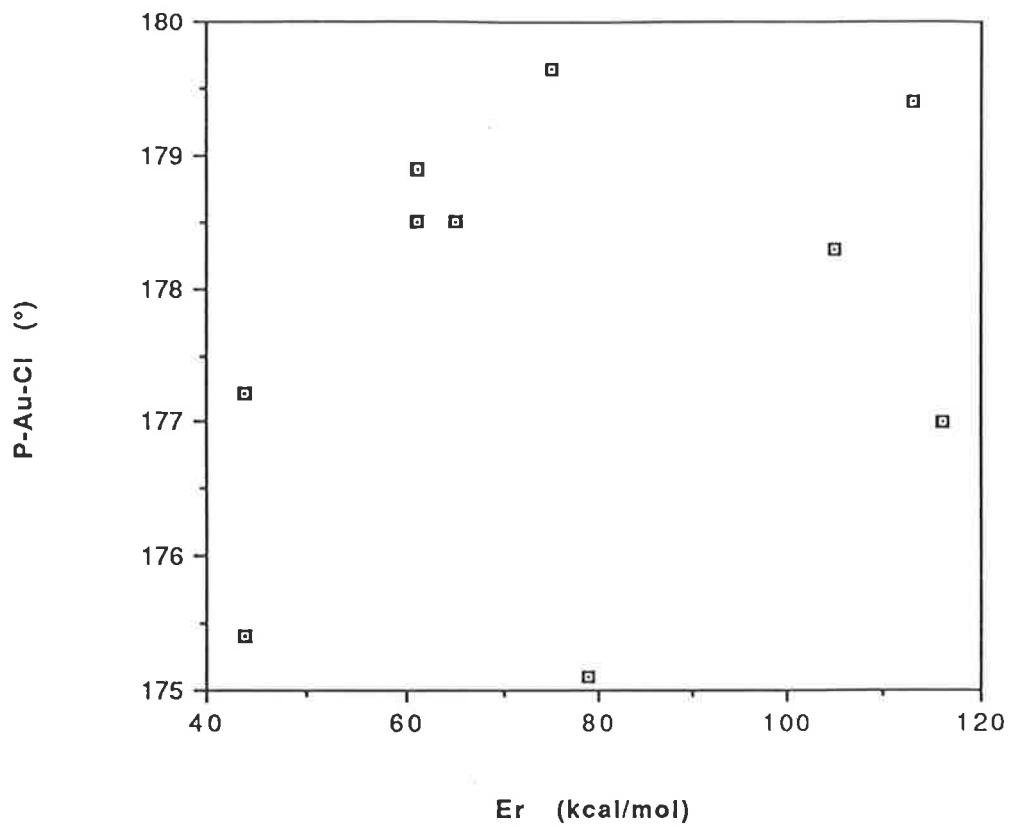
Figure 3.4 *(continued)*

P–Au versus θ plot, indicating that steric effects on the P–Au bond in the [R$_3$PAuCl] complexes are also negligible.

The two exceptions to the general trends were found for the [(PhO)$_3$PAuCl] and [PhMe$_2$PAuCl] complexes. In the paper by Brown[51], phosphite ligands were noted as exceptions due to the flexibility of C–O–P linkages, which can easily 'absorb' steric effects by adopting a variety of conformations not available to phosphines. Hence, neither θ nor E$_R$ can adequately express the steric or electronic factors of the (PhO)$_3$P ligand. PhMe$_2$P is classed as a small phosphine, and gold(I) chloride complexes of these phosphines often crystallize in such an arrangement to allow the closest Au...Au interaction possible in the lattice, usually resulting in dimers[46]. As discussed earlier in this chapter, the structure determination of [PhMe$_2$PAuCl] revealed that such dimers were present, with an Au(1)...Au(2) interaction of 3.262(1) Å, less than the sum of the van der Waals radii (3.40 Å). Such a small distance is not often observed for complexes of larger phosphines, and so in this complex the intermolecular interaction may be a determining factor for the anomalous P–Au bond length. [Et$_3$PAuCl] also contains a small phosphine[48], but the cone angle is considerably greater. The closest Au...Au interaction here is 3.615(2) Å, significantly larger than 3.40 Å, and [Et$_3$PAuCl] is consistent with the linear trend of the graph. Thus, it can be postulated that, since [PhMe$_2$PAuCl] is anomalous for both E$_R$ and θ, electronic factors from intermolecular Au...Au interactions have a significant influence on the length of the P–Au bond in complexes of small phosphines. Neither E$_R$ nor θ are adequate quantities for accommodating such intermolecular interactions.

The Au–Cl bond length should manifest electronic effects of the phosphine ligand on the P–Au–Cl moiety more than steric effects, as it occupies a position *trans* to the phosphorus atom. The plots involving Au–Cl (i.e. Figure 3.4) show that there is no clear trend. In fact, all the values lie within experimental error. This indicates that, even in complexes with significant intermolecular interactions in the lattice, the Au–Cl bond length is largely independent of the steric and electronic effects of the phosphine ligand.

The P–Au–Cl bond angle displays a relatively large spread of values. However, there is no noticeable trend based on the nature of the phosphine ligand coordinated to the gold centre. The values for [(PhO)$_3$PAuCl] and [PhMe$_2$PAuCl] are not exceptional, indicating that conformations and intermolecular interactions do not affect this aspect of the chromophore in any special way.

Based on the examples studied, the important results are: 1) the P–Au bond length is independent of the steric and electronic effects of the phosphine ligand, but can reflect the electronic environment about the gold atom if significant intermolecular Au...Au interactions are present; 2) the Au–Cl bond length remains invariant, regardless of intermolecular interactions and the steric or electronic profiles of the phosphine ligand; 3) the P–Au–Cl bond angle shows a range of values, but this angle is not clearly related to any steric or electronic property of the phosphine ligand; and 4) the ligand repulsive energy, E_R, as calculated by Brown from energy-minimization models, has a good correlation with the cone-angle of phosphines but is no better than this angle for observing how the steric nature of a phosphine affects the intramolecular characteristics of triorganophosphinegold(I) chlorides.

CHAPTER 4

Spectroscopic Characterization of the Triorganophosphinegold(I) 6-mercaptopurinate Complexes

4.1 *Introduction*

In this chapter the results obtained from the spectroscopic analysis of the complexes with the general formulae [R$_3$PAu(6-MP)] (where R$_3$P = Et$_3$P, Cycl$_3$P, PhMe$_2$P, Ph$_3$P, (*o*-Tol)$_3$P, (*m*-Tol)$_3$P or (*p*-Tol)$_3$P), [(Ph$_2$P(CH$_2$)$_n$PPh$_2$)(AuCl)(Au(6-MP))] (where n = 2 or 3) and [(Ph$_2$P(CH$_2$)$_n$PPh$_2$)(Au(6-MP))$_2$] (where n = 1, 2 or 3) will be tabulated and discussed, with emphasis on how these results indicate product formation and what they reveal about the coordinated 6-mercaptopurinate ligand. A general introduction concerning the 6-mercaptopurine ligand itself and its chemistry as related to this project will be given first to help illustrate the points discussed later.

4.2 *An overview of the 6-mercaptopurine ligand*

6-Mercaptopurine, 6-MPH, shown in Figure 4.2.1, is a member of the class of nucleobases known as purines. These compounds consist of a six-membered heterocyclic ring fused to a
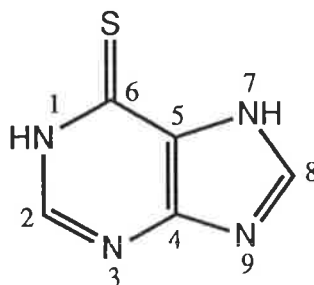
Figure 4.2.1: *Labelling Scheme For 6-mercaptopurine.*

five membered ring at the 4 and 5 positions, as shown in Figure 4.2.1, thus resulting in a nine membered skeletal structure. Purines are characterized by the 1, 3, 7, 9 substitution pattern of nitrogens for carbons.

The systematic name for 6-MPH is 1,7-dihydro-6H-purine-6-thione, which indicates that the two protonated nitrogens are at positions 1 and 7. This finding is based on crystal structure determinations[57,58], but determinations on complexes containing 6-MP show that it is possible for the protons to be bound to the other nitrogens alternatively. Tautomeric studies on the free ligand in solution[59] have shown that the most dominant tautomer is in fact the 1,9-dihydro-form, suggesting the protons may be sufficiently labile to suit the requirements of a given reaction mechanism: four tautomers of 6MPH are shown in Figure 4.2.2. It is therefore also possible for the 6-thione group to exist as the thiol, although in a proportionately low quantity[59].
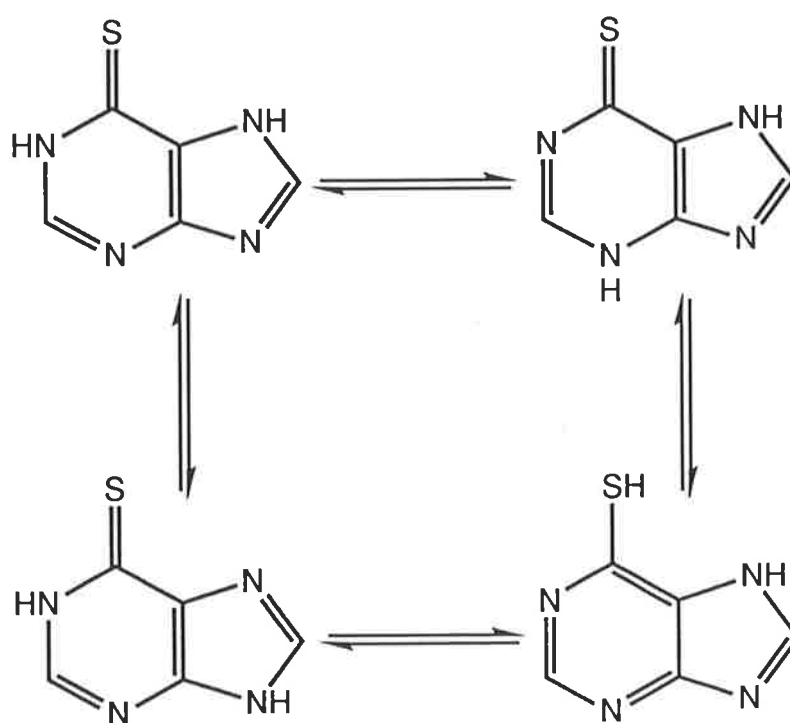
Figure 4.2.2: *Tautomeric Structures For 6-mercaptopurine.*

For the preparation of the compounds in this thesis, a metathetical reaction involving base was utilized. This involves the exchange of a chloride ion for the 6-MP ligand, though it is not clear whether the reaction is S_N1 or S_N2. In either mechanism, the 6-MPH molecule must be

deprotonated. Studies on the pK_a values for the protonated nitrogen centres indicate that N^1 is the more acidic atom[59]. Deprotonation here can result in the formal negative charge being located on the sulphur atom through resonance (see Figure 4.2.3), thus leading to coordination to the gold centre. This is verified by the crystal structure determinations presented in Chapter 5.
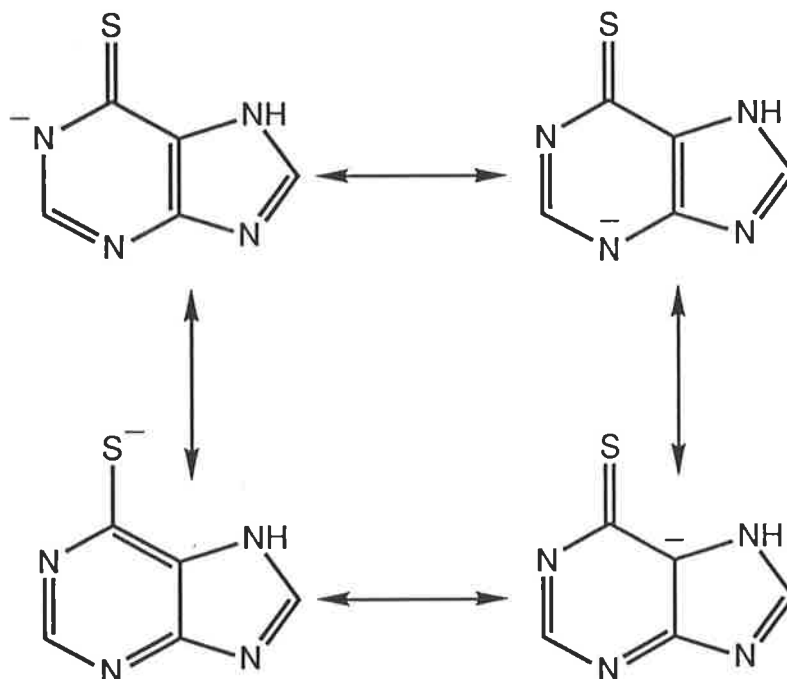
Figure 4.2.3: *Resonance Contributors To The 6-mercaptopurine Anion.*

The electron density in the 6-mercaptopurine ring system is likely to be altered when gold(I) is coordinated by the sulphur atom, leading to greater delocalization of electron density in the six-membered ring system. The changes in electron density should be detectable via spectroscopy.

4.3 Infrared spectroscopy

The heterocyclic, aromatic nature of the 6-mercaptopurine ring system lends itself to a great many possible absorptions in the infrared spectrum. Chromophores such as C=N, C=C and other groups have all been observed to absorb strongly in purines and related thionucleobases[60,61,62]. Due to the overlapping of many of the absorptions, coupling effects, as noted by Thakur and Singh[63], are likely to occur in 6-mercaptopurine and its complexes, leading to complicated spectra. Reports in the literature often conflict with each other as to where certain absorptions occur in the spectra, and on the identities of certain strong

absorptions[64,65]. The 'thioamide bands'[63,66], which result from the coupling of various absorption modes of delocalized N–C–S groups, have not been generally reported for complexes of 6-mercaptopurine, although they are noted for other thionucleobases[60,61,62]. The thioamide absorption is usually divided into four bands (I, II, III and IV)[63], which differ in their frequency ranges due to the constituent absorptions that are coupled. Bands III and IV are usually observed at lower wavenumbers, around the finger-print region, and thus they are not considered here as their assignments would be too tentative. The major contribution to band I is from the ν(C=N) vibrational mode, and band II from ν(C=S). Hence coordination of 6-mercaptopurine to gold via sulphur should be observable through changes to the absorption frequencies of these two bands.

The lack of definitive data in the literature has resulted in uncertainty as to how the infrared data for the complexes in this thesis should be presented. The scheme thus chosen is to list the data in two tables: 1) Table 4.3.1 presenting the absorptions due to the phosphine moieties (from comparisons with the spectra of the corresponding triorganophosphinegold(I) chloride species); and 2) Table 4.3.2 presenting the absorptions due to the purine group. In the latter table, the absorptions for the thioamide bands I and II, ν(N–C–S), have been resolved from the phosphine peaks by comparison with the spectra of the corresponding gold(I) chloride complexes, but the other absorptions are listed together under the classification of 'purine ring vibrations'. Bands I and II assignments are those peaks occuring in the range where this absorption is observed for analogous heterocycles e.g. for thionucleobase gold(I) complexes[60,61,62]. These should not be regarded as definitive assignments, but they are likely to be representative of the important thioamide chromophore.

A broad absorption band occurs in many of the spectra at ca 3400 cm^{-1}, due to water molecules of hydration, or moisture in the spectrometer environment. This band, when present, overlaps with that of the N–H stretching mode. The ν(N–H) absorption in all the spectra occurs over a broad range of approximately 3300 to 2200 cm^{-1} of medium intensity; such a wide range has been observed before in complexes of 6-MP via sulphur coordination[64,65]. However, the ν(C–H) absorption also occurs in this range[34,35], so the broad absorption in this region should

Table 4.3.1: *Infrared Data For The Phosphine Moieties.*

Complex	ν(C–H)	ν(C=C)	ν(P–C), ν(C–C) and δ(C–H)
[Et$_3$PAu(6-MP)]	3099m, 3055m, 2964s, 2931s	-	1456m, 1418m, 1384m, 1268m
[Cycl$_3$PAu(6-MP)]	3099w, 3041w, 2926vs, 2853s	-	1446m, 1417w, 1385s, 1176w
[PhMe$_2$PAu(6-MP)]	3053s, 2952s, 2925s	1465w	1436m, 1419m, 1384m, 1110w
[Ph$_3$PAu(6-MP)]	3054m, 2967m, 2929m	1479m	1434vs, 1421m, 1381s, 1181w, 1100s
[(*o*-Tol)$_3$PAu(6-MP)]	3054m, 2964m, 2927m	1590s, 1470m	1449s, 1410m, 1384s
[(*m*-Tol)$_3$PAu(6-MP)]	3035m, 2921m	1477m	1447m, 1418m, 1384m, 1108m
[(*p*-Tol)$_3$PAu(6-MP)]	3097s, 3035s, 2917s	1597s, 1497s	1441m, 1418s, 1397s, 1384s, 1187s, 1102vs
[dppe(AuCl)(Au(6-MP))]	3055m, 2924s	1575m, 1481m	1435vs, 1384s,sh, 1173s, 1104s
[dppp(AuCl)(Au(6-MP))]	3056m, 2924s, 2851m	1481m	1434vs, 1404m, 1384s, 1104s
[dppm(Au(6-MP))$_2$]	3050s, 2927s, 2923s, 2853s	1483m, 1467m	1436vs, 1421s, 1384vs, 1191m, 1102s
[dppe(Au(6-MP))$_2$]	3050m, 2972m	1481w, 1468w	1436s, 1410m, 1384vs, 1171w, 1104m
[dppp(Au(6-MP))$_2$]	3050s, 2924s, 2852m	1482m	1436vs, 1420s, 1384s, 1186m, 1104s

Note: Units are wavenumbers (cm^{-1}).

Table 4.3.2: *Infrared Data For The 6-mercaptopurinate Moieties.*

Complex	ν(N–C–S) band I	band II	Purine vibrational modes.
6-MPH	1615s, 1575s, 1558m	1346s	1224s, 1156m, 1147m, 1123m, 1276m, 1529s, 1472m, 1409vs
[Et₃PAu(6-MP)]	1586s, 1557vs	1320m	1238m, 1208m, 1155w, 1132w
[Cycl₃PAu(6-MP)]	1585m, 1554s	1320m	1269w, 1214w, 1207w, 1176w, 1132w, 1113w
[PhMe₂PAu(6-MP)]	1586m, 1558s	1319s	1269w, 1238w, 1208w,1132w
[Ph₃PAu(6-MP)]	1591s, 1559vs	1321s	1244s, 1236s, 1210m, 1157w, 1133w
[(o-Tol)₃PAu(6-MP)]	1617m, 1554vs	1322m	1277w, 1241m, 1229m, 1211m, 1164w
[(m-Tol)₃PAu(6-MP)]	1587m, 1555s	1319m	1268w, 1234m, 1207m
[(p-Tol)₃PAu(6-MP)]	1585s, 1556vs	1319s	1269m, 1234s, 1208s, 1120w
[dppe(AuCl)(Au(6-MP))]	1616s, 1595s, 1558m	1335m	1311m, 1276m, 1217m, 1159m, 1122m
[dppp(AuCl)(Au(6-MP))]	1594m, 1558m	1318w	1347w, 1274w, 1240w, 1209w
[dppm(Au(6-MP))₂]	1586s, 1558vs	1320s	1270m, 1236s, 1207m, 1161w
[dppe(Au(6-MP))₂]	1587s, 1558s	1319m	1275w, 1236m,br, 1209m, 1122w
[dppp(Au(6-MP))₂]	1585s, 1558vs	1319s	1269m, 1238s, 1208m

Note: Units are wavenumbers (cm^{-1}).

be assigned to the overlapping vibrational modes of both ν(N–H) and ν(C–H). This absorption can be seen most clearly for 6-mercaptopurine in Figure 4.3.1 and for [Ph$_3$PAu(6-MP)] in Figure 4.3.2. In the latter spectra the ν(C–H) absorptions from the phosphine moiety can also be observed as sharper peaks around 3000 to 2900 cm^{-1}, an observation that is suggestive of product formation. Further confirmation arises from inspection of the thioamide peaks in these two spectra; the differences in absorption frequencies for band I at 1575 cm^{-1} for 6-MPH and 1591 cm^{-1} for [Ph$_3$PAu(6-MP)] for example. This suggests an increase in bond order of the C=N chromophore, which is expected since the electron density in the aromatic system increases upon coordination. The C=S bond approaches single bond character when the sulphur atom coordinates to gold, and this is observed via band II; the 1346 cm^{-1} peak moves down to 1321 cm^{-1} in the [Ph$_3$PAu(6-MP)] complex. Similar trends are observed for these peaks in all spectra, suggesting product formation in all cases. The deduced changes in bond lengths will be verified in the crystallographic examples in Chapter 5; N(1)–C(6) undergoes a decrease in length of around 0.040 to 0.045 Å, and C(6)–S(6) increases by approximately 0.039 to 0.052 Å upon coordination.

As expected, the frequencies of the phosphine vibrational modes are observed to be independent of the coordination of the purine molecule to the gold atom. From the foregoing discussion, infrared spectroscopy confirms product formation via the appearance of both phosphine and 6-mercaptopurine absorptions in the spectra, and by the frequency shifts of the thioamide absorption bands, which also confirm the expected increase in electron density in the ring system upon complexation.

4.4 ^1H NMR spectroscopy

The data obtained from the proton NMR spectra of the complexes studied in this thesis are reported in Tables 4.4.1 and 4.4.2. The solvent utilized was d$_6$-dimethylsulphoxide as this proved to be the only common solvent into which 6-mercaptopurine and the gold complexes would dissolve. NMR studies on these and other analogous complexes were also performed in other solvents (e.g. (CD$_3$)$_2$CO and CDCl$_3$) which showed that there was no obvious solvent
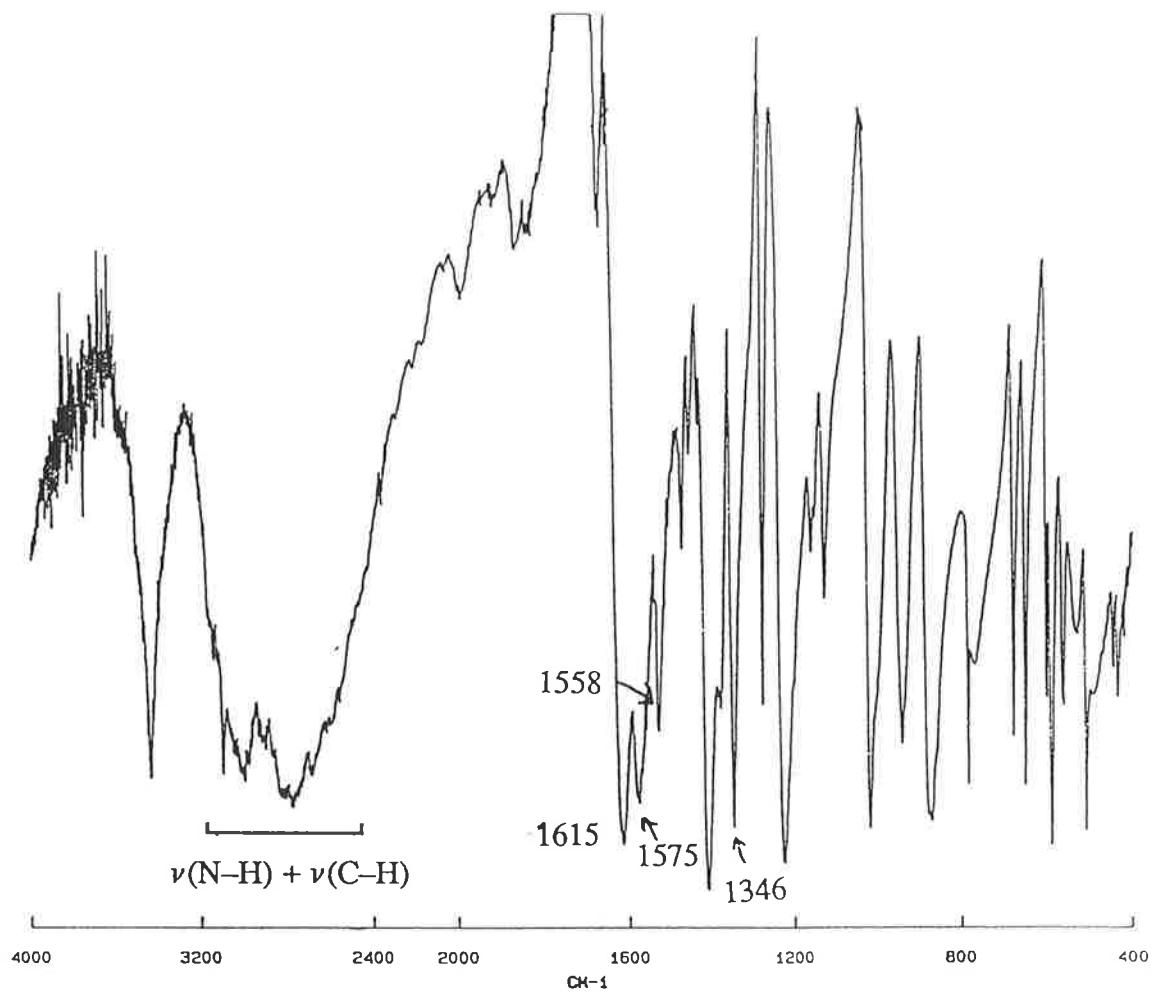
Figure 4.3.1: *IR Spectrum Of 6-mercaptopurine, 6-MPH.*
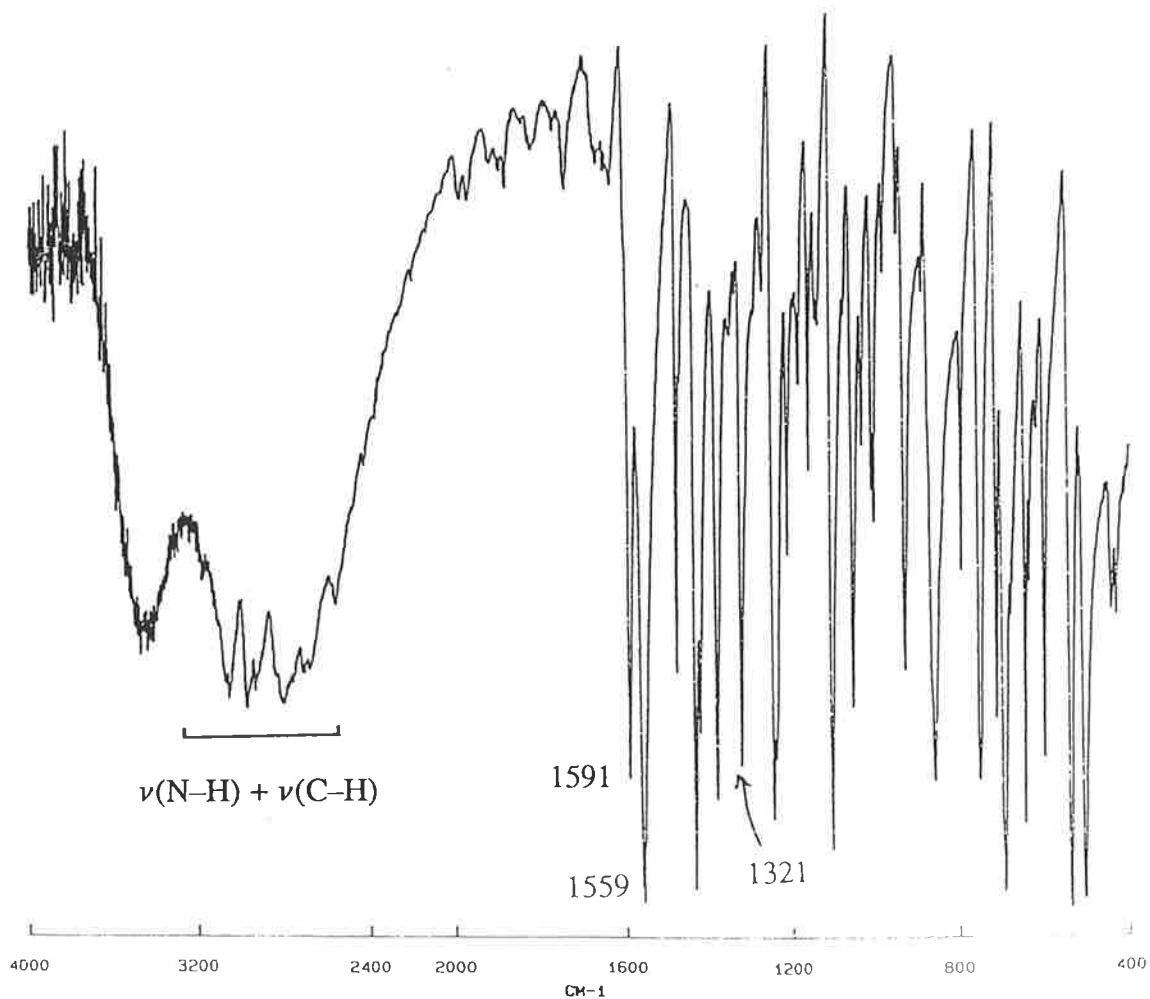
Figure 4.3.2: *IR Spectrum Of 6-mercaptopurinato(triphenylphosphine)gold(I),*
$[Ph_3PAu(6-MP)]$.

Table 4.4.1: *^1H NMR Chemical Shift Values (ppm) For The [$R_3PAu(6\text{-}MP)$] Complexes.*

R_3P	H^2	H^9	H^8	H_α	H_β	H_γ	H_δ	H_{CH3}
6-MPH	8.45(s)	13.62(br,s)	8.26(s)	-	-	-	-	-
Et_3P	8.41(s)	13.21(br,s)	8.31(s)	1.95(m)	1.19(dt) (7.68)[a] (18.35)[b]	-	-	-
$Cycl_3P$	8.34(s)	13.12(br,s)	8.19(s)	2.17(m)	1.89(m)	1.57(m)	1.32(m)	-
Ph_3P	8.51(s)	13.35(br,s)	8.31(s)	-	7.73 - 7.64(br,m)			-
$(o\text{-}Tol)_3P$	8.35(s)	13.14(br,s)	7.87(s)	-	7.61 - 7.02(br,m)			2.64(s)
$(m\text{-}Tol)_3P$	8.45(s)	13.32(br,s)	8.25(s)	-	7.53 - 7.38(br,m)			2.28(s)
$(p\text{-}Tol)_3P$	8.46(s)	13.32(br,s)	8.32(s)	-	7.58 - 7.40(br,m)			2.37(s)
$PhMe_2P$	8.45(s)	13.20(br,s)	8.33(s)	-	8.02 - 7.58(br,m)			1.95(d) (10.63)[c]

Note: Coupling constants, in parentheses, are in units of Hertz: a: $^3J_{H\text{-}H}$, b: $^3J_{P\text{-}H}$ and c: $^2J_{P\text{-}H}$.

Table 4.4.2: *^1H NMR Chemical Shift Values (ppm) For The [($Ph_2P(CH_2)_nPPh_2$)- (AuCl)(Au(6-MP))] And [($Ph_2P(CH_2)_nPPh_2$)(Au(6-MP))$_2$] Complexes.*

Complex	H^2	H^9	H^8	Phenyl Protons	H_a	H_b
6-MPH	8.45(s)	13.62(br,s)	8.26(s)	-	-	-
[dppe(AuCl)(Au(6-MP))]	8.36(s)	13.12(br,s)	8.17(s)	7.95 - 7.37(br,m)	3.04(m)	-
[dppp(AuCl)(Au(6-MP))]	8.36(s)	13.25(br,s)	8.09(s)	7.87 - 7.47(br,m)	3.02(m)	-
[dppm(Au(6-MP))$_2$]	8.37(s)	13.13(br,s)	8.24(s)	7.89 - 7.49(br,m)	4.64(m)	-
[dppe(Au(6-MP))$_2$]	8.40(s)	13.22(br,s)	8.20(s)	7.74 - 7.50(br,m)	3.07(m)	1.73(m)
[dppp(Au(6-MP))$_2$]	8.38(s)	13.18(br,s)	8.19(s)	7.83 - 7.42(br,m)	3.16(m)	1.89(m)

Note: Coupling constants, in parentheses, are in units of Hertz: a: $^3J_{H\text{-}H}$, b: $^3J_{P\text{-}H}$ and c: $^2J_{P\text{-}H}$.

effects[62]. The labelling scheme adopted is the same as that described in Chapter 3 for the phosphine moieties, and the protons of the 6-MP moiety are labelled as in Figure 4.2.2. *4.2.1* Crystal structure determinations on [Ph$_3$PAu(6-MP)].C$_2$H$_5$OH and [(o-Tol)$_3$PAu(6-MP)].C$_2$H$_5$OH (see Chapter 5) revealed that the protonated imadazole nitrogen in these complexes is H^9, whereas it was H^7 in 6-mercaptopurine. Therefore the H^9 resonance given for 6-mercaptopurine in Tables 4.4.1 and 4.4.2 corresponds to H^7.

As for the triorganophosphinegold(I) chloride analogues, the phenyl regions are not very informative due to the complicated coupling patterns which lead to broad multiplets. This applies also to the spectrum of [Cycl$_3$PAu(6-MP)], where broad and complex multiplets are still observed. If there is an effect on coupling and chemical shifts in the phosphine ligand when 6-MP substitutes for the chloride on the gold centre, then it would best be observed in the spectrum of [Et$_3$PAu(6-MP)], where phosphorus-proton coupling is most clearly illustrated. Table 4.4.3 shows the coupling constants involved with [Et$_3$PAuCl] and [Et$_3$PAu(6-MP)].

Table 4.4.3: *Coupling Constants (Hz) Associated With The Et$_3$P Moiety.*

Complex	$^3J_{PH}$	$^3J_{HH}$	δH_α	δH_β
[Et$_3$PAuCl]	18.89	7.71	1.94(m)	1.10(dt)
[Et$_3$PAu(6-MP)]	18.35	7.68	1.95(m)	1.19(dt)

It was not possible to determine clearly the values for $^2J_{PH}$ (which are typically in the order of 10-11 Hz)[60,62], but the data from the table suggest there is little effect on the coupling and shielding factors of the phosphine moiety between chloride and 6-MP substituted complexes. Hence, the phosphine chemical shifts between the corresponding chloride and 6-MP substituted complexes are fairly similar.

The proton resonances arising from the 6-mercaptopurine moiety give rise to simple peaks in the spectra. The free ligand contains two N–H protons, nominally defined as H^1 and H^7, which occur together as a very broad resonance centred at δ 13.62 ppm. This phenomenon has been

reported in the literature before, at δ 13.5 ppm in d_6-dmso[67]. On complexation H^1 is removed, but the single N–H resonance for H^9 is still broad, and is indeed almost unresolved in some of the spectra. Where observed, it resonates in the approximate range of δ 13.10 to δ 13.35 ppm. An example in the literature where 6-MP is complexed via the sulphur atom to a tungsten atom, $[W(CO)_5(6\text{-}MP)]^{[68]}$, gives this proton resonance at δ 14.37 ppm. The high value of the chemical shift is indicative of both the aromatic environment and of the electronegative nitrogen, which both give rise to a deshielding effect. The H^2 and H^8 resonances in the free ligand occur as singlets at δ 8.45 and δ 8.26 ppm respectively (the literature example gives δ 8.35 and $\delta 8.15$ ppm)[67], with the H^8 resonance being slightly broader and smaller. This is illustrated in Figure 4.4.1 for $[(m\text{-}Tol)_3PAu(6\text{-}MP)]$, where the broad appearance of H^9 and the complex phenyl region can also be observed. The small difference in shape allowed identification of these peaks in the complexes, where the H^2 resonance was still observed to be further downfield (the tungsten complex has values of δ 9.23 and δ 8.60 ppm, respectively). The values for both these protons vary between the complexes, and so is no real guide as to whether complexation has occurred; however, the appearance of both phosphine and purine resonances in each spectra and the resultant integration allowed the confirmation of product formation.

4.5 ^{13}C $\{^1H\}$ NMR spectroscopy

The labelling system used is the same as that for the triorganophosphinegold(I) chloride precursors in Chapter 3 and that for the purine in Figure 4.2.2. Tables 4.5.1 and 4.5.2 show the assigned resonances and coupling constants.

The resonances due to the phosphine moiety are consistent with those obtained for the triorganophosphinegold(I) chloride precursors in terms of chemical shift values. In the complexes, the alpha carbon resonates approximately 1 ppm further downfield when R = Ph, o-Tol, m-Tol or p-Tol, and around 0.4 ppm for the other complexes when compared with the triorganophosphinegold(I) chloride precursors. The beta, gamma and delta carbon resonances show no significant changes. However, it is still notable that C_δ for the dppm, dppe and dppp complexes experiences a general upfield shift of 0.5 to 0.7 ppm. The phenyl resonances in
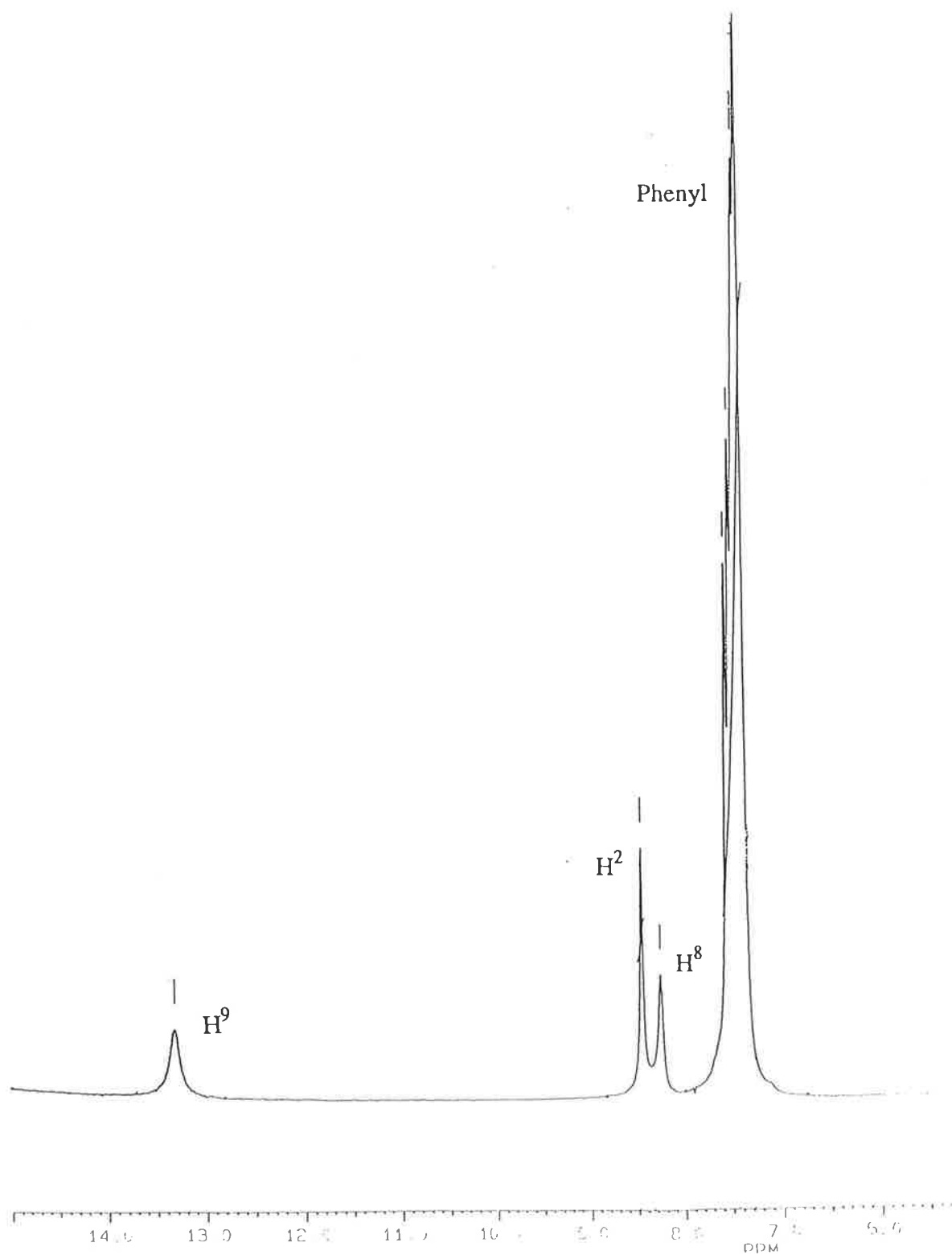
Figure 4.4.1: *^1H NMR Spectrum Of 6-mercaptopurinato[tri(m-tolyl)phosphine]gold(1),*

[(m-Tol)$_3$PAu(6-MP)].

Table 4.5.1: ^{13}C $\{^{1}H\}$ *And* $^{31}P\{^{1}H\}$ *Chemical Shifts (ppm) For The Complexes Of The General Formula* $[R_3PAu(6\text{-}MP)]$.

Complex	C^2	C^4	C^5	C^6	C^8	C_α	C_β	C_γ	C_δ	C_ϵ	C_ζ	-CH$_3$	^{31}P
6-mercaptopurine	144.6	151.0	127.9	170.8	144.6	-	-	-	-	-	-	-	-
[Et$_3$PAu(6-MP)]	141.3	151.1	132.7	171.0	149.1	17.3(d) (33.81)a	8.92	-	-	-	-	-	37.52
[Cycl$_3$PAu(6-MP)]	140.8	150.8	132.7	170.8	149.1	32.6(d) (28.53)a	26.4(d) (12.08)b	30.1	25.5	30.1	26.4(d) (12.08)b	-	57.23
[Ph$_3$PAu(6-MP)]	141.6	151.4	132.4	170.1	149.2	129.4(d) (56.38)a	133.9(d) (14.19)b	129.6(d) (11.24)c	132.0	129.6(d) (11.24)c	133.9(d) (14.19)b	-	37.53
[(o-Tol)$_3$PAu(6-MP)]	140.6	150.6	Obs.	169.5	148.7	125.4(d) (60.99)a	142.3(d) (12.53)b	132.3(d) (8.30)c	131.9	126.9(d) (9.66)c	133.1(d) (9.43)b	22.3(d) (10.94)c	19.15
[(m-Tol)$_3$PAu(6-MP)]	141.3	151.0	132.4	170.2	149.0	129.2(d) (57.06)a	138.8(d) (11.85)b	130.9(d) (12.91)c	132.5	129.2(d) (11.85)c	134.1(d) (14.94)b	21.0	37.36
[(p-Tol)$_3$PAu(6-MP)]	141.5	150.9	132.4	170.4	149.0	126.3(d) (59.70)a	133.6(d) (14.19)b	130.0(d) (11.93)c	141.9	130.0(d) (11.93)c	133.6(d) (14.19)b	20.9	35.61
[PhMe$_2$PAu(6-MP)]	141.4	150.9	Obs.	170.4	149.2	132.9(d) (56.15)a	131.9(d) (13.21)b	128.9(d) (11.02)c	131.3(d) (1.43)d	128.9(d) (11.02)c	131.9(d) (13.21)b	14.8(d) (36.53)a	9.21

Note: ^{31}P-^{13}C coupling constants, in parentheses, are in Hertz, where: a = $^{1}J_{PC}$; b = $^{2}J_{PC}$; c = $^{3}J_{PC}$; d = $^{4}J_{PC}$.

Table 4.5.2: *$^{13}C\ \{^1H\}$ And $^{31}P\ \{^1H\}$ Chemical Shifts (ppm) For The Complexes Of The General Formulae [(Ph$_2$P(CH$_2$)$_n$PPh$_2$)(AuCl)(Au(6-MP))] And [(Ph$_2$P(CH$_2$)$_n$PPh$_2$)(Au(6-MP))$_2$].*

Complex	C^2	C^4	C^5	C^6	C^8	C_α	C_β	C_γ	C_δ	C_a	C_b	^{31}P
6-mercaptopurine	144.6	151.0	127.9	170.8	144.6	-	-	-	-	-	-	-
[dppe(AuCl)(Au(6-MP))]	141.5	150.6	Obs.	170.1	149.0	129.2(d) (56.00)^a	133.2(t) (6.87)	129.2(t) (5.66)	131.9	22.7(t) (19.93)^a	-	31.6
[dppp(AuCl)Au(6-MP))]	142.0	150.9	Obs.	171.3	150.9	129.1(d) (56.83)^a	133.0(d) (13.13)^b	129.3(d) (11.10)^c	131.9	26.5(dd) (36.08)^a (12.76)^c	19.9(m)	28.5
[dppm(Au(6-MP))$_2$]	141.0	150.7	132.5	170.5	149.1	Obs.	133.5(t) (6.72)	128.9(t) (5.38)	131.6	24.9(m)	-	31.3
[dppe(Au(6-MP))$_2$]	142.5	150.3	133.0	169.0	149.0	129.3(d) (56.08)^a	133.2(t) (6.87)	129.2(t) (5.59)	131.9	22.6(m)	-	33.6
[dppp(Au(6-MP))$_2$]	141.3	150.9	132.7	170.4	149.8	129.0(d) (55.85)^a	133.1(d) (13.28)^b	129.1(d) (11.25)^c	131.6	26.6(d) (30.52)^a	19.5(m)	31.4

Note: ^{31}P-^{13}C coupling constants, in parentheses, are in Hertz, where: a = $^1J_{PC}$; b = $^2J_{PC}$; c = $^3J_{PC}$. Obs. indicates obscured.

these complexes again display the coupling pattern due to isotopic asymmetry observed for the triorganophosphinegold(I) chloride precursors. It is also notable that the complex multiplet that might have been expected in the $[(Ph_2P(CH_2)_nPPh_2)(AuCl)(Au(6\text{-}MP))]$ complexes due to overlapping phenyl regions is not observed, indicating that all the phenyl rings give equivalent resonance values in solution, hence suggesting that the gold ligands are fluctional; this is supported by evidence from the phosphorus-31 nmr studies (see later). The resonances for C_a and C_b are usually observed as complex multiplets which, like the methyl groups on the tolyl phosphine complexes, do not experience significant changes in chemical shift or coupling constants after complexation.

The five carbon resonances for the 6-MP moiety occur as broad peaks at greater than δ 130 ppm due to the deshielding environment of the aromatic system. The relevant spectral region for $[Ph_3PAu(6\text{-}MP)]$ is shown in Figure 4.5.1, which demonstrates how the purine resonances have a small and broad appearance. This feature is due to the Nuclear-Overhauser Effect[69], and arises because the rigid structure of the ring system does not allow efficient dissipation of the spin energies via thermal motion, causing these nuclei to have long relaxation times and hence to occur as broad resonances. The resonances for 6-mercaptopurine are given in Tables 4.4.1 and 4.4.2, and agree with the literature reports that indicate that C^2 and C^8 occur at the same chemical shift value, i.e. δ 144.8 ppm[70]. These peaks are resolved in the complexes as the resonance for C^8 is shifted downfield and that for C^2 is shifted upfield. The chemical shifts of the C^4 and C^6 atoms do not change significantly upon complexation, whereas C^5 is shifted downfield in value by approximately 5 ppm. What follows is a rationalization of the shifts in resonance values observed for each nuclei in going from the free purine to the complexes.

Complexation of 6-mercaptopurine to the gold atom via the sulphur atom causes significant delocalization within the six membered ring system, which results in C^2 experiencing a greater share of electron density, the effect being a slight shielding of the nucleus and so a shift upfield in the spectra. The resonance for C^6 might be expected to change for the same reasons, however, the reduction of double bond character of the C=S bond has an opposing effect on

Figure 4.5.1: *^{13}C NMR Spectrum Of 6-mercaptopurinato(triphenylphosphine)gold(I),*
[Ph$_3$PAu(6-MP)].
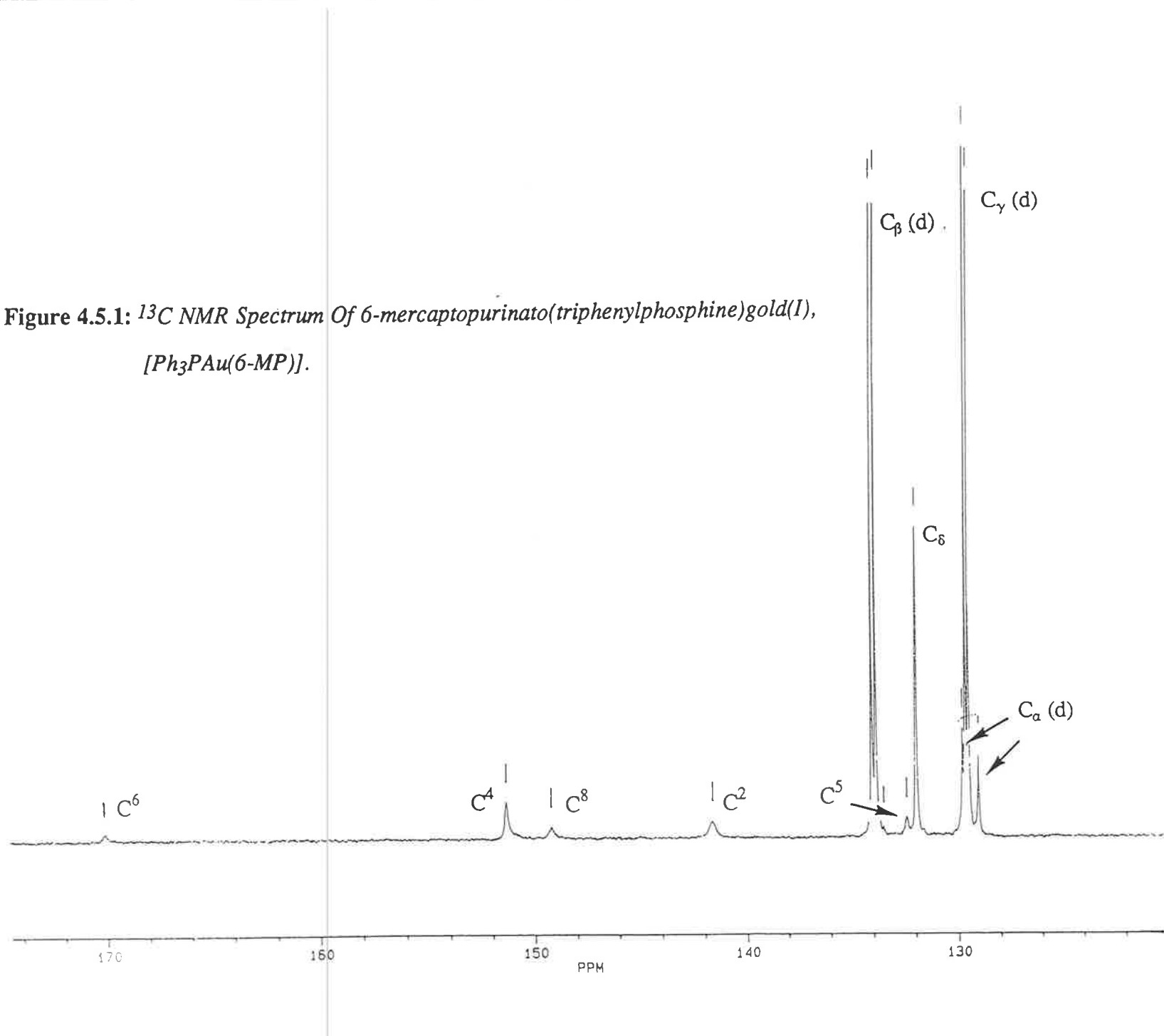
electron density, and so the chemical shift value undergoes no significant change. The resonances for C^4 and C^5 will experience a similar even distribution of electron density, however, although the C^5 resonance is indeed observed to move upfield, the signal for C^4 remains fairly static. The delocalization of electron density in the six-membered ring creates an electron withdrawing effect on the atoms in the imadazole ring, thus resulting in a downfield shift for the C^8 resonance.

In fact, the shifts in resonance observed are really only minor, but are large enough to suggest that complexation to gold via sulphur has occurred for all the complexes; the resonances for C^5 and C^8 are the most indicative of product formation. The occurrence of both phosphine and purine resonances in the spectra is further verification for product formation.

4.6 ^{31}P {^{1}H} NMR spectroscopy

The chemical shifts observed in the ^{31}P proton decoupled spectra of the complexes are listed in Tables 4.5.1 and 4.5.2. All the resonances are singlets, as coupling to carbon-13 nuclei is not observed owing to the low natural abundance of this isotope. The spectra are also diagnostic in terms of purity of the complexes.

The resonances can often appear broad: Figures 4.6.1 and 4.6.2 show the spectra of [Ph₃PAu(6-MP)] and [(m-Tol)₃PAu(6-MP)], the latter resonance having the broader appearance. The chemical shift values vary appreciably between the complexes, as the phosphorus nucleus is sensitive to changes outside the coordination sphere[71], such as the cone-angle of the phosphine and the electronic environment of the adjacent atoms.

Of note are the spectra of the complexes [dppe(AuCl)(Au(6-MP))] and [dppp(AuCl)(Au(6-MP))], where two types of phosphorus nuclei occur in the molecule but only a single resonance is observed at ambient temperature. Low temperature NMR studies on a representative molecule i.e. [dppe(AuCl)(Au(6-MP))] resolved this resonance into two peaks that differed by approximately 4 ppm at 190 K, suggesting that 6-mercaptopurinate and chloride
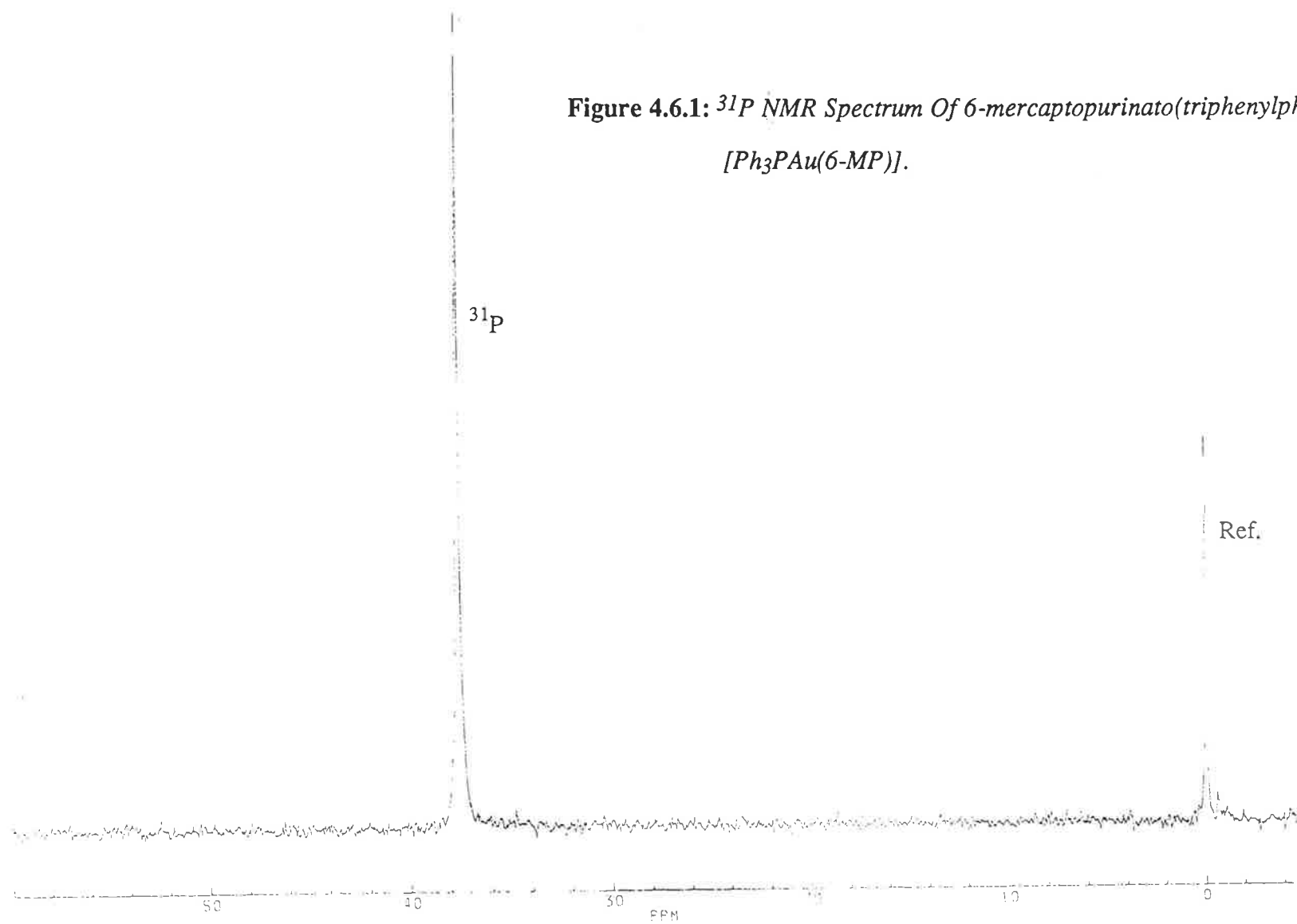
Figure 4.6.1: *^{31}P NMR Spectrum Of 6-mercaptopurinato(triphenylphosphine)gold(I),*

[Ph₃PAu(6-MP)].

Figure 4.6.2: *31P NMR Spectrum Of 6-mercaptopurinato(tri(p-tolyl)phosphine)gold(I),*

[(p-Tol)₃PAu(6-MP)].

Ref.

³¹P

x

50   40   30   20   10   0

PPM
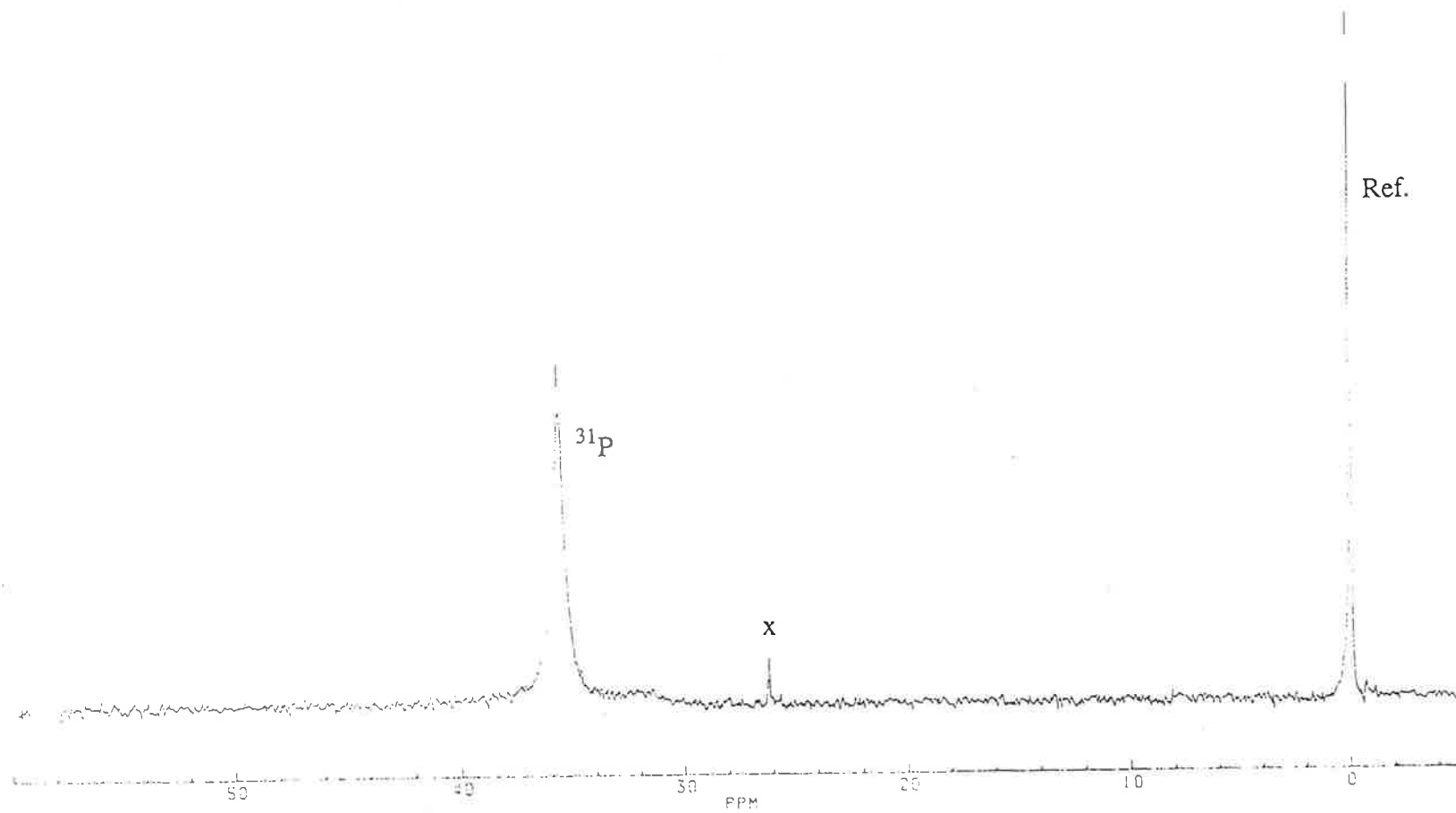
ligands are fluctional at ambient temperatures. The results from the carbon-13 NMR studies on the phenyl regions of these complexes supports this hypothesis.

4.7 *Fast Atom Bombardment mass spectroscopy*

The technique of Fast Atom Bombardment mass spectroscopy (FAB-MS) involves the bombardment of gaseous molecules by high energy particles, to produce a series of ions that can be observed on a spectrum with respect to their mass/charge ratio and their intensity. The positively charged ions produced are accelerated through a magnetic field in a gaseous state, and so collide with each other and fragment or aggregate according to the stabilities of the resulting ions. The detector in the spectrometer records those ions that reach it as a peak on the spectrum, the most intense of which is assigned an intensity of 100%.

Previous work on monomeric triorganophosphinegold(I) thionucleobases of the general formula $[R_3PAuSR']$[60,62] revealed that high nuclearity aggregates involving phosphorus, gold and sulphur can occur in relatively high abundance, indicating not only that such ions are stable but also that both sulphur and phosphorus have an affinity for gold(I), as discussed in Chapter 1. Examples of the types of ions observed are given below:

$$[R_3PAu]^+ \qquad\qquad [(R_3P)_2Au]^+$$

$$[(R_3P)_2AuS]^+ \qquad\qquad [(R_3PAu)_2S]^+$$

$$[(R_3PAu)_2AuS]^+ \qquad\qquad [(R_3PAu)_3S]^+$$
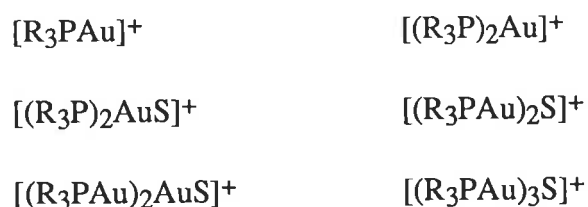
Tables 4.7.1 and 4.7.2 list the m/e values, intensity (as a percentage of the height of the most intense peak) and the assignment of the most significant ions found in the FAB spectra of the complexes. For those complexes of the general formula $[R_3PAu(6\text{-MP})]$ where $R_3P = Et_3P$, $Cycl_3P$, $PhMe_2P$, Ph_3P, $(o\text{-Tol})_3P$, $(m\text{-Tol})_3P$ or $(p\text{-Tol})_3P$, Table 4.7.1 shows that the molecular ion, $[M]^+$, is observed for all the complexes, suggesting product formation. A selection of the type of fragments listed above are observed in these spectra, suggesting that the binding force between the sulphur and gold atoms is independent of the nature of the thionucleobase. However, fragments analogous to $[(R_3PAu)_2(6\text{-MP})]^+$ were not observed for

Table 4.7.1: *Mass Spectral Data For The Complexes Of The General Formula*

[R₃PAu(6-MP)].

R_3P	$[R_3PAu]^+$	$[M]^+$	$[(R_3P)_2Au]^+$	$[(R_3PAu)_2(6\text{-}MP)]^+$	$[(R_3PAu)_2S]^+$	$[(R_3PAu)_3S]^+$
Et_3P	315, 77%	466, 96%	433, 100%	780, 79%	-	977, 13%
$Cycl_3P$	477, 60%	628, 90%	757, 100%	1104, 90%	-	1463, 20%
$PhMe_2P$	335, 62%	486, 19%	-	-	702, 8%	1037, 15%
Ph_3P	459, 59%	610, 100%	721, 27%	1068, 27%	-	-
$(o\text{-}Tol)_3P$	501, 24%	652, 33%	805, 100%	1152, 10%	-	-
$(m\text{-}Tol)_3P$	501, 100%	652, 90%	805, 51%	1152, 62%	-	-
$(p\text{-}Tol)_3P$	501, 40%	652, 51%	805, 100%	1152, 6%	-	-

Table 4.7.2: *Mass Spectral Data For The Complexes Of The General Formulae*

[(Ph₂P(CH₂)ₙPPh₂)(AuCl)(Au(6-MP))] and [(Ph₂P(CH₂)ₙPPh₂)(Au(6-MP))₂].

Complex	$[dpp n Au]^+$	$[dpp n AuS]^+$	$[PhP_2(CH_2)_{(n+1)}Au]^+$	$[(dpp n Au)_2]^+$	$[dpp n Au_2S]^+$
[dppm(Au(6-MP))₂]	581, 8%	-	-	-	-
[dppe(AuCl)(Au(6-MP))]	-	-	378, 5%	-	824, 25%
[dppe(Au(6-MP))₂]	-	-	-	-	824, 8%
[dppp(AuCl)(Au(6-MP))]	609, 11%	641, 4%	-	-	838, 8%
[dppp(Au(6-MP))₂]	609, 16%	-	392, 87%	1218, 3%	-

Table 4.7.2: *(cont.)*

Complex	$[dpp n Au_2(6\text{-}MP)]^+$	$[Ph_3P(CH_2)_n Au_2S(6\text{-}MP)]^+$
[dppm(Au(6-MP))₂]	929, 100%	-
[dppe(AuCl)(Au(6-MP))]	943, 100%	898, 5%
[dppe(Au(6-MP))₂]	943, 100%	-
[dppp(AuCl)(Au(6-MP))]	957, 100%	912, 15%
[dppp(Au(6-MP))₂]	957, 56%	912, 6%

Note: The symbol *n* represents m, e, or p for the corresponding complex in that row. *n+1* indicates an extra methylene group. When used as a subscript, $n = 1$ for dppm complexes, $n = 2$ for dppe complexes and so on.

other thionucleobases, suggesting that the stability of the S–C^6 bond is higher for 6-mercaptopurine under the conditions of the spectrometer.

The results from Table 4.7.1 suggest, from inspection of the composition of the fragments, that phosphorus forms a strong interaction with gold(I) more often in a 1:1 ratio, but that sulphur has the ability to coordinate to as many as three gold atoms.

The spectra for the complexes of the general formula [(Ph$_2$P(CH$_2$)$_n$PPh$_2$)(AuCl)(Au(6-MP))] and [(Ph$_2$P(CH$_2$)$_n$PPh$_2$)(Au(6-MP))$_2$], the results of which are summarized in Table 4.7.2, show a variety of peaks, the results having less in common between the compounds than observed in Table 4.7.1. The molecular ion is never observed with any significant abundance: for the mono-substituted complexes, this might be attributable to the chloride ion being readily lost in the conditions of the spectrometer. Notable is the appearance of the [dpp$n$Au$_2$(6-MP)]$^+$ fragment in high abundance in all the spectra. This fragment is analogous to the [(R$_3$PAu)$_2$(6-MP)]$^+$ fragment observed in Table 4.7.1, perhaps indicative of a strong interaction between the gold atom and the 6-mercaptopurine moiety.

The combined spectroscopic evidence presented in this chapter is in accordance with the data for analogous compounds in the literature and suggests product formation for the complexes with the general formulae [R$_3$PAu(6-MP)] (where R$_3$P = Et$_3$P, Cycl$_3$P, PhMe$_2$P, Ph$_3$P, (o-Tol)$_3$P, (m-Tol)$_3$P or (p-Tol)$_3$P), [(Ph$_2$P(CH$_2$)$_n$PPh$_2$)(AuCl)(Au(6-MP))] (where n = 2 or 3) and [(Ph$_2$P(CH$_2$)$_n$PPh$_2$)(Au(6-MP))$_2$] (where n = 1, 2 or 3). The results also indicate the presence of the P–Au–S chromophore with 6-mercaptopurine as the sulphur donor. This chromophore is usually observed to be linear in related structures; the next chapter discusses the structure determinations of two of the complexes listed above, and confirms the spectroscopic results.

CHAPTER 5

Crystallographic Investigations of the Complexes [Ph$_3$PAu(6-MP)].C$_2$H$_5$OH and [(o-Tol)$_3$PAu(6-MP)].C$_2$H$_5$OH

5.1 *Introduction*

In this section the crystal structures of the complexes [Ph$_3$PAu(6-MP)].C$_2$H$_5$OH and [(o-Tol)$_3$PAu(6-MP)].C$_2$H$_5$OH and will be discussed. The methods concerned with the data collection and refinement procedures for these structures have already been outlined in Chapter 2. The effects of coordination to gold on the 6-mercaptopurinate moiety will be discussed as a separate section.

5.2 *Crystal structure of [Ph$_3$PAu(6-MP)].C$_2$H$_5$OH*

Crystals of the complex [Ph$_3$PAu(6-MP)].C$_2$H$_5$OH were grown from the slow evaporation of a concentrated ethanolic solution of [Ph$_3$PAu(6-MP)]. The complex crystallizes in the triclinic space group P$\bar{1}$ (C$_i^1$, No. 2)[44]; crystal and refinement data are listed in Table 5.2.1 and the derived results are given in Tables 5.2.2 to 5.2.7. Unlike the other structures featured in this thesis, the structure was solved by Patterson methods, using the program DIRDIF92 PATTY[72]. Calculated and observed structure factors are listed in the Appendix. The crystallographic numbering scheme as drawn with the ORTEP[45] program is shown in Figure 5.2.1.

Figure 5.2.2 shows the unit cell contents with 15 % thermal ellipsoids. The triclinic space group P$\bar{1}$ is centrosymmetric, and this is demonstrated clearly in Figure 5.2.2. There are two

Table 5.2.1: *Crystallographic Parameters for the [Ph₃PAu(6-MP)].C₂H₅OH Complex.*

Data	$[Ph_3PAu(6\text{-}MP)].C_2H_5OH$
Formula	$C_{25}H_{24}AuSPON_4$
Formula weight	656.5
Crystal shape	octahedral
Crystal dimensions (mm)	0.07 x 0.11 x 0.29
Crystal system	triclinic
Space group	$P\bar{1}$ (C_i^1, No. 2)
a (Å)	11.066(3)
b (Å)	13.552(3)
c (Å)	8.705(2)
α (°)	91.51(2)
β (°)	113.06(2)
γ (°)	89.69(2)
V (Å³)	1200.8(5)
Z	2
$\rho_{calc.}$ (g cm⁻³)	1.816
F(000)	640
μ (cm⁻¹)	63.27
θ limits, cell (°)	7.51 to 12.82
θ limits, data (°)	1.5 to 28.7
hkl range	0 to 14, -18 to 18, -11 to 10
Range of transmission factors	0.964 to 1.016
Scan technique	ω:2θ
No. of data measured	6297
No. of unique data	5989
R_{amal}	0.033
No. of unique data used	3978
Criterion of observability	$I \geq 3.0\sigma(I)$
No. of parameters	298
R	0.034
R_w	0.029
Residual electron density (e Å⁻³)	-0.98 to 0.72

Table 5.2.2: *Fractional Atomic Coordinates For The [Ph₃PAu(6-MP)].C₂H₅OH Complex.*

Atom	x	y	z
Au	0.10466(2)	-0.22959(2)	-0.00005(3)
S(6)	-0.0379(2)	-0.3205(1)	-0.2211(2)
P(1)	0.2556(2)	-0.1366(1)	0.1981(2)
O(41)	0.7564(5)	0.4593(3)	0.4445(5)
N(1)	-0.2015(5)	-0.4645(4)	-0.2436(5)
N(3)	-0.2628(6)	-0.5303(4)	-0.0324(6)
N(7)	-0.0271(5)	-0.3431(3)	0.1643(5)
N(9)	-0.1475(5)	-0.4520(4)	0.2358(5)
C(2)	-0.2659(7)	-0.5257(5)	-0.1846(8)
C(4)	-0.1778(6)	-0.4651(4)	0.0697(7)
C(5)	-0.1043(5)	-0.3985(4)	0.0263(6)
C(6)	-0.1182(5)	-0.3987(4)	-0.1382(6)
C(8)	-0.0567(6)	-0.3789(5)	0.2828(7)
C(11)	0.4109(5)	-0.1995(4)	0.2864(6)
C(12)	0.4960(7)	-0.1823(5)	0.4499(7)
C(13)	0.6143(7)	-0.2308(5)	0.5115(8)
C(14)	0.6469(7)	-0.2948(5)	0.4109(9)
C(15)	0.5622(7)	-0.3118(5)	0.2515(8)
C(16)	0.4439(6)	-0.2646(5)	0.1883(7)
C(21)	0.2909(6)	-0.0202(4)	0.1290(7)
C(22)	0.4141(6)	0.0105(5)	0.1581(8)
C(23)	0.4355(8)	0.1011(6)	0.1034(9)
C(24)	0.3327(9)	0.1588(5)	0.0194(9)
C(25)	0.2100(8)	0.1286(5)	-0.0102(9)
C(26)	0.1878(7)	0.0396(5)	0.0435(9)

Table 5.2.2 (*continued*)

C(31)	0.2123(6)	-0.1065(5)	0.3719(7)
C(32)	0.2333(8)	-0.0148(5)	0.4489(9)
C(33)	0.2036(9)	0.0031(7)	0.5858(10)
C(34)	0.1534(9)	-0.0708(8)	0.6458(10)
C(35)	0.1368(11)	-0.1604(8)	0.5731(11)
C(36)	0.1639(9)	-0.1781(6)	0.4345(9)
C(41)	0.5805(11)	0.3773(8)	0.2306(12)
C(42)	0.6319(12)	0.4197(7)	0.3923(11)

Table 5.2.3: *Anisotropic Thermal Parameters For The [Ph₃PAu(6-MP)].C₂H₅OH Complex.*

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Au	0.0484(1)	0.0500(1)	0.0367(1)	-0.0138(1)	0.01005(9)	-0.00523(9)
S(6)	0.059(1)	0.064(1)	0.0324(7)	-0.0208(8)	0.0102(7)	-0.0032(7)
P(1)	0.050(1)	0.048(1)	0.0369(8)	-0.0140(7)	0.0137(7)	-0.0072(7)
O(41)	0.093(4)	0.084(3)	0.045(3)	-0.029(3)	0.025(3)	-0.005(2)
N(1)	0.067(3)	0.061(3)	0.036(3)	-0.023(3)	0.010(2)	-0.007(2)
N(3)	0.086(4)	0.069(4)	0.044(3)	-0.035(3)	0.017(3)	-0.003(3)
N(7)	0.064(3)	0.054(3)	0.032(3)	-0.015(3)	0.010(2)	-0.007(2)
N(9)	0.070(3)	0.058(3)	0.035(3)	-0.010(3)	0.017(2)	-0.001(2)
C(2)	0.085(5)	0.072(5)	0.046(4)	-0.047(4)	0.014(4)	-0.010(3)
C(4)	0.062(4)	0.043(3)	0.037(3)	0.001(3)	0.015(3)	0.002(3)
C(5)	0.047(3)	0.038(3)	0.033(3)	-0.000(3)	0.006(2)	-0.002(2)
C(6)	0.045(3)	0.039(3)	0.038(3)	0.000(3)	0.011(3)	0.003(2)
C(8)	0.070(4)	0.061(4)	0.039(3)	-0.003(3)	0.016(3)	-0.005(3)
C(11)	0.050(3)	0.044(3)	0.037(3)	-0.014(3)	0.010(3)	-0.001(3)
C(12)	0.070(5)	0.056(4)	0.044(4)	-0.007(4)	0.001(3)	-0.013(3)
C(13)	0.071(5)	0.068(4)	0.049(4)	0.002(4)	-0.003(3)	0.005(3)
C(14)	0.064(5)	0.057(4)	0.073(5)	-0.002(4)	0.014(4)	0.006(4)
C(15)	0.070(5)	0.062(4)	0.058(4)	0.001(4)	0.019(4)	-0.005(3)
C(16)	0.068(4)	0.056(4)	0.039(3)	-0.018(3)	0.017(3)	-0.006(3)
C(21)	0.056(4)	0.038(3)	0.039(3)	-0.010(3)	0.018(3)	-0.007(3)
C(22)	0.057(4)	0.059(4)	0.059(4)	-0.011(3)	0.021(3)	0.001(3)
C(23)	0.083(5)	0.066(5)	0.087(6)	-0.024(4)	0.039(5)	0.001(4)
C(24)	0.121(7)	0.048(4)	0.080(5)	-0.011(5)	0.059(5)	-0.003(4)
C(25)	0.094(6)	0.053(5)	0.087(6)	0.016(4)	0.037(5)	0.013(4)
C(26)	0.064(4)	0.061(5)	0.076(5)	-0.004(4)	0.029(4)	0.001(4)

Table 5.2.3 (*continued*)

C(31)	0.054(4)	0.072(4)	0.039(3)	-0.015(3)	0.016(3)	-0.009(3)
C(32)	0.107(6)	0.069(5)	0.066(5)	-0.019(4)	0.046(5)	-0.019(4)
C(33)	0.127(8)	0.101(7)	0.090(6)	-0.014(6)	0.061(6)	-0.033(5)
C(34)	0.126(8)	0.148(9)	0.066(5)	-0.046(7)	0.059(6)	-0.034(6)
C(35)	0.21(1)	0.17(1)	0.088(7)	-0.12(1)	0.100(8)	-0.052(7)
C(36)	0.165(9)	0.106(6)	0.068(5)	-0.078(6)	0.071(6)	-0.036(5)
C(41)	0.19(1)	0.15(1)	0.092(7)	-0.083(8)	0.037(7)	-0.029(7)
C(42)	0.20(1)	0.120(8)	0.071(6)	-0.078(8)	0.057(7)	-0.035(5)

Table 5.2.4: *Hydrogen Atom Parameters For The [Ph$_3$PAu(6-MP)].C$_2$H$_5$OH Complex.*

Atom	x	y	z	B(eq)
H(2)	-0.3228	-0.5735	-0.2649	6.4
H(8)	-0.0163	-0.3550	0.3975	6.1
H(9)	-0.1830	-0.4871	0.3047	12.4
H(12)	0.4724	-0.1366	0.5211	6.0
H(13)	0.6743	-0.2192	0.6267	6.4
H(14)	0.7310	-0.3282	0.4538	6.4
H(15)	0.5856	-0.3578	0.1806	6.1
H(16)	0.3834	-0.2776	0.0738	5.3
H(22)	0.4880	-0.0314	0.2177	5.3
H(23)	0.5240	0.1231	0.1258	7.0
H(24)	0.3467	0.2223	-0.0202	6.9
H(25)	0.1359	0.1706	-0.0704	6.8
H(26)	0.0986	0.0186	0.0210	6.1
H(32)	0.2695	0.0377	0.4057	6.8
H(33)	0.2179	0.0682	0.6391	7.1
H(34)	0.1302	-0.0589	0.7410	9.8
H(35)	0.1052	-0.2142	0.6194	12.7
H(36)	0.1475	-0.2429	0.3806	9.7
H(41b)	0.5784	0.4268	0.1507	13.2
H(41c)	0.6354	0.3229	0.2238	9.2
H(41a)	0.4923	0.3538	0.2057	13.2
H(42a)	0.6350	0.3691	0.4699	10.8
H(42b)	0.5740	0.4722	0.3975	10.8

Table 5.2.5: *Bond Distances (Å) For The [Ph₃PAu(6-MP)].C₂H₅OH Complex.*

Atom		Atom	Distance	Atom		Atom	Distance
Au	–	S(6)	2.287(1)	C(11)	–	C(16)	1.358(8)
Au	–	P(1)	2.237(2)	C(12)	–	C(13)	1.375(9)
S(6)	–	C(6)	1.728(5)	C(13)	–	C(14)	1.362(9)
P(1)	–	C(11)	1.804(6)	C(41)	–	C(42)	1.40(1)
P(1)	–	C(21)	1.801(6)	C(14)	–	C(15)	1.351(8)
P(1)	–	C(31)	1.794(6)	C(15)	–	C(16)	1.368(9)
O(41)	–	C(42)	1.38(1)	C(21)	–	C(22)	1.352(8)
N(1)	–	C(2)	1.332(7)	C(21)	–	C(26)	1.366(8)
N(1)	–	C(6)	1.338(6)	C(22)	–	C(23)	1.383(9)
N(3)	–	C(2)	1.315(7)	C(23)	–	C(24)	1.34(1)
N(3)	–	C(4)	1.329(7)	C(24)	–	C(25)	1.34(1)
N(7)	–	C(5)	1.376(6)	C(25)	–	C(26)	1.363(9)
N(7)	–	C(8)	1.303(7)	C(31)	–	C(32)	1.373(8)
N(9)	–	C(4)	1.358(6)	C(31)	–	C(36)	1.337(9)
N(9)	–	C(8)	1.352(7)	C(32)	–	C(33)	1.371(9)
C(4)	–	C(5)	1.373(7)	C(33)	–	C(34)	1.36(1)
C(5)	–	C(6)	1.379(7)	C(34)	–	C(35)	1.33(1)
C(11)	–	C(12)	1.379(7)	C(35)	–	C(36)	1.37(1)

Table 5.2.6: *Bond Angles (°) For The [Ph₃PAu(6-MP)].C₂H₅OH Complex.*

Atom	Atom	Atom	Angle	Atom	Atom	Atom	Angle
S(6)	– Au	– P(1)	173.71(6)	P(1)	– C(11)	– C(16)	118.7(4)
Au	– S(6)	– C(6)	105.9(2)	C(12)	– C(11)	– C(16)	119.8(6)
Au	– P(1)	– C(11)	111.4(2)	C(11)	– C(12)	– C(13)	119.6(6)
Au	– P(1)	– C(21)	114.9(2)	C(12)	– C(13)	– C(14)	120.0(6)
Au	– P(1)	– C(31)	113.3(2)	C(13)	– C(14)	– C(15)	119.9(7)
C(11)	– P(1)	– C(21)	105.7(3)	C(14)	– C(15)	– C(16)	120.9(6)
C(11)	– P(1)	– C(31)	105.2(3)	C(11)	– C(16)	– C(15)	119.8(6)
C(21)	– P(1)	– C(31)	105.4(3)	P(1)	– C(21)	– C(22)	123.0(5)
C(2)	– N(1)	– C(6)	118.7(5)	P(1)	– C(21)	– C(26)	118.1(5)
C(2)	– N(3)	– C(4)	111.0(5)	C(22)	– C(21)	– C(26)	118.8(6)
C(5)	– N(7)	– C(8)	102.8(5)	C(21)	– C(22)	– C(23)	120.5(6)
C(4)	– N(9)	– C(8)	104.0(5)	C(22)	– C(23)	– C(24)	119.7(7)
N(1)	– C(2)	– N(3)	128.9(5)	C(23)	– C(24)	– C(25)	120.0(7)
N(3)	– C(4)	– N(9)	126.5(6)	C(24)	– C(25)	– C(26)	120.8(7)
N(3)	– C(4)	– C(5)	126.2(5)	C(21)	– C(26)	– C(25)	120.2(7)
N(9)	– C(4)	– C(5)	107.3(5)	P(1)	– C(31)	– C(32)	122.9(5)
N(7)	– C(5)	– C(4)	110.1(5)	P(1)	– C(31)	– C(36)	118.4(5)
N(7)	– C(5)	– C(6)	132.2(5)	C(32)	– C(31)	– C(36)	118.6(6)
C(4)	– C(5)	– C(6)	117.7(5)	C(31)	– C(32)	– C(33)	120.6(7)
S(6)	– C(6)	– N(1)	116.9(4)	C(32)	– C(33)	– C(34)	119.5(8)
S(6)	– C(6)	– C(5)	125.6(4)	C(33)	– C(34)	– C(35)	119.5(8)
N(1)	– C(6)	– C(5)	117.5(5)	C(34)	– C(35)	– C(36)	121.1(8)
N(7)	– C(8)	– N(9)	115.8(5)	C(31)	– C(36)	– C(35)	120.6(8)
P(1)	– C(11)	– C(12)	121.5(5)	O(41)	– C(42)	– C(41)	116.1(9)

Table 5.2.7: *Mean Plane Data For The [Ph$_3$PAu(6-MP)].C$_2$H$_5$OH Complex.*

Plane number 1: Least-squares plane through the 6-mercaptopurinate moiety.

Atoms Defining Plane	Distance (Å)	esd (Å)
S(6)	-0.0024	0.0018
N(1)	0.0192	0.0054
N(3)	-0.0226	0.0062
N(7)	0.0110	0.0051
N(9)	-0.0094	0.0052
C(2)	0.0202	0.0079
C(4)	-0.0124	0.0059
C(5)	-0.0003	0.0054
C(6)	0.0085	0.0054
C(8)	0.0148	0.0065
Additional Atoms	Distance (Å)	
Au	0.1465	

Mean deviation from plane is 0.0121 Å.

Chi-squared: 56.4.

Table 5.2.7 *(continued)*

<u>Plane number 2:</u> Least-squares plane through the phenyl ring defined by the atoms C(11) to C(16).

Atoms Defining Plane	Distance (Å)	esd (Å)
C(11)	0.0047	0.0051
C(12)	-0.0023	0.0067
C(13)	-0.0050	0.0074
C(14)	0.0060	0.0067
C(15)	-0.0003	0.0068
C(16)	-0.0048	0.0057
Additional Atom	Distance (Å)	
P(1)	0.0342	

Mean deviation from plane is 0.0039 (Å).

Chi-squared: 2.8.

<u>Plane number 3:</u> Least-squares plane through the phenyl ring defined by the atoms C(21) to C(26).

Atoms Defining Plane	Distance (Å)	esd (Å)
C(21)	0.0014	0.0051
C(22)	-0.0023	0.0062
C(23)	0.0020	0.0073
C(24)	-0.0005	0.0068
C(25)	0.0001	0.0073
C(26)	-0.0010	0.0067
Additional Atom	Distance (Å)	
P(1)	0.0118	

Mean deviation from plane is 0.0012 Å.

Chi-squared: 0.3.

Table 5.2.7 (*continued*)

Plane number 4: Least-squares plane through the phenyl ring defined by the atoms C(31) to C(36).

Atoms Defining Plane	Distance (Å)	esd (Å)
C(31)	-0.0031	0.0061
C(32)	0.0062	0.0081
C(33)	-0.0002	0.0094
C(34)	-0.0111	0.0100
C(35)	0.0177	0.0126
C(36)	-0.0024	0.0101
Additional Atom	Distance (Å)	
P(1)	0.0790	

Mean deviation from plane is 0.0068 Å.

Chi-squared: 3.5.
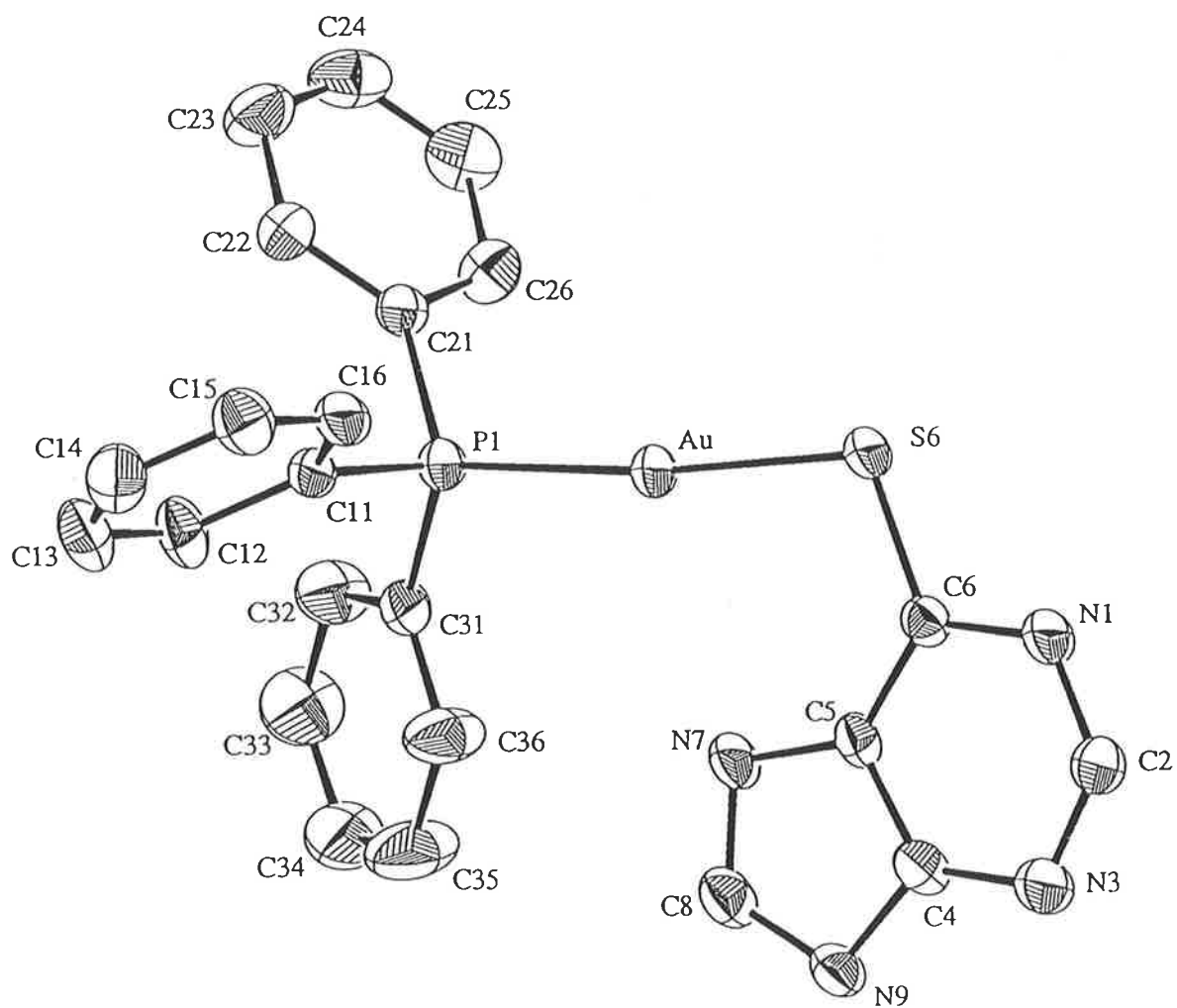
Figure 5.2.1: *Molecular Structure And Crystallographic Numbering Scheme For*

[Ph₃PAu(6-MP)].
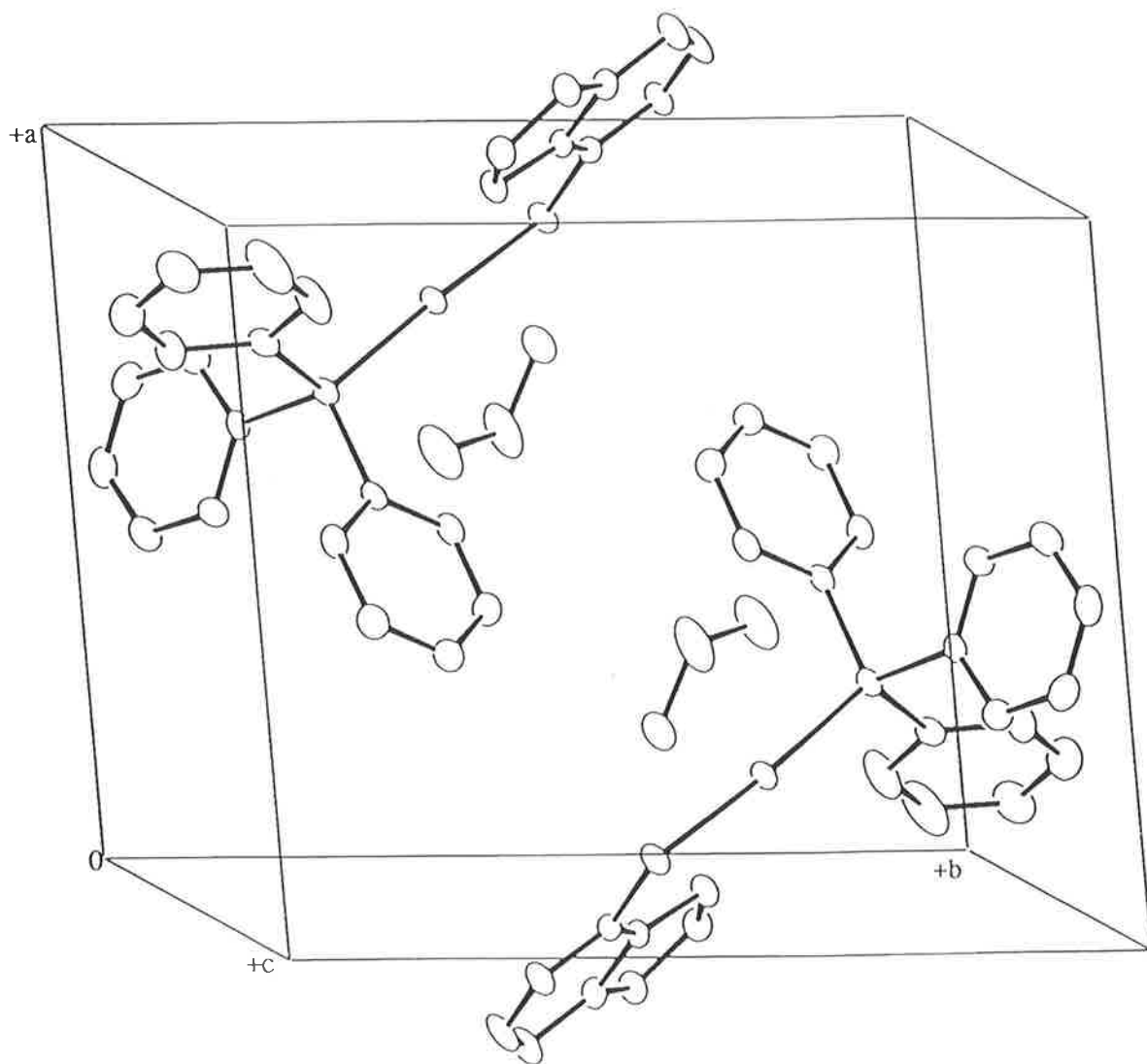
Figure 5.2.2: *Unit Cell Diagram Of [Ph₃PAu(6-MP)].C₂H₅OH.*

ethanol solvent molecules of crystallization in the unit cell such that the ratio of complex to ethanol molecules is 1:1. Hydrogen bonding is observed to occur between O(41) of the ethanol molecule and H(9) of the 6-mercaptopurinate moiety, at a distance of 1.77 Å; this is demonstrated in the extended lattice diagram of Figure 5.2.3. Hydrogen bonding might be expected to occur between nearby purine moieties; however, the planes of any two purine rings that are nearest neighbours are only parallel, not co-planar. Figure 5.2.3 also indicates how the molecules pack in such a way in the lattice such that the phosphine groups form a layer, and the more polar gold(I), purine and ethanol regions form another layer. There are no significant Au...Au interactions in the lattice: the closest such interaction is 6.628(1) Å, which is larger than range of Au...Au contacts of 2.75 to 3.25 Å normally considered to indicate a 'significant' interaction[46].

Figure 5.2.1 is an ORTEP[45] diagram of [Ph3PAu(6-MP)] plotted with 30% probability ellipsoids. The gold atom exists in the expected linear geometry defined by the P(1) atom of the triphenylphosphine ligand and the S(6) atom derived from the 6-mercaptopurinate moiety, with a P–Au–S angle of 173.71(6)°. The deviation from ideal geometry may be related to the presence of the close intramolecular Au...N(7) contact. The intramolecular distance is 2.884(5) Å, less than the sum of the van der Waals radii of Au and N of 3.25 Å, but not suggestive of a significant interaction. The length of the P(1)–Au bond is found to be 2.237(1) Å, which is equivalent within standard deviation to the value of 2.235(3) Å for [Ph3PAuCl][47]. Comparison between the Ph3P moieties of [Ph3PAuCl] and [Ph3PAu(6-MP)] reveals that this region is virtually identical in both complexes; hence, coordination of the 6-MP ligand to gold has a negligible effect on the electronic factors of the Ph3P ligand.

As expected, the phenyl rings of the phosphine moiety are all planar; the maximum mean deviation is 0.01(1) Å for the ring defined by atoms C(31) to C(36). The maximum deviation of P(1) out of this ring is 0.079 Å. The internal bond distances and bond angles are all typical of electron delocalization in the six-membered aromatic system.
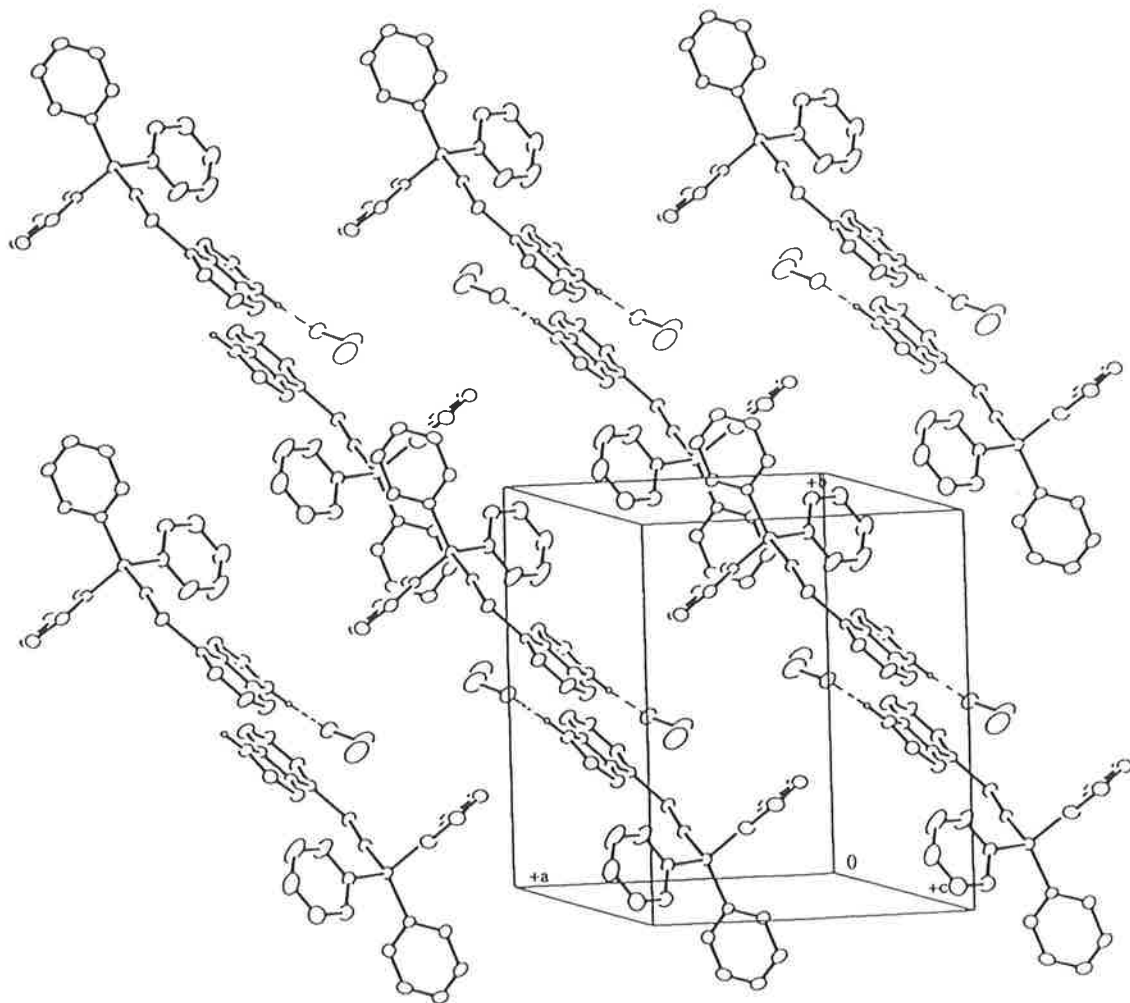
Figure 5.2.3: *Lattice Diagram Of [Ph3PAu(6-MP)].C2H5OH.*

The Au–S bond distance is 2.287(1) Å, which is a typical value for triorganophosphinegold(I) thionucleobase complexes; examples of these will be given in Chapter 6. The intramolecular parameters of the 6-mercaptopurinate moiety will be discussed in detail in section 5.4.

5.3 *Crystal Structure of [(o-Tol)₃PAu(6-MP)].C₂H₅OH.*

Crystals of the complex [(o-Tol)₃PAu(6-MP)].C₂H₅OH, grown from the slow evaporation of a concentrated ethanolic solution of the compound, crystallize in the monoclinic space group P2₁/n (C_{2h}^5, No. 14)[44]. Crystal and refinement data are listed in Table 5.3.1 and the derived parameters are given in Tables 5.3.2 to 5.3.7. Calculated and observed structure factors can be found in the Appendix. The crystallographic numbering scheme is shown in the ORTEP diagram in Figure 5.3.1.

The contents of the unit cell are illustrated in Figure 5.3.2. The ethanol and 6-mercaptopurinate regions are observed to be associated as a layer, as are the phosphine moieties. Hydrogen bonding occurs between H(9) and N(3) of nearby purine rings, at a intermolecular distance of 1.93 Å. This association is possible as the purine ring systems are close to co-planar; Figure 5.3.3 shows this interaction in detail. The closest Au...Au contact in the lattice is at a distance of 7.821(2) Å; as for [Ph₃PAu(6-MP)].C₂H₅OH this distance is not indicative of a significant interaction.

Figure 5.3.1 shows an ORTEP diagram of the complex with 30% thermal ellipsoids. Notable is the similarity in appearance with [Ph₃PAu(6-MP)]. As expected, the P–Au–S chromophore is nearly linear, with an angle of 177.03(8)°. This is closer to linearity than for [Ph₃PAu(6-MP)]; this may be due to the different hydrogen bonding interactions, or is perhaps due to the larger cone angle of (o-Tol)₃P and the possible consequent steric interactions. The N(7) atom is directed towards the gold centre at a distance of 2.860(7) Å, again less than the sum of the van der Waals radii, but not suggestive of any significant bonding interaction[46].

Table 5.3.1: *Crystallographic Parameters for the [(o-Tol)$_3$PAu(6-MP)].C$_2$H$_5$OH Complex.*

Data	[(o-Tol)$_3$PAu(6-MP)].C$_2$H$_5$OH
Formula	C$_{28}$H$_{30}$AuSPON$_4$
Formula weight	698.6
Crystal shape	hexagonal
Crystal dimensions (mm)	0.07 x 0.11 x 0.35
Crystal system	monoclinic
Space group	P2$_1$/n (C$_{2h}^5$, No. 14)
a (Å)	10.067(2)
b (Å)	10.518(2)
c (Å)	25.416(4)
β (°)	98.42(2)
V (Å^3)	2662.1(9)
Z	4
$\rho_{calc.}$ (g cm^{-3})	~~1.778~~ 1.743
F(000)	~~1404~~ 1376
μ (cm^{-1})	57.16
θ limits, cell (°)	7.7 to 12.8
θ limits, data (°)	1.5 to 27.9
hkl range	0 to 12, 0 to 13, -33 to 33
Range of transmission factors	0.939 to 1.070
Scan technique	ω:2θ
No. of data measured	6280
No. of unique data	5913
R$_{amal}$	0.025
No. of unique data used	4183
Criterion of observability	$I \geq 3.0\sigma(I)$
No. of parameters	325
R	0.040
R$_w$	0.041
Residual electron density (e Å^{-3})	3.51

Table 5.3.2: *Fractional Atomic Coordinates For The [(o-Tol)₃PAu(6-MP)].C₂H₅OH Complex.*

Atom	x	y	z
Au	0.34432(3)	0.51852(3)	0.14775(1)
S(6)	0.1721(2)	0.6422(2)	0.1099(1)
P(1)	0.5073(2)	0.3918(2)	0.1878(1)
O(41)	0.1220(7)	0.2139(6)	-0.0267(3)
N(1)	0.1579(7)	0.8334(6)	0.0445(3)
N(3)	0.3315(8)	0.9469(7)	0.0122(3)
N(7)	0.4869(7)	0.6950(6)	0.0912(3)
N(9)	0.5481(7)	0.8552(7)	0.0425(3)
C(2)	0.2072(10)	0.9250(9)	0.0176(4)
C(4)	0.4130(9)	0.8625(8)	0.0393(4)
C(5)	0.3778(8)	0.7632(7)	0.0693(3)
C(6)	0.2430(8)	0.7502(7)	0.0717(3)
C(8)	0.5863(9)	0.7533(9)	0.0744(4)
C(11)	0.5543(7)	0.4320(7)	0.2573(3)
C(12)	0.5587(8)	0.3363(8)	0.2951(4)
C(13)	0.5845(10)	0.3647(9)	0.3476(4)
C(14)	0.6032(10)	0.4863(11)	0.3635(4)
C(15)	0.6004(9)	0.5808(8)	0.3272(4)
C(16)	0.5769(8)	0.5574(7)	0.2743(4)
C(17)	0.5825(8)	0.6639(7)	0.2363(4)
C(21)	0.4648(8)	0.2248(6)	0.1868(3)
C(22)	0.5554(8)	0.1387(7)	0.1696(3)
C(23)	0.5256(10)	0.0122(8)	0.1666(4)
C(24)	0.4045(10)	-0.0294(8)	0.1792(4)

Table 5.3.2 (*continued*)

C(25)	0.3166(9)	0.0545(8)	0.1955(4)
C(26)	0.3445(8)	0.1820(7)	0.2006(3)
C(27)	0.2468(8)	0.2677(8)	0.2212(4)
C(31)	0.6580(8)	0.4081(7)	0.1575(3)
C(32)	0.7749(8)	0.4418(7)	0.1869(3)
C(33)	0.8892(9)	0.4634(9)	0.1673(5)
C(34)	0.8828(11)	0.4515(9)	0.1135(6)
C(35)	0.7668(11)	0.4161(9)	0.0814(4)
C(36)	0.6526(9)	0.3935(8)	0.1036(4)
C(37)	0.5280(11)	0.3565(9)	0.0668(4)
C(41)	0.1443(14)	0.2360(12)	0.0655(5)
C(42)	0.1396(12)	0.3009(12)	0.0152(5)

Table 5.3.3: *Anisotropic Thermal Parameters For The [(o-Tol)₃PAu(6-MP)].C₂H₅OH Complex.*

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Au	0.0425(2)	0.0445(2)	0.0442(2)	0.0005(2)	0.0064(2)	0.0099(1)
S(6)	0.040(1)	0.073(2)	0.099(2)	0.004(1)	0.011(1)	0.045(2)
P(1)	0.038(1)	0.037(1)	0.034(1)	-0.0008(9)	0.008(1)	0.0038(9)
O(41)	0.082(5)	0.104(5)	0.042(5)	0.014(4)	0.012(4)	-0.009(4)
N(1)	0.063(5)	0.058(4)	0.048(5)	0.005(4)	0.016(4)	0.017(4)
N(3)	0.066(5)	0.067(5)	0.062(6)	0.005(4)	0.017(5)	0.025(4)
N(7)	0.042(4)	0.064(5)	0.064(6)	0.002(4)	0.009(4)	0.008(4)
N(9)	0.063(5)	0.066(5)	0.050(6)	-0.011(4)	0.015(4)	0.009(4)
C(2)	0.071(7)	0.064(6)	0.058(7)	0.003(5)	0.009(6)	0.019(5)
C(4)	0.058(6)	0.059(5)	0.039(6)	-0.006(5)	0.018(5)	-0.001(4)
C(5)	0.053(5)	0.049(5)	0.035(6)	-0.004(4)	0.006(4)	0.003(4)
C(6)	0.051(5)	0.054(5)	0.042(6)	0.000(4)	0.013(5)	0.009(4)
C(8)	0.058(6)	0.071(6)	0.050(7)	0.001(5)	0.014(5)	0.010(5)
C(11)	0.036(4)	0.045(4)	0.028(5)	-0.001(3)	0.010(4)	-0.001(3)
C(12)	0.058(6)	0.053(5)	0.042(6)	-0.006(4)	0.008(5)	0.006(4)
C(13)	0.074(7)	0.084(7)	0.031(6)	-0.015(6)	-0.000(5)	0.012(5)
C(14)	0.071(6)	0.108(8)	0.029(6)	-0.015(6)	0.010(5)	-0.015(6)
C(15)	0.064(6)	0.067(6)	0.036(6)	-0.006(5)	0.012(5)	-0.017(5)
C(16)	0.040(5)	0.047(5)	0.043(6)	-0.003(4)	0.009(4)	-0.004(4)
C(17)	0.059(6)	0.043(5)	0.062(7)	0.002(4)	0.007(5)	-0.006(4)
C(21)	0.049(5)	0.035(4)	0.034(5)	-0.004(3)	0.003(4)	0.001(3)
C(22)	0.054(5)	0.046(5)	0.044(6)	0.002(4)	0.012(5)	-0.000(4)
C(23)	0.090(7)	0.047(5)	0.057(7)	0.013(5)	0.025(6)	-0.005(5)
C(24)	0.088(7)	0.042(5)	0.048(6)	-0.011(5)	0.007(6)	-0.002(4)

Table 5.3.3 (*continued*)

C(25)	0.067(6)	0.054(5)	0.055(7)	-0.011(5)	0.017(5)	0.011(5)
C(26)	0.053(5)	0.044(4)	0.036(6)	-0.002(4)	0.013(4)	0.006(4)
C(27)	0.055(6)	0.063(5)	0.062(7)	-0.008(4)	0.034(5)	0.004(5)
C(31)	0.044(5)	0.042(4)	0.033(5)	-0.005(4)	0.019(4)	0.004(4)
C(32)	0.048(5)	0.047(4)	0.045(6)	0.001(4)	0.021(4)	-0.000(4)
C(33)	0.053(6)	0.068(6)	0.086(9)	-0.013(5)	0.017(6)	-0.005(6)
C(34)	0.074(8)	0.071(7)	0.10(1)	-0.016(6)	0.051(7)	-0.007(7)
C(35)	0.092(8)	0.079(7)	0.058(8)	-0.013(6)	0.045(7)	-0.007(6)
C(36)	0.057(6)	0.056(5)	0.052(7)	-0.009(4)	0.021(5)	-0.001(5)
C(37)	0.093(8)	0.095(7)	0.038(7)	-0.011(6)	0.017(6)	-0.005(5)
C(41)	0.16(1)	0.13(1)	0.07(1)	0.00(1)	0.02(1)	-0.022(8)
C(42)	0.088(9)	0.13(1)	0.056(9)	-0.014(7)	0.011(7)	0.004(8)

Table 5.3.4: *Hydrogen Atom Parameters For The [(o-Tol)₃PAu(6-MP)].C₂H₅OH Complex.*

Atom	x	y	z	B(eq)
H(2)	0.1419	0.9838	-0.0006	6.1
H(8)	0.6791	0.7269	0.0837	5.6
H(9)	0.6060	0.9110	0.0256	5.6
H(12)	0.5431	0.2487	0.2839	4.8
H(13)	0.5895	0.2972	0.3738	6.0
H(14)	0.6189	0.5063	0.4012	6.6
H(15)	0.6156	0.6677	0.3394	5.2
H(17a)	0.6714	0.7016	0.2420	5.2
H(17b)	0.5633	0.6321	0.2002	5.2
H(17c)	0.5164	0.7277	0.2420	5.2
H(22)	0.6394	0.1690	0.1598	4.5
H(23)	0.5892	-0.0480	0.1557	6.0
H(24)	0.3819	-0.1191	0.1764	5.6
H(25)	0.2314	0.0234	0.2038	5.5
H(27a)	0.2804	0.3543	0.2222	5.5
H(27b)	0.1613	0.2635	0.1981	5.5
H(27c)	0.2351	0.2413	0.2568	5.5
H(32)	0.7764	0.4510	0.2250	4.3
H(33)	0.9718	0.4862	0.1900	6.5
H(34)	0.9626	0.4686	0.0974	7.4
H(35)	0.7657	0.4071	0.0434	6.9
H(37a)	0.4551	0.3428	0.0872	7.1
H(37b)	0.5038	0.4240	0.0412	7.1
H(37c)	0.5446	0.2788	0.0482	11.0
H(41a)	0.0606	0.1908	0.0662	11.0

Table 5.3.4 *(continued)*

H(41b)	0.2182	0.1758	0.0697	11.0
H(41c)	0.1574	0.2974	0.0942	11.0
H(42a)	0.2230	0.3468	0.0148	8.6
H(42b)	0.0652	0.3605	0.0110	8.6

Table 5.3.5: *Bond Distances (Å) For The [(o-Tol)₃PAu(6-MP)].C₂H₅OH Complex.*

Atom		Atom	Distance	Atom		Atom	Distance
Au	–	S(6)	2.266(2)	C(14)	–	C(15)	1.36(1)
Au	–	P(1)	2.239(2)	S(6)	–	C(6)	1.715(8)
C(15)	–	C(16)	1.35(1)	P(1)	–	C(11)	1.809(8)
P(1)	–	C(21)	1.808(7)	C(16)	–	C(17)	1.49(1)
P(1)	–	C(31)	1.808(8)	O(41)	–	C(42)	1.40(1)
N(1)	–	C(2)	1.32(1)	N(1)	–	C(6)	1.343(9)
C(21)	–	C(22)	1.40(1)	N(3)	–	C(2)	1.30(1)
C(21)	–	C(26)	1.38(1)	N(3)	–	C(4)	1.33(1)
C(22)	–	C(23)	1.36(1)	N(7)	–	C(5)	1.36(1)
N(7)	–	C(8)	1.30(1)	C(23)	–	C(24)	1.38(1)
N(9)	–	C(4)	1.35(1)	N(9)	–	C(8)	1.37(1)
C(24)	–	C(25)	1.36(1)	C(25)	–	C(26)	1.37(1)
C(4)	–	C(5)	1.37(1)	C(5)	–	C(6)	1.37(1)
C(26)	–	C(27)	1.49(1)	C(11)	–	C(12)	1.39(1)
C(11)	–	C(16)	1.40(1)	C(12)	–	C(13)	1.36(1)
C(31)	–	C(32)	1.35(1)	C(31)	–	C(36)	1.37(1)
C(13)	–	C(14)	1.35(1)	C(32)	–	C(33)	1.34(1)
C(33)	–	C(34)	1.37(1)	C(34)	–	C(35)	1.37(1)
C(35)	–	C(36)	1.37(1)	C(36)	–	C(37)	1.50(1)
C(41)	–	C(42)	1.44(2)				

Table 5.3.6: *Bond Angles (°) For The [(o-Tol)₃PAu(6-MP)].C₂H₅OH Complex.*

Atom	Atom	Atom	Angle	Atom	Atom	Atom	Angle
S(6)	– Au	– P(1)	177.03(8)	C(11)	– C(12)	– C(13)	120.3(8)
Au	– S(6)	– C(6)	105.3(3)	C(12)	– C(13)	– C(14)	120.2(9)
Au	– P(1)	– C(11)	112.0(2)	C(13)	– C(14)	– C(15)	120.3(9)
Au	– P(1)	– C(21)	114.6(3)	C(14)	– C(15)	– C(16)	121.8(8)
Au	– P(1)	– C(31)	110.7(3)	C(11)	– C(16)	– C(15)	118.5(8)
C(11)	– P(1)	– C(21)	105.6(4)	C(11)	– C(16)	– C(17)	122.1(8)
C(11)	– P(1)	– C(31)	106.1(4)	C(15)	– C(16)	– C(17)	119.4(8)
C(21)	– P(1)	– C(31)	107.3(4)	P(1)	– C(21)	– C(22)	118.0(6)
C(2)	– N(1)	– C(6)	118.9(8)	P(1)	– C(21)	– C(26)	121.7(6)
C(2)	– N(3)	– C(4)	110.9(8)	C(22)	– C(21)	– C(26)	120.2(7)
C(5)	– N(7)	– C(8)	103.4(7)	C(21)	– C(22)	– C(23)	120.0(8)
C(4)	– N(9)	– C(8)	105.8(7)	C(22)	– C(23)	– C(24)	119.5(8)
N(1)	– C(2)	– N(3)	128.7(9)	C(23)	– C(24)	– C(25)	120.2(8)
N(3)	– C(4)	– N(9)	127.4(8)	C(24)	– C(25)	– C(26)	122.1(9)
N(3)	– C(4)	– C(5)	127.4(9)	C(21)	– C(26)	– C(25)	117.9(8)
N(9)	– C(4)	– C(5)	105.2(8)	C(21)	– C(26)	– C(27)	122.8(7)
N(7)	– C(5)	– C(4)	111.7(8)	C(25)	– C(26)	– C(27)	119.3(8)
N(7)	– C(5)	– C(6)	132.3(8)	P(1)	– C(31)	– C(32)	120.5(6)
C(4)	– C(5)	– C(6)	115.9(8)	P(1)	– C(31)	– C(36)	120.2(6)
S(6)	– C(6)	– N(1)	115.8(6)	C(32)	– C(31)	– C(36)	119.2(8)
S(6)	– C(6)	– C(5)	125.9(7)	C(31)	– C(32)	– C(33)	124.6(9)
N(1)	– C(6)	– C(5)	118.2(8)	C(32)	– C(33)	– C(34)	116(1)
N(7)	– C(8)	– N(9)	113.8(8)	C(33)	– C(34)	– C(35)	122.0(9)
P(1)	– C(11)	– C(12)	118.9(6)	C(34)	– C(35)	– C(36)	120(1)
P(1)	– C(11)	– C(16)	122.1(6)	C(31)	– C(36)	– C(35)	118.5(9)
C(12)	– C(11)	– C(16)	118.9(8)	C(31)	– C(36)	– C(37)	123.9(8)
C(35)	– C(36)	– C(37)	118(1)	O(41)	– C(42)	– C(41)	110(1)

Table 5.3.7 (*continued*)

Plane number 2: Least-squares plane through the *ortho*-tolyl ring defined by the atoms C(11) to C(16).

Atoms Defining Plane	Distance (Å)	esd (Å)
C(11)	-0.0041	0.0071
C(12)	-0.0017	0.0086
C(13)	0.0106	0.0100
C(14)	-0.0089	0.0099
C(15)	-0.0011	0.0091
C(16)	0.0056	0.0076
Additional Atoms	Distance (Å)	
P(1)	-0.1466	
C(17)	0.0901	

Mean deviation from plane is 0.0053 (Å).

Chi-squared: 2.5.

Table 5.3.7: *Mean Plane Data For The [(o-Tol)$_3$PAu(6-MP)].C$_2$H$_5$OH Complex.*

Plane number 1: Least-squares plane through the 6-mercaptopurine moiety.

Atoms Defining Plane	Distance (Å)	esd (Å)
S(6)	0.0134	0.0031
N(1)	-0.0479	0.0076
N(3)	0.0324	0.0083
N(7)	-0.0363	0.0077
N(9)	0.0282	0.0076
C(2)	0.0058	0.0104
C(4)	0.0196	0.0086
C(5)	-0.0223	0.0082
C(6)	-0.0503	0.0086
C(8)	0.0016	0.0097
Additional Atom	Distance (Å)	
Au	-0.0444	

Mean deviation from plane is 0.0258 (Å).

Chi-squared: 156.3.

Table 5.3.7: (*continued*)

Plane number 3: Least-squares plane through the *ortho*-tolyl ring defined by the atoms C(21) to C(26).

Atoms Defining Plane	Distance (Å)	esd (Å)
C(21)	-0.0039	0.0078
C(22)	-0.0062	0.0084
C(23)	0.0131	0.0098
C(24)	-0.0029	0.0092
C(25)	-0.0105	0.0094
C(26)	0.0111	0.0082
Additional Atoms	Distance (Å)	
C(27)	0.0711	
P(1)	-0.0856	

Mean deviation from plane is 0.0080 (Å).

Chi-squared: 5.3.

Table 5.3.7 (*continued*)

Plane number 4: Least-squares plane through the *ortho*-tolyl ring defined by the atoms C(31) to C(36).

Atoms Defining Plane	Distance (Å)	esd (Å)
C(31)	-0.0048	0.0070
C(32)	0.0001	0.0074
C(33)	0.0086	0.0093
C(34)	-0.0093	0.0100
C(35)	-0.0004	0.0099
C(36)	0.0070	0.0083
Additional Atoms	Distance (Å)	
P(1)	-0.1298	
C(37)	0.0010	

Mean deviation from plane is 0.0050 (Å).

Chi-squared: 2.6.
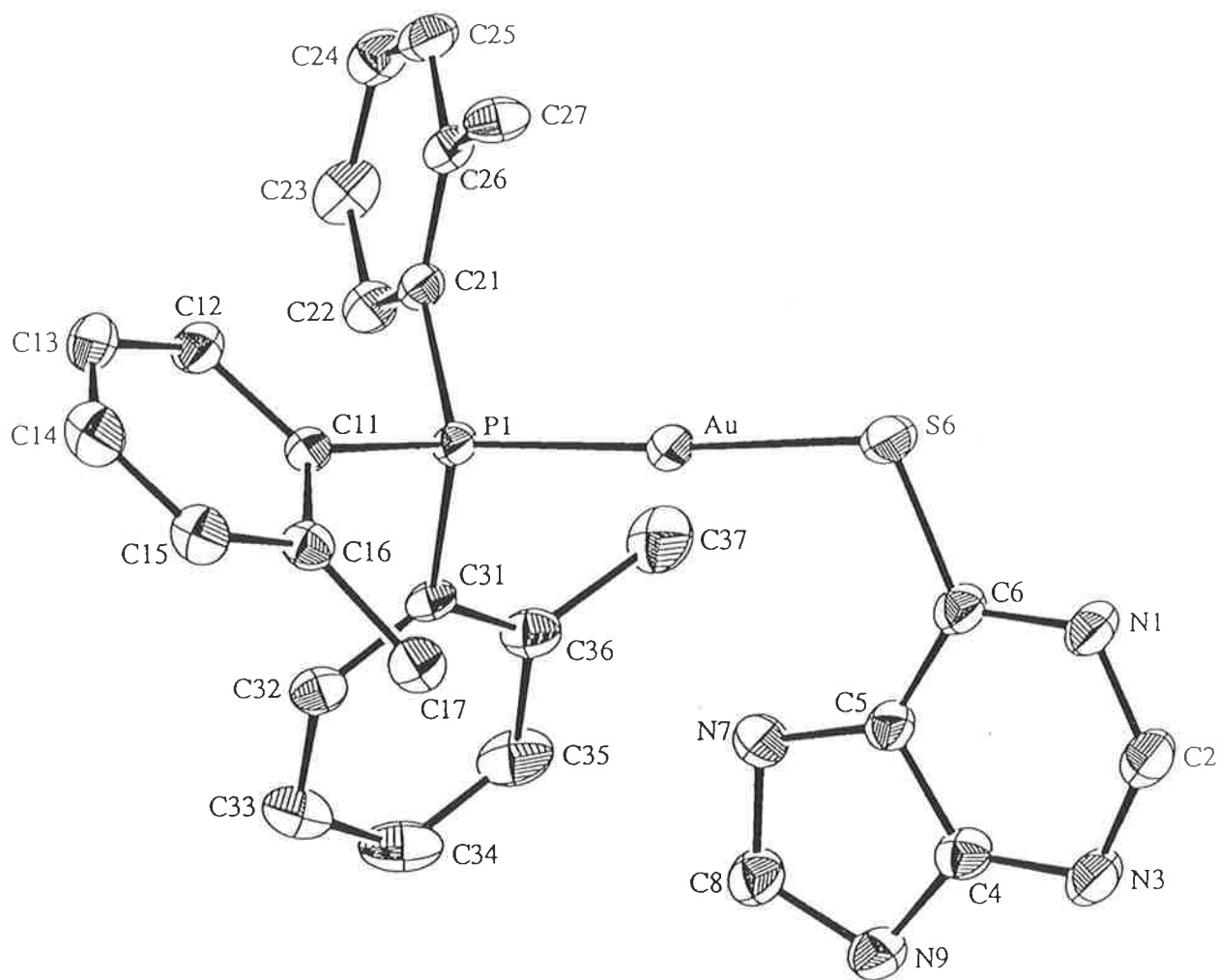
Figure 5.3.1: *Molecular Structure And Crystallographic Numbering Scheme For*

[(o-Tol)₃PAu(6-MP)].
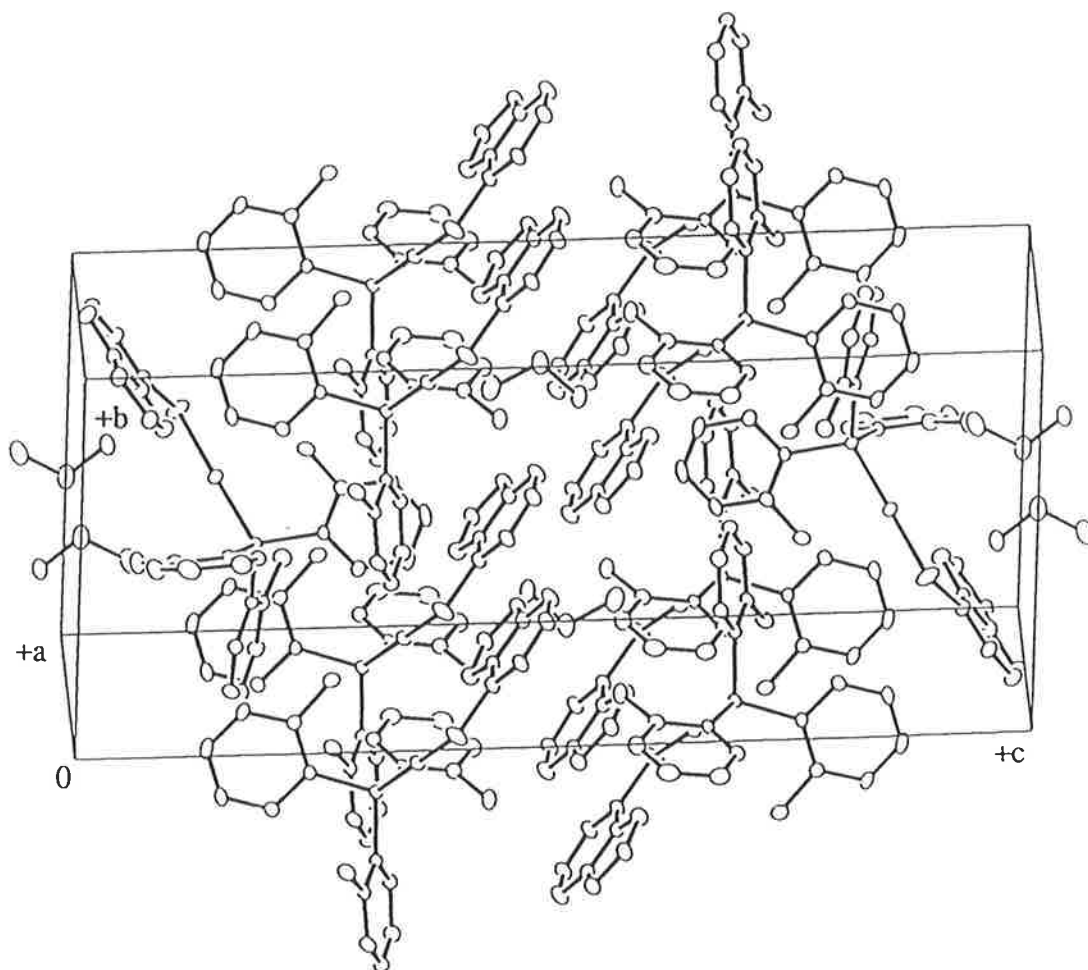
Figure 5.3.2: *Unit Cell Diagram Of [(o-Tol)₃PAu(6-MP)].C₂H₅OH.*
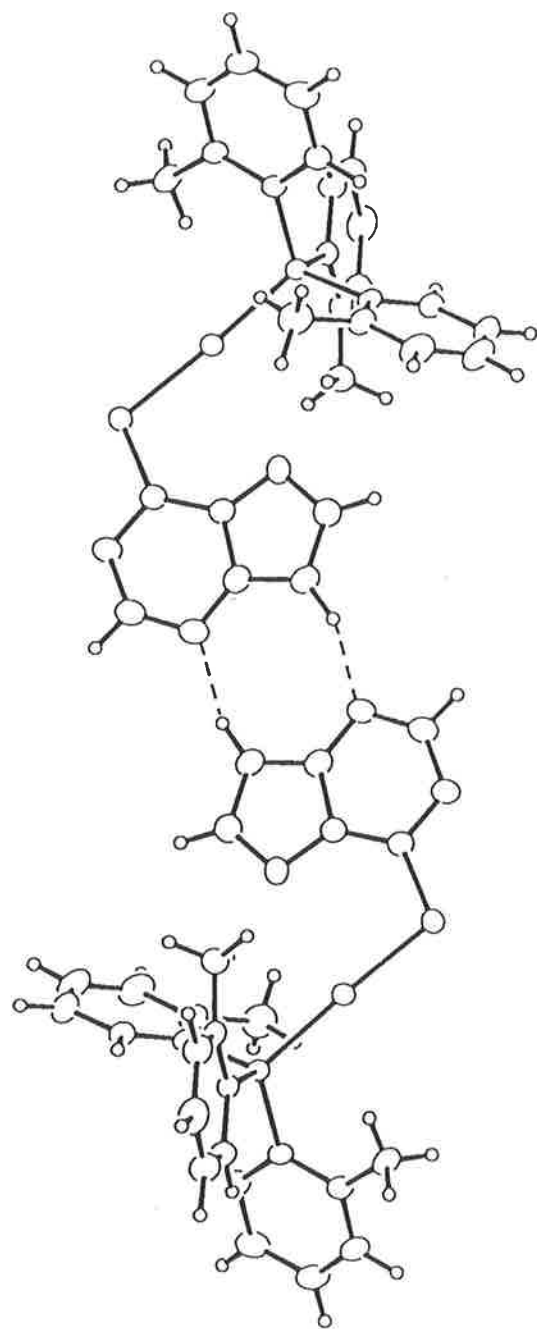
Figure 5.3.3: *Diagram Illustrating Intermolecular Hydrogen Bonding (indicated by dashed lines).*

The P(1)–Au distance is 2.239(2) Å, which is equivalent within standard deviation to the value of 2.243(2) Å for [(*o*-Tol)₃PAuCl][55]. It is also equivalent to the corresponding value of 2.237(2) Å for [Ph₃PAu(6-MP)], suggesting that not only does the coordination of the 6-MP ligand to the gold centre have little electronic effect on the phosphine moiety but also that the size of the phosphine cone angle affects the P–Au bond to a negligible extent. This latter observation is in accordance with the results obtained from the cone angle correlation for triorganophosphinegold(I) chlorides in Chapter 3. The P–C bond distances also display equivalent values.

The *ortho*-tolyl rings are all planar; the maximum deviation from planarity is observed for the ring defined by the atoms C(21) to C(26), of the value 0.008(9) Å. The phosphorus atom lies out of the plane to a maximum value of 0.147 Å for the ring defined by the atoms C(11) to C(16). The methyl groups on all three ring systems only deviate from the plane by less than 0.1 Å, which is expected as the C(16), C(26) and C(36) atoms are all sp^2 hybridized in the aromatic system, as evidenced by the corresponding angles all being equal to 120° within standard deviation.

The Au–S bond length is 2.266(2) Å, a value which is significantly shorter than 2.287(1) Å for [Ph₃PAu(6-MP)]. Again, this may be attributable to the relative cone-angles of (*o*-Tol)₃P and Ph₃P, which are 194 and 145° respectively[49], possibly giving rise to differing steric interactions. The effect of coordination on the 6-mercaptopurinate moiety is discussed in the next section.

5.4 *Comparison between the 6-mercaptopurinate moiety in the free ligand and in the complexes.*

Crystallographic data for the free 6-mercaptopurine ligand has been obtained from the reference of Sletten, Sletten and Jensen[57] on the analysis of 6-mercaptopurine monohydrate. Tables 5.4.1 and 5.4.2 give the bond distances and bond angles for 6-mercaptopurine monohydrate. These values are also given pictorially in Figures 5.4.1 and 5.4.2. Alongside

Table 5.4.1: *Bond Distances (Å) For 6-mercaptopurine Monohydrate*[57].

Atom	Atom	Distance	Atom	Atom	Distance
N(1)	– C(2)	1.350(2)	C(6)	– S(6)	1.676(2)
C(2)	– N(3)	1.307(2)	C(5)	– N(7)	1.370(2)
N(3)	– C(4)	1.364(2)	N(7)	– C(8)	1.346(2)
C(4)	– C(5)	1.397(2)	C(8)	– N(9)	1.326(2)
C(5)	– C(6)	1.396(2)	N(9)	– C(4)	1.363(2)
C(6)	– N(1)	1.384(2)			

Table 5.4.2: *Bond Angles (°) For 6-mercaptopurine Monohydrate*[57].

Atom	Atom	Atom	Angle	Atom	Atom	Atom	Angle
C(6)	– N(1)	– C(2)	125.4(1)	C(6)	– C(5)	– N(7)	132.2(1)
N(1)	– C(2)	– N(3)	125.1(1)	C(4)	– C(5)	– N(7)	105.9(1)
C(2)	– N(3)	– C(4)	113.0(1)	C(5)	– N(7)	– C(8)	106.1(1)
N(3)	– C(4)	– C(5)	124.2(1)	N(7)	– C(8)	– N(9)	113.6(1)
C(4)	– C(5)	– C(6)	121.9(1)	C(8)	– N(9)	– C(4)	104.5(1)
C(5)	– C(6)	– N(1)	110.4(1)	N(9)	– C(4)	– C(5)	109.9(1)
C(5)	– C(6)	– S(6)	127.0(1)	N(9)	– C(4)	– N(3)	125.9(1)
N(1)	– C(6)	– S(6)	122.6(1)				

6-mercaptopurine

[Ph₃PAu(6-MP)]
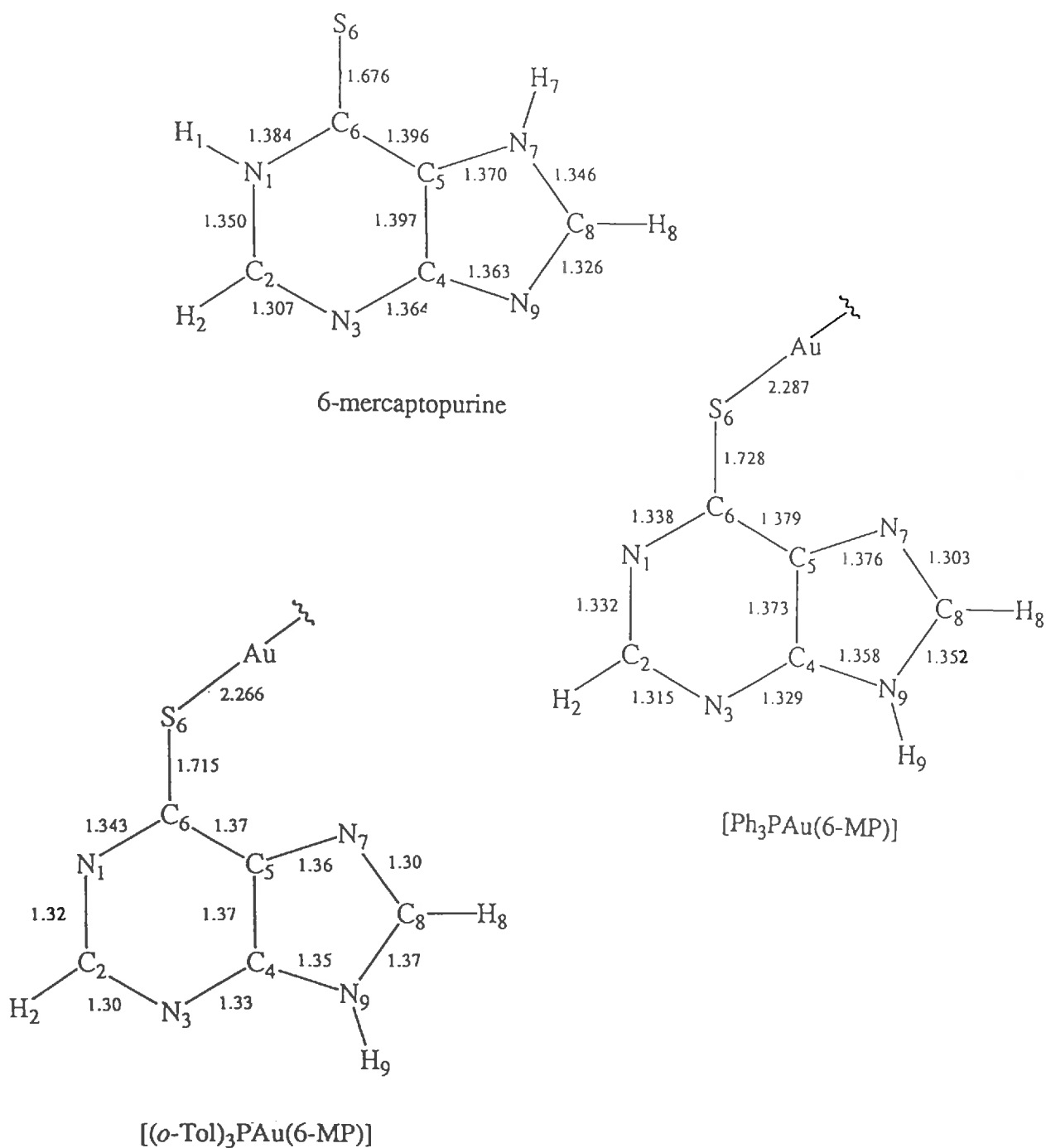
[(o-Tol)₃PAu(6-MP)]

Figure 5.4.1: *Schematic Representation Of The Bond Distances (Å) In The Purine Moiety Of 6-mercaptopurine Monohydrate, [Ph₃PAu(6-MP)].C₂H₅OH and [(o-Tol)₃PAu(6-MP)].C₂H₅OH.*
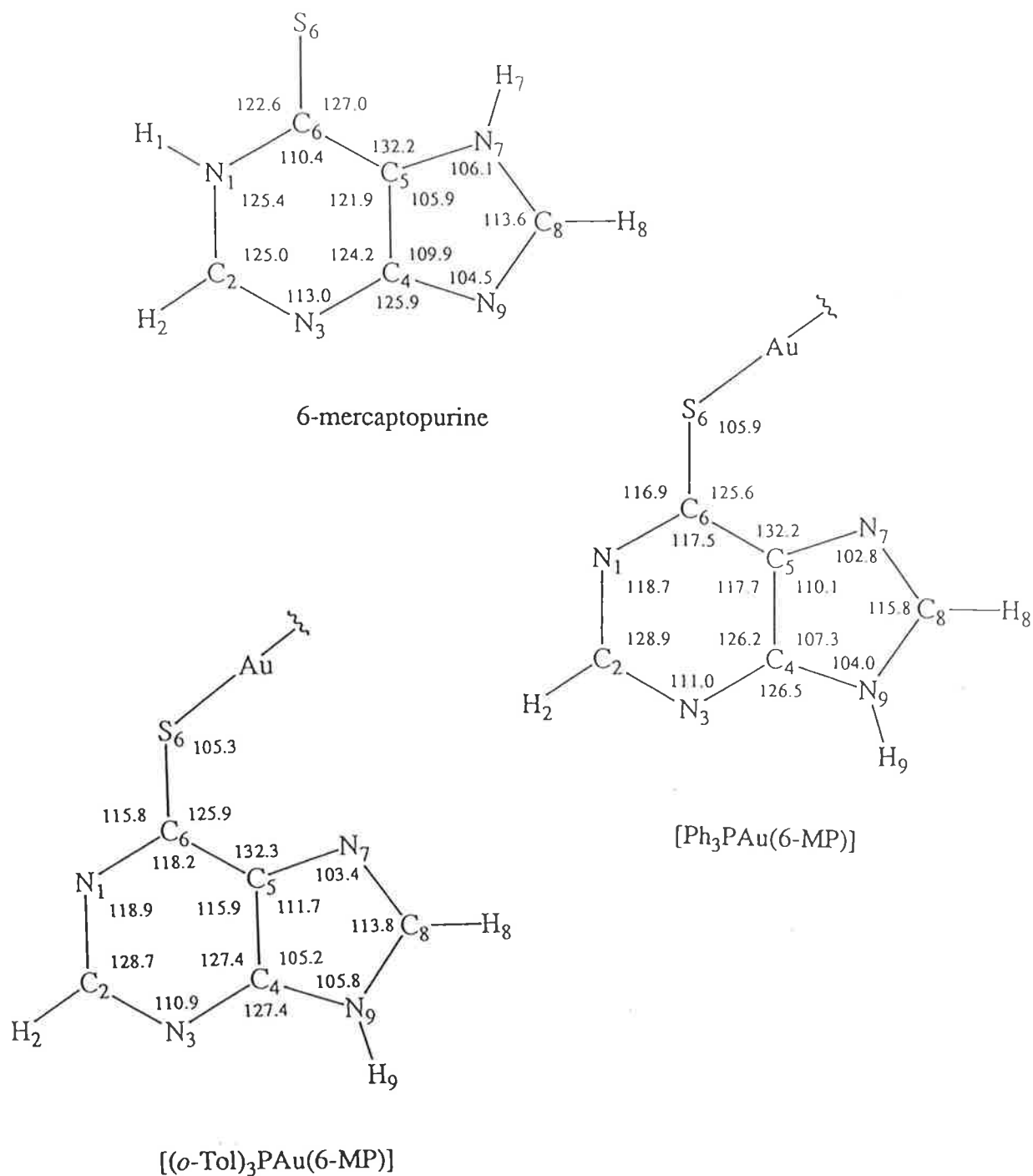
Figure 5.4.2: *Schematic Representation Of The Bond Angles (°) In The Purine Moiety Of 6-mercaptopurine Monohydrate, [Ph₃PAu(6-MP)].C₂H₅OH and [(o-Tol)₃PAu(6-MP)].C₂H₅OH.*

these diagrams are shown the 6-mercaptopurinate regions of the two complexes. The estimated standard deviations for the values of the complexes have not been given for reasons of clarity but they can be found in the tables on the previous pages.

Analysis of Figure 5.4.1 indicates how the internal molecular structure of the ring system is altered upon complexation of the 6-mercaptopurinate ligand to the gold atom via the sulphur atom. The most significant observation is that concerning the C(6)–S(6) bond. In 6-MPH, the C(6)–S(6) bond length is 1.676(2) Å, a value indicative of its significant double-bond character. Upon complexation, the length of this bond increases appreciably, to 1.728(5) Å for [Ph$_3$PAu(6-MP)] and to 1.715(8) Å for [(o-Tol)$_3$PAu(6-MP)]. Hence, as expected the C(6)–S(6) bond approaches single-bond character as the sulphur atom binds to the gold atom. The general increase in electron delocalization in the six-membered ring of 6-mercaptopurine upon complexation leads to the N(1)–C(6) and C(5)–C(6) bonds increasing in multiple-bond character, which in turn lessens the bond order of the C(6)–S(6) interaction. All the bonds in the six-membered ring system except for C(2)–N(3) demonstrate a decrease in length; N(1)–C(6) undergoes the greatest change. In the five-membered ring, the bonds of C(5)–N(7) and C(4)–N(9) vary only slightly. An increase in the bond length of C(8)–N(9) and a decrease in N(7)–C(8) is observed; the bond character in these two bonds has essentially been exchanged from the free ligand to the complex. The movement in electron density thus suggests that it is N(9) which is protonated in the complexes, whereas N(7) was protonated in the free ligand, and justifies the placement of H(9) at this position, with the N–H bond distance fixed at 0.95 Å.

The change in the internal angles, as illustrated in Figure 5.4.2, confirms what the previous paragraph suggested. The internal angles of the six-membered ring all appear to converge to 120°, consistent with an increase in aromaticity in the ring. For both complexes the angles C(4)–C(5)–N(7) and C(5)–C(4)–N(9) increase and decrease in size respectively upon complexation, which is consistent with the movement of the amino hydrogen from N(7) to N(9).

The arguments above are consistent with the data obtained via the spectral characterization of the complexes. Contraction of N(1)–C(6) upon complexation, which indicates an increase in double bond character, was manifested in the infrared spectra by a higher absorption frequency of the thioamide band I vibrational mode. Similarly, the decrease in double bond character of C(6)–S(6) is reflected by the decreasing absorption frequency of the thioamide band II chromophore in the complexes. The observed overall contraction in size of the ring system also supports the arguments made in Chapter 4 concerning the electronic effects of complexation via sulphur on the resonance frequencies of the carbon-13 nuclei. Hence, as these interpretations are now vindicated by the crystallographic evidence, then the identity of all the other complexes prepared can be confirmed by extrapolation.

Even with the inclusion of the sulphur atom as part of the ring system, the purine group in each of the molecules is planar; the mean deviation from the mean planes for [Ph$_3$PAu(6-MP)] and [(o-Tol)$_3$PAu(6-MP)] being 0.012 and 0.026 Å respectively. When excluded, calculations show that the system appears to be more planar e.g. in [Ph$_3$PAu(6-MP)] the mean deviation is 0.009 Å. Either way, the mean deviations are small.

All the effects noticed are expected for complexation to gold(I) via the sulphur atom, consistent with the structures of other triorganophosphinegold(I) thiolate complexes. However, a variety of coordination modes exist for crystal structures involving 6-mercaptopurine-type thionucleobases in the literature. One example is coordination via N(9) e.g. 6-mercaptopurine riboside[73], and another common type is the ligand acting in bidentate fashion, coordinating to the metal atom via the S(6) and N(7) atoms, e.g. dichloro-(6-mercapto-9-methylpurine)copper(II)[74], (6-mercaptopurine)diaquodicadmium(II)[75] and bis(6-mercapto-9-benzylpurine)palladium(II)-dimethylacetamide[76]. In these cases the internal structure of the purine moiety is similar to those discussed above given the changes. An example of metal to sulphur coordination has been reported for dichloro(6-mercaptopurinium)copper(I)[13], where the 6-MP is in a protonated form; the effects here on the internal structure of the

6-mercaptopurinate moiety are many ways the opposite to the effects observed for deprotonation.

The crystallographic investigations of $[Ph_3PAu(6\text{-}MP)].C_2H_5OH$ and $[(o\text{-}Tol)_3PAu(6\text{-}MP)].C_2H_5OH$ has revealed a number of observations. As expected, the P–Au–S chromophore is a near linear group, consistent with previously observed data for analogous structures. The bond distances within the 6-mercaptopurinate moiety undergo a general contraction upon complexation, a result which is expected as the electron density increases within the ring structure. The ligand coordinates exclusively in the monodentate mode; the N(7) atom is oriented towards the gold centre in the solid state, although not at a intramolecular distance indicative of a significant interaction. The spectroscopic data concerning these complexes is consistent with the observed intramolecular parameters.

CHAPTER 6

Crystallographic Investigations of Triorganophosphinegold(I) Thiolates

6.1 *Introduction*

There are now several examples of crystal structures of triorganophosphinegold(I) thiolates with the general formula [R$_3$PAu(SR')] in the literature. Common to all these complexes is the SR' moiety coordinating in a monodentate mode, as a thiolate ligand, i.e. with an Au–S–R' linkage, and an invariably linear P–Au–S chromophore. Such structural characteristics were also observed in Chapter 5 for the [Ph$_3$PAu(6-MP)] and [(*o*-Tol)$_3$PAu(6-MP)] complexes. Thus, in a similar fashion to the triorganophosphinegold(I) chlorides analyzed in Chapter 3, a study may be performed on these complexes to determine whether any simple relationship exists between the steric effects of the phosphine and thiolate groups, and the intramolecular parameters of   P–Au, Au–S, P–Au–S and possibly the Au...N interaction observed in most of the complexes; such a study is performed in this chapter. In order to gain additional information on complexes possessing the Cycl$_3$P phosphine group, the crystal structure determination of the complex 6-n-propyl-2-thiouracilato(tricyclohexylphosphine)gold(I), [Cycl$_3$PAu(6p2-TU)], was performed.

6.2 *Crystal structure of the [Cycl$_3$PAu(6p2-TU)] complex*

The complex [Cycl$_3$PAu(6p2-TU)] was prepared by the literature method[19]; crystals of the complex were obtained from the slow evaporation of a saturated ethanolic solution of the compound, and the complex crystallizes in the monoclinic space group $P2_1/c$ (C$_{2h}^5$, No. 14)[44].

Table 6.2.1: *Crystallographic Parameters For The [Cycl₃PAu(6p2-TU)] Complex.*

Data	[Cycl₃PAu(6p2-TU)]
Formula	$C_{25}H_{42}AuSPON_2$
Formula weight	646.6
Crystal shape	rectangular prism
Crystal dimensions (mm)	0.16 x 0.16 x 0.29
Crystal system	monoclinic
Space group	$P2_1/c$ (C_{2h}^5, No. 14)
a (Å)	9.539(2)
b (Å)	16.452(4)
c (Å)	16.880(2)
β (°)	95.37(2)
V (Å³)	2637.4(8)
Z	4
$\rho_{calc.}$ (g cm⁻³)	1.628
F(000)	~~324~~ 1296
μ (cm⁻¹)	57.56
θ limits, cell (°)	13.1 to 15.4
θ limits, data (°)	1.5 to 27.9
hkl range	0 to 12, 0 to 21, -20 to 20
Range of transmission factors	0.985 to 1.012
Scan technique	$\omega:2\theta$
No. of data measured	6899
No. of unique data	6524
R_{amal}	0.060
No. of unique data used	3695
Criterion of observability	$I \geq 3.0\sigma(I)$
No. of parameters	280
R	0.043
R_w	0.039
Residual electron density (e Å⁻³)	-1.28 to 0.90

Crystal and refinement data are listed in Table 6.2.1, and the derived results are given in Tables 6.2.2 to 6.2.7. The observed and calculated structure factors can be found in the Appendix. The crystallographic numbering scheme is shown in the ORTEP[45] diagram in Figure 6.2.1, plotted with 30 % thermal ellipsoids.

The unit cell contents of [Cycl$_3$PAu(6p2-TU)] are displayed in Figure 6.2.2 and are clearly demonstrative of the P2$_1$/c space group. As observed in other triorganophosphinegold(I) derivatives containing the thiouracilate anion[9,19,61], centrosymmetrically related molecules are associated via hydrogen bonding contacts in the lattice. They involve the N(3)–H(3) and O(4') atoms such that the H(3)...O(4') separation is 1.90 Å and the N(3)–H(3)...O(4') angle is 161° (symmetry operation for O(4') is -x, 1-y, -z). The closest gold to gold interaction is 8.460(1) Å, which is too large to be considered as a 'significant' interaction[46].

The molecular structure of [Cycl$_3$PAu(6p2-TU)] is shown in Figure 6.2.2. As expected, the P–Au–S chromophore is linear, the angle being 177.6(1)°. The P(1)–Au and Au–S(2) bond lengths are 2.248(3) and 2.302(3) Å respectively. These values are equivalent to those observed for the related complex [Cycl$_3$PAu(6m2-TU)][77]; the implications of this will be discussed in the next section. The three P–C bond lengths are all equivalent to within standard deviation, suggesting the electronic environment about these bonds is identical. The cyclohexyl groups exist in the 'chair' conformation; relatively large thermal motion is associated with these atoms.

The 6-n-propyl-2-thiouracilate moiety is coordinated as expected to the gold centre via the sulphur atom, as a thiolate rather than a thione. The two bond distances of N(1)–C(2) and N(3)–C(2) are 1.28(1) and 1.37(1) Å respectively, indicating the former has greater double bond character. Hence deprotonation of the free ligand occurs at N(1), consistent with results observed for other triorganophosphinegold(I) thiouracilates[9,19,62,78]. The distance between N(1) and Au is 3.061(9) Å, less than the sum of the van der Waal radii, but, like with the two 6-mercaptopurinate complexes in Chapter 5 and other analogous complexes, not indicative of a

Table 6.2.2: *Fractional Atomic Coordinates For The [Cycl3PAu(6p2-TU)] Complex.*

Atom	x	y	z
Au	0.40117(4)	0.71525(3)	0.22652(3)
S(2)	0.2653(3)	0.6070(2)	0.1792(2)
P(1)	0.5417(3)	0.8183(2)	0.2714(2)
O(4)	-0.0151(9)	0.5635(5)	-0.0732(5)
N(1)	0.2145(9)	0.7192(6)	0.0689(6)
N(3)	0.1137(8)	0.5937(5)	0.0415(5)
C(2)	0.1957(9)	0.6458(7)	0.0896(6)
C(4)	0.0525(13)	0.6143(8)	-0.0323(8)
C(5)	0.0743(15)	0.6972(9)	-0.0507(8)
C(6)	0.1523(14)	0.7461(9)	-0.0009(9)
C(11)	0.7079(10)	0.8113(6)	0.2279(6)
C(12)	0.8076(11)	0.8823(7)	0.2425(7)
C(13)	0.9317(12)	0.8727(8)	0.1928(8)
C(14)	1.0081(12)	0.7950(10)	0.2090(8)
C(15)	0.9106(13)	0.7232(8)	0.2002(7)
C(16)	0.7821(11)	0.7306(7)	0.2450(6)
C(21)	0.5778(14)	0.8208(8)	0.3794(7)
C(22)	0.6144(14)	0.9027(8)	0.4149(8)
C(23)	0.6442(26)	0.8949(11)	0.5056(10)
C(24)	0.6002(24)	0.8381(15)	0.5457(10)
C(25)	0.5671(18)	0.7615(10)	0.5100(9)
C(26)	0.5342(25)	0.7634(11)	0.4218(9)
C(31)	0.4687(10)	0.9161(6)	0.2395(6)
C(32)	0.3266(12)	0.9291(7)	0.2674(8)
C(33)	0.2670(12)	1.0126(8)	0.2380(11)

Table 6.2.2 (*continued*)

C(34)	0.2619(17)	1.0240(9)	0.1533(10)
C(35)	0.4042(15)	1.0090(9)	0.1268(8)
C(36)	0.4580(12)	0.9267(7)	0.1505(7)
C(61)	0.1764(21)	0.8342(10)	-0.0176(11)
C(62)	0.1260(26)	0.8678(12)	-0.0779(16)
C(63)	0.1669(22)	0.9509(11)	-0.0911(14)

Table 6.2.3: *Anisotropic Thermal Parameters For The [Cycl₃PAu(6p2-TU)] Complex.*

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Au	0.0382(2)	0.0390(2)	0.0547(2)	-0.0046(3)	-0.0015(2)	-0.0068(3)
S(2)	0.052(2)	0.042(2)	0.065(2)	-0.007(1)	-0.013(2)	0.000(1)
P(1)	0.042(2)	0.038(2)	0.046(2)	-0.005(1)	0.003(1)	-0.006(1)
O(4)	0.108(7)	0.074(7)	0.091(7)	-0.033(6)	-0.047(6)	0.013(6)
N(1)	0.060(6)	0.046(6)	0.075(7)	-0.013(6)	-0.011(5)	0.008(6)
N(3)	0.043(6)	0.041(6)	0.066(7)	-0.005(4)	-0.013(5)	0.005(5)
C(2)	0.024(6)	0.044(7)	0.067(8)	-0.000(5)	-0.003(5)	-0.012(6)
C(4)	0.060(9)	0.07(1)	0.07(1)	-0.015(7)	-0.023(7)	-0.002(8)
C(5)	0.11(1)	0.07(1)	0.10(1)	-0.02(1)	-0.04(1)	0.04(1)
C(6)	0.09(1)	0.07(1)	0.10(1)	-0.017(8)	-0.032(9)	0.011(9)
C(11)	0.037(6)	0.048(7)	0.049(7)	-0.001(5)	0.005(5)	0.005(5)
C(12)	0.036(7)	0.064(9)	0.09(1)	-0.007(6)	0.008(6)	-0.010(7)
C(13)	0.048(9)	0.07(1)	0.13(1)	-0.009(7)	0.029(8)	-0.00(1)
C(14)	0.052(8)	0.10(1)	0.13(1)	-0.012(9)	0.034(8)	-0.04(1)
C(15)	0.068(9)	0.08(1)	0.09(1)	0.017(9)	0.024(8)	-0.015(9)
C(16)	0.052(8)	0.06(1)	0.068(8)	0.013(6)	0.017(6)	-0.007(7)
C(21)	0.13(1)	0.062(9)	0.049(8)	-0.044(8)	0.021(8)	-0.016(7)
C(22)	0.12(1)	0.08(1)	0.06(1)	-0.013(9)	0.004(8)	-0.009(8)
C(23)	0.41(3)	0.10(2)	0.06(1)	-0.06(2)	0.00(2)	-0.04(1)
C(24)	0.23(2)	0.23(3)	0.06(1)	-0.09(2)	0.01(1)	0.06(2)
C(25)	0.16(2)	0.10(1)	0.08(1)	-0.06(1)	-0.00(1)	0.01(1)
C(26)	0.43(3)	0.16(2)	0.04(1)	-0.16(2)	0.01(1)	0.02(1)
C(31)	0.043(7)	0.046(7)	0.051(7)	-0.005(6)	0.007(6)	-0.013(6)
C(32)	0.050(8)	0.061(9)	0.11(1)	0.004(7)	0.001(8)	-0.023(8)
C(33)	0.043(9)	0.047(9)	0.22(2)	0.017(7)	-0.01(1)	-0.04(1)

Table 6.2.3 *(continued)*

C(34)	0.12(1)	0.07(1)	0.12(1)	0.02(1)	-0.06(1)	0.01(1)
C(35)	0.10(1)	0.08(1)	0.10(1)	0.02(1)	-0.02(1)	0.024(9)
C(36)	0.070(9)	0.066(9)	0.066(9)	0.021(7)	-0.009(7)	0.007(7)
C(61)	0.25(2)	0.07(1)	0.15(2)	-0.08(1)	-0.12(2)	0.07(1)
C(62)	0.30(3)	0.11(2)	0.30(3)	-0.07(2)	-0.12(2)	0.13(2)
C(63)	0.28(3)	0.09(2)	0.29(3)	-0.04(2)	-0.03(2)	0.11(2)

Table 6.2.4: *Hydrogen Atom Parameters For The [Cycl₃PAu(6p2-TU)] Complex.*

Atom	x	y	z	B(eq)
H(3)	0.0983	0.5403	0.0606	5.2
H(5)	0.0309	0.7187	-0.1007	9.1
H(11)	0.6835	0.8113	0.1710	4.5
H(12a)	0.7592	0.9325	0.2277	6.1
H(12b)	0.8429	0.8843	0.2984	6.1
H(13a)	0.8977	0.8745	0.1369	7.8
H(13b)	0.9975	0.9173	0.2047	7.8
H(14a)	1.0794	0.7895	0.1719	8.2
H(14b)	1.0532	0.7962	0.2629	8.2
H(15a)	0.8807	0.7166	0.1441	7.4
H(15b)	0.9637	0.6755	0.2193	7.4
H(16a)	0.8115	0.7267	0.3016	5.7
H(16b)	0.7187	0.6867	0.2291	19.8
H(21)	0.6743	0.8015	0.3805	7.2
H(22a)	0.6973	0.9239	0.3922	7.7
H(22b)	0.5365	0.9396	0.4033	7.7
H(23a)	0.7488	0.8927	0.5152	16.4
H(23b)	0.6130	0.9448	0.5278	4.2
H(24a)	0.5164	0.8585	0.5663	14.9
H(24b)	0.6726	0.8285	0.5896	14.9
H(25a)	0.4859	0.7404	0.5333	10.0
H(25b)	0.6471	0.7256	0.5225	10.0
H(26a)	0.4335	0.7627	0.4121	18.0
H(26b)	0.5735	0.7136	0.4020	18.0
H(31)	0.5304	0.9582	0.2629	4.5

Table 6.2.4 (*continued*)

H(32b)	0.2628	0.8864	0.2463	7.2
H(32a)	0.3329	0.9276	0.3251	7.2
H(33a)	0.1719	1.0180	0.2545	8.7
H(33b)	0.3260	1.0548	0.2635	8.7
H(34a)	0.1927	0.9860	0.1275	9.4
H(34b)	0.2300	1.0791	0.1405	9.4
H(35a)	0.3970	1.0137	0.0694	8.7
H(35b)	0.4671	1.0498	0.1506	8.7
H(36a)	0.5502	0.9201	0.1321	6.5
H(36b)	0.3943	0.8859	0.1260	7.2
H(61a)	0.1410	0.8639	0.0265	15.1
H(61b)	0.2761	0.8412	-0.0167	15.1
H(62a)	0.1496	0.8361	-0.1226	19.8
H(62b)	0.0226	0.8671	-0.0765	19.8
H(63a)	0.2661	0.9548	-0.0876	17.8
H(63b)	0.1255	0.9678	-0.1439	17.8
H(63c)	0.1281	0.9857	-0.0515	20.8

Table 6.2.5: *Bond Distances (Å) For The [Cycl₃PAu(6p2-TU)] Complex.*

Atom		Atom	Distance	Atom		Atom	Distance
Au	–	S(2)	2.302(3)	C(13)	–	C(14)	1.48(2)
Au	–	P(1)	2.248(3)	C(14)	–	C(15)	1.50(2)
S(2)	–	C(2)	1.72(1)	C(32)	–	C(33)	1.55(2)
P(1)	–	C(11)	1.81(1)	C(33)	–	C(34)	1.44(2)
P(1)	–	C(21)	1.82(1)	C(34)	–	C(35)	1.49(2)
P(1)	–	C(31)	1.82(1)	C(35)	–	C(36)	1.49(2)
O(4)	–	C(4)	1.23(1)	C(61)	–	C(62)	1.22(2)
N(1)	–	C(2)	1.28(1)	C(62)	–	C(63)	1.44(2)
N(1)	–	C(6)	1.34(1)	C(15)	–	C(16)	1.50(1)
N(3)	–	C(2)	1.37(1)	C(21)	–	C(22)	1.50(2)
N(3)	–	C(4)	1.37(1)	C(21)	–	C(26)	1.28(2)
C(4)	–	C(5)	1.42(2)	C(22)	–	C(23)	1.54(2)
C(5)	–	C(6)	1.34(2)	C(23)	–	C(24)	1.25(2)
C(6)	–	C(61)	1.50(2)	C(24)	–	C(25)	1.42(2)
C(11)	–	C(12)	1.51(1)	C(25)	–	C(26)	1.49(2)
C(11)	–	C(16)	1.52(1)	C(31)	–	C(32)	1.49(1)
C(12)	–	C(13)	1.52(1)	C(31)	–	C(36)	1.51(1)

Table 6.2.6: *Bond Angles (°) For The [Cycl₃PAu(6p2-TU)] Complex.*

Atom		Atom		Atom	Angle	Atom		Atom		Atom	Angle
S(2)	–	Au	–	P(1)	177.6(1)	C(11)	–	C(12)	–	C(13)	110(1)
Au	–	S(2)	–	C(2)	100.2(4)	C(12)	–	C(13)	–	C(14)	112(1)
Au	–	P(1)	–	C(11)	109.4(3)	C(13)	–	C(14)	–	C(15)	112(1)
Au	–	P(1)	–	C(21)	113.9(4)	C(14)	–	C(15)	–	C(16)	114(1)
Au	–	P(1)	–	C(31)	111.6(3)	C(11)	–	C(16)	–	C(15)	111(1)
C(11)	–	P(1)	–	C(21)	108.4(5)	P(1)	–	C(21)	–	C(22)	115.7(9)
C(11)	–	P(1)	–	C(31)	105.2(5)	P(1)	–	C(21)	–	C(26)	120(1)
C(21)	–	P(1)	–	C(31)	107.9(5)	C(22)	–	C(21)	–	C(26)	121(1)
C(2)	–	N(1)	–	C(6)	119(1)	C(21)	–	C(22)	–	C(23)	110(1)
C(2)	–	N(3)	–	C(4)	124(1)	C(22)	–	C(23)	–	C(24)	124(2)
S(2)	–	C(2)	–	N(1)	122.7(8)	C(23)	–	C(24)	–	C(25)	120(2)
S(2)	–	C(2)	–	N(3)	116.1(8)	C(24)	–	C(25)	–	C(26)	115(1)
N(1)	–	C(2)	–	N(3)	121(1)	C(21)	–	C(26)	–	C(25)	122(2)
O(4)	–	C(4)	–	N(3)	120(1)	P(1)	–	C(31)	–	C(32)	111.6(8)
O(4)	–	C(4)	–	C(5)	128(1)	P(1)	–	C(31)	–	C(36)	112.7(7)
N(3)	–	C(4)	–	C(5)	112(1)	C(32)	–	C(31)	–	C(36)	108.7(9)
C(4)	–	C(5)	–	C(6)	122(1)	C(31)	–	C(32)	–	C(33)	110(1)
N(1)	–	C(6)	–	C(5)	122(1)	C(32)	–	C(33)	–	C(34)	114(1)
N(1)	–	C(6)	–	C(61)	115(1)	C(33)	–	C(34)	–	C(35)	109(1)
C(5)	–	C(6)	–	C(61)	123(1)	C(34)	–	C(35)	–	C(36)	112(1)
P(1)	–	C(11)	–	C(12)	116.5(8)	C(31)	–	C(36)	–	C(35)	111(1)
P(1)	–	C(11)	–	C(16)	112.8(7)	C(6)	–	C(61)	–	C(62)	123(2)
C(12)	–	C(11)	–	C(16)	111.7(8)	C(61)	–	C(62)	–	C(63)	118(2)

Table 6.2.7: *Mean Plane Data For The [Cycl$_3$PAu(6p2-TU)] Complex.*

Least squares plane through the 6-n-propyl-2-thiouracilate moiety.

Atoms Defining Plane	Distance (Å)	esd (Å)
N(1)	0.0075	0.0092
N(3)	-0.0156	0.0085
C(2)	0.0059	0.0095
C(4)	0.0294	0.0130
C(5)	-0.0075	0.0155
C(6)	-0.0203	0.0149
Additional Atoms	Distance (Å)	
Au	0.1910	
S(2)	-0.0235	
P(1)	0.4893	
O(4)	0.0583	
C(61)	-0.0760	
C(62)	-0.1189	
C(63)	-0.0444	

Mean deviation from plane is 0.0144 (Å).

Chi-squared: 9.9.
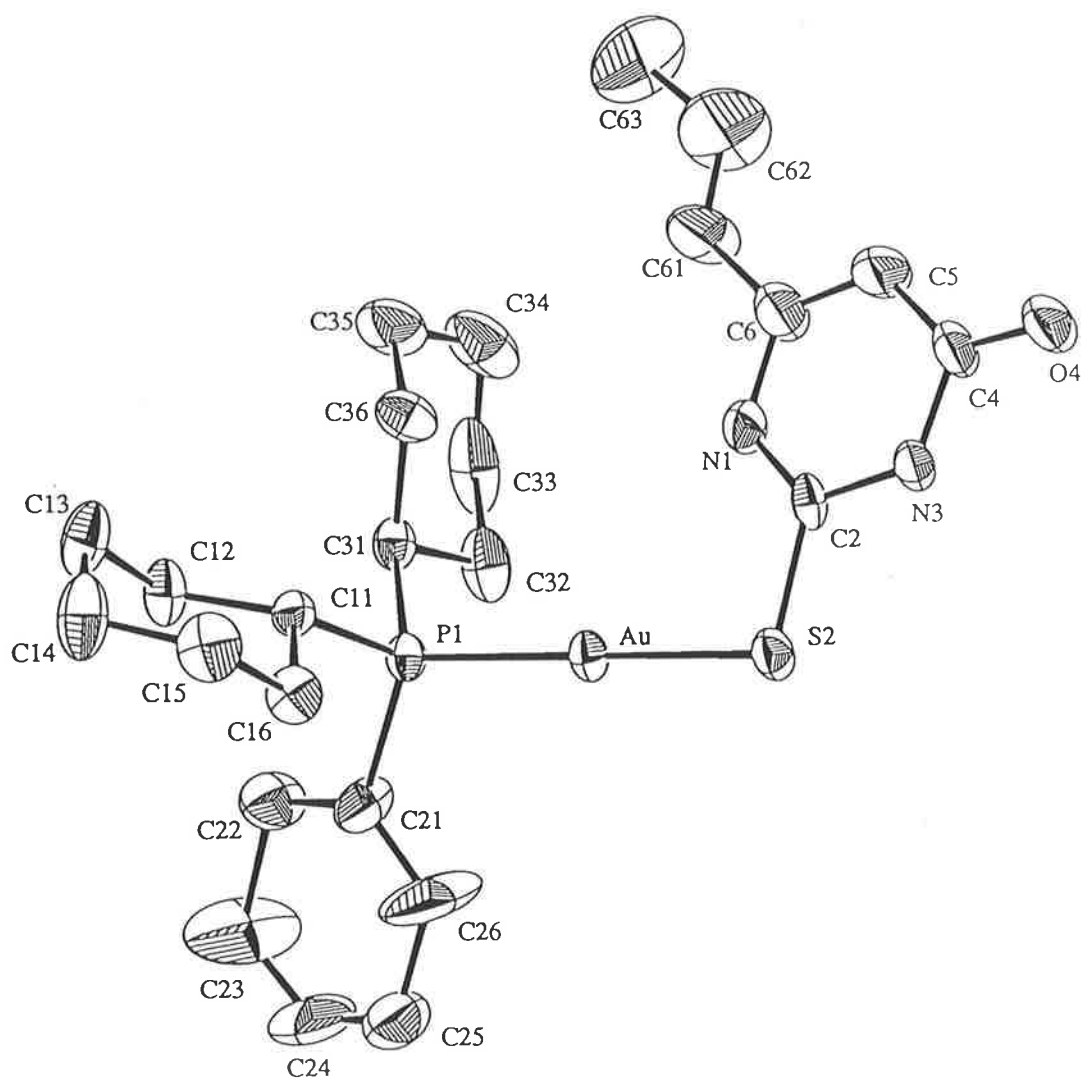
Figure 6.2.1: *Molecular Structure And Crystallographic Numbering Scheme For*

[Cycl₃PAu(6p2-TU)].
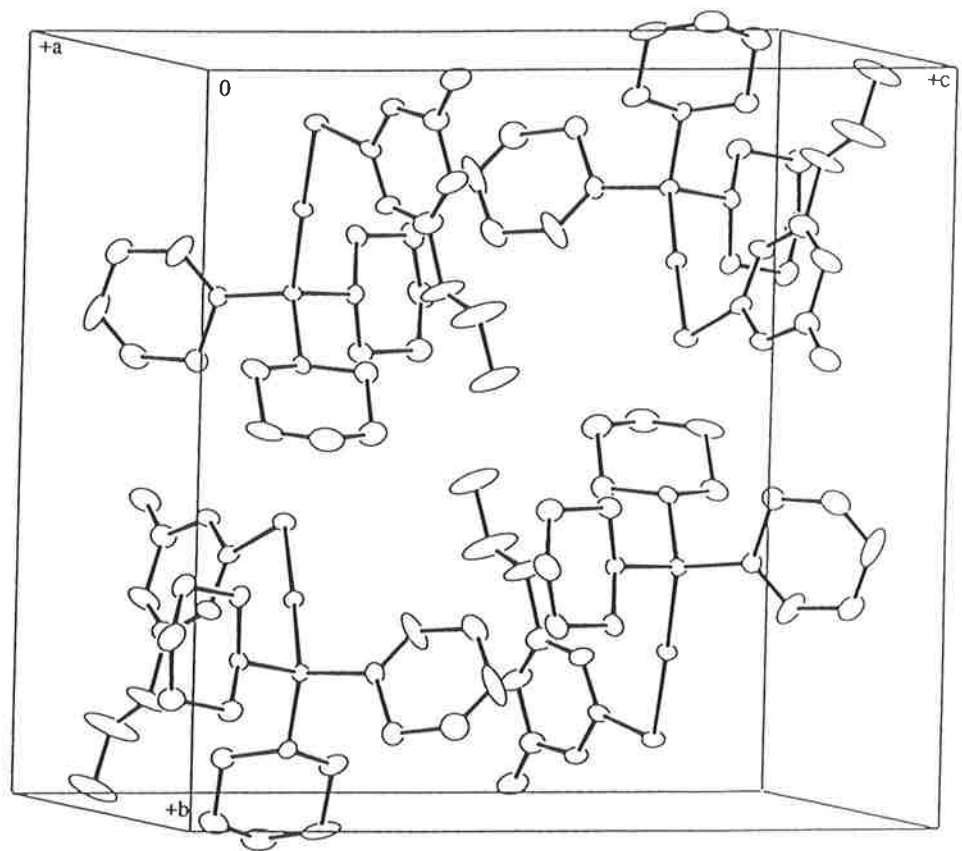
Figure 6.2.2: *Unit Cell Diagram Of [Cycl₃PAu(6p2-TU)].*

bonding interaction. High thermal motion is noted for the carbon atoms of the propyl chain; this was also observed in the [Et₃PAu(6p2-TU)][61] complex.

The crystal structure of 6-n-propyl-2-thiouracil has been reported in the literature[78]; however, the relatively high errors associated with the light atom positions in the complex and those in the structure of the thionucleobase itself preclude a meaningful discussion concerning the derived parameters. The structure of this complex is closely related to [Cycl₃PAu(6m2-TU)][77] (1), [Et₃PAu(6p2-TU)][61] (2), [Et₃PAu(2-TU)][9] (3) and [Ph₃PAu(2-TU)][19] (4). Comparisons can hence be made between these complexes for the thiolate group. Table 6.2.8 shows the intramolecular bond distances involved.

Table 6.2.8: *Bond Distances (Å) For The Thiouracilate Moiety.*

	[Cycl₃PAu(6p2-TU)]	1	2	3	4
S(2)-C(2)	1.72(1)	1.73(1)	1.71(2), 1.74(2)	1.72(1)	1.722(8), 1.765(7)
N(1)-C(2)	1.28(1)	1.29(1)	1.33(2), 1.30(2)	1.31(1)	1.33(1), 1.29(1)
N(1)-C(6)	1.34(1)	1.37(1)	1.37(2), 1.38(2)	1.37(1)	1.37(1), 1.39(1)
N(3)-C(2)	1.37(1)	1.35(1)	1.37(2), 1.36(2)	1.35(1)	1.36(1), 1.34(1)
N(3)-C(4)	1.37(1)	1.40(1)	1.43(2), 1.36(2)	1.38(1)	1.37(1), 1.40(1)
C(4)-C(5)	1.42(2)	1.39(1)	1.43(2), 1.39(2)	1.40(1)	1.41(1), 1.41(5)
C(4)-O(4)	1.23(1)	1.23(1)	1.25(2), 1.23(2)	1.24(1)	1.25(1), 1.24(1)
C(5)-C(6)	1.34(2)	1.34(2)	1.33(2), 1.35(2)	1.35(2)	1.35(1), 1.34(1)

It is evident from Table 6.2.8 that most of the constituent distances are equivalent within standard deviation between the three complexes (both [Et₃PAu(6p2-TU)] and [Ph₃PAu(2-TU)] contained two molecules each in their asymmetric crystallographic units). The electron density around the ring is also identical, with C(4)–O(4) and C(5)–C(6) possessing the expected double bond character in all the structures. This suggests that the internal structure of ligands based on 2-thiouracilate is independent of the nature of the phosphine group and of the alkyl groups

external to the aromatic system. Mean plane calculations show that the six atoms of the thionucleobase in [Cycl$_3$PAu(6p2-TU)] form a planar system, with a mean deviation of 0.01(1) Å. The O(4), C(61) and S(2) atoms lie out of the plane by 0.0583, 0.0760 and 0.0235 Å, respectively.

6.3 *Cone-angle correlation for triorganophosphinegold(I) thiolates*

As discussed in Chapter 3, the cone-angle is a parameter that quantifies the steric effect of bulky phosphine groups. Triorganophosphinegold(I) thiolates of the general formula [R$_3$PAu(SR')], where the SR' group is a thionucleobase derivative, contain two bulky ligands, as the thiolate moiety can have significant size. The cone-angle correlation study for triorganophosphinegold(I) chlorides indicated that the P–Au bond distance in these complexes is invariant when the individual molecules crystallize as discrete molecules, i.e. with no significant intermolecular interactions such as close Au...Au contacts. However, the presence of another bulky ligand bound to the gold centre may cause a variation in the P–Au values in a series of complexes, or result in noticeable trends in the Au–S or P–Au–S chromophores.

Table 6.3.1 shows the important intramolecular parameters for a representative selection of triorganophosphinegold(I) thiolates reported in the literature. No significant Au...Au interactions were reported for any of these complexes. The cone-angles for Et$_3$P, Ph$_3$P, Cycl$_3$P and (*o*-Tol)$_3$P are 132, 145, 170 and 194 ° respectively[49], and the complexes are listed in Table 6.3.1 in order of increasing cone angle. The P–Au bond distance ranges in length from 2.248(2) to 2.255(5) Å for the Et$_3$P complexes, 2.237(2) to 2.260(3) Å for Ph$_3$P, 2.244(3) to 2.292(3) Å for Cycl$_3$P and 2.239(2) Å for [(*o*-Tol)$_3$PAu(6-MP)]. Not considering the value for [Ph$_3$PAu(6-MP)], the values for the other Ph$_3$P complexes are all equivalent within standard deviation, and this is also the case for the two Et$_3$P complexes. The P–Au range for the Cycl$_3$P complexes appears large; however, [Cycl$_3$PAu(2mba)] displays intermolecular hydrogen bonding, and 1-methyl-2-mercaptoimidazole is not a true thionucleobase derivative. Notable is that these two complexes possess no close Au...N interactions. Also notable is that the Au...N contacts for [Ph$_3$PAu(6-MP)] and [(*o*-Tol)$_3$PAu(6-MP)], which display the shortest P–Au

Table 6.3.1: *Intramolecular Parameters Of The P–Au–S Chromophore.*

Complex	Au–P (Å)	Au–S (Å)	P–Au–S (°)	Au...N (Å)	Ref.
[Et$_3$PAu(2-TU)]	2.248(2)	2.310(2)	176.9(1)	3.113(2)	[9]
[Et$_3$PAu(6p2-TU)]	2.249(5)	2.328(4)	175.0(2)	3.12(1)	[61]
	2.255(5)	2.314(5)	176.9(2)	3.11(1)	
[Ph$_3$PAu(2-TU)]	2.248(2)	2.296(2)	175.4(2)	3.23(1)	[19]
	2.248(2)	2.300(2)	177.0(2)	3.13(1)	
[Ph$_3$PAu(2-pymS)]	2.253(2)	2.310(3)	174.7(1)	2.951(8)	[62]
[Ph$_3$PAuL^1]	2.256(2)	2.308(2)	178.6(2)	3.312(4)	[79]
[Ph$_3$PAu(2-pyS)]	2.258(1)	2.297(2)	177.9(1)	3.118(4)	[62]
[Ph$_3$PAuL^2]	2.258(2)	2.299(2)	176.43(8)	3.414(4)	[80]
[Ph$_3$PAu(S-C$_6$H$_5$)]	2.259(2)	2.296(2)	179.12(7)	-	[81]
	2.258(2)	2.302(2)	175.79(6)	-	
[Ph$_3$PAu(S-2,4,6-C$_6$H$_2$Me$_3$)]	2.255(2)	2.284(2)	175.24(7)	-	[81]
[Ph$_3$PAu(S-2,4,6-C$_6$H$_2$Et$_3$)]	2.260(3)	2.288(4)	176.2(1)	-	[81]
[Ph$_3$PAu(S-2,4,6-C$_6$H$_2$iPr$_3$)]	2.255(2)	2.284(2)	176.35(5)	-	[81]
[Ph$_3$PAu(6-MP)]	2.237(2)	2.287(1)	173.71(6)	2.884(5)	This work
[Cycl$_3$PAu(2mba)]	2.271(1)	2.313(1)	176.8(1)	-	[62]
[Cycl$_3$PAuL^3]	2.292(3)	2.330(3)	172.0(1)	3.641(5)	[82]
[Cycl$_3$PAu(6m2-TU)]	2.244(3)	2.299(3)	176.1(1)	3.095(8)	[77]
[Cycl$_3$PAu(6p2-TU)]	2.248(3)	2.302(3)	177.6(1)	3.061(9)	This work
[(o-Tol)$_3$PAu(6-MP)]	2.239(2)	2.266(2)	177.03(8)	2.860(7)	This work

Note: L^{1}H = 8-mercaptotheophylline, L^{2}H = 2-mercaptobenzoxazole and L^{3}H = 1-methyl-2-mercaptoimidazole.

distances, are significantly shorter than in the other complexes. Hence, the P–Au bond distance appears to be independent of the cone-angle for those complexes containing six-membered aromatic thionucleobase derivatives.

The Au–S bond distance shows a greater variation between the complexes, with a range extending from 2.266(2) to 2.330(3) Å. However, the variation is not related to the size of the phosphine cone-angle, nor does it appear to depend on the size of the thiolate e.g. in the series represented by the complexes of the general formula $[Ph_3PAu(S-2,4,6-C_6H_2R_3)]$[81] where R = H, Me, Et or iPr, the $2,4,6-C_6H_2i$Pr$_3$ ligand would intuitively have the larger steric effects, but the C_6H_5 ligand gives rise to the longest Au–S bond in the resultant complexes. The P–Au–S bond angle displays the range of values 172.0(1) to 179.12(7)°. These values also appear to be independent of the bulkiness of the two ligands bound to the gold. The Au...N intramolecular contact varies largely in size, but maintains a relatively narrow range of 3.061(9) to 3.23(1) Å when the thiolate is a derivative of 2-thiouracil.

The conclusions from the analysis of monodentate triorganophosphinegold(I) thiolates based on thionucleobase related moieties are as follows: the linearity of the P–Au–S moiety is largely unaffected by the nature of the phosphine or thiolate bound to the gold centre; the P–Au and Au–S bond distances are independent of the cone-angle of the phosphine, but can be affected by the nature of the coordinated thiolate; and the Au...N interaction is of a secondary nature. The intramolecular parameters of the P–Au–S are thus not determined by steric factors but are more likely determined by the electronic effects of the coordinating thiolate.

CHAPTER 7

Assessment of Anti-Arthritic Activity

The effectiveness of the complexes described in this thesis against rheumatoid arthritis was determined via *in vivo* biological testing. The assessment was performed by Dr. M.W. Whitehouse and co-workers at the Department of Pathology, The University of Adelaide.

The complexes were tested on both male and female Dark Agouti rats. The choice of these rodents is based on the knowledge that Dark Agouti rats possess an immune response to rheumatoid arthritis which resembles closely that of humans, and this particular breed has been found to be sensitive to gold-based drugs. Hence, any positive results obtained may be extrapolated to give justification for later testing on humans.

Tests are continuing at the time of writing, but some interesting results have already been obtained for a selection of complexes. The protocol of testing involves injection of an arthritogen into the hind leg to induce swelling in the tail base and hind quarter joints. In a preliminary trial, the complex [Ph$_3$PAu(6-MP)], as 100 mg in saline solution, was co-administered with the arthritogen as a single dose to a female specimen. 6-mercaptopurine (6MPH), Auranofin and [Au(CN)$_2$]$^-$ were similarly injected and assayed against an untreated specimen. The results are summarized in Table 7.1.

The untreated specimen, injected only with arthritogen, suffered weight loss and a significant increase in swelling in the hind quarters, an obviously adverse reaction. By comparison, the other complexes produced greater than 50% less swelling, indicating the complexes were

Table 7.1: *Biological Data For Female Dark Agouti Rats After Anti-arthritic Treatment.*

Complex	milligram dose	Δweight (g)	Δpaw swelling (mm)
[Ph$_3$PAu(6-MP)]	100	+09	0.37
6MPH	25	+09	0.51
Auranofin	100	+03	0.71
[Au(CN)$_2$]$^-$	20	+14	0.10
Untreated	-	-11	1.83

negating the effects of the arthritogen to a large extent. [Au(CN)$_2$]$^-$ was most successful, being the species mentioned in Chapter 1 as being perhaps the main active species in the inflammation reduction process. [Ph$_3$PAu(6-MP)] leads to only half the swelling than for Auranofin in these trials, and to an increase in weight, so that the rat is generally healthier. Auranofin has also been observed to be toxic to specimens when given as multiple doses[8]. Therefore [Ph$_3$PAu(6-MP)], on the basis of these results, appears to be more successful than Auranofin in treating rheumatoid arthritis, at least in this model. 6-mercaptopurine itself also appears to be beneficial.

Three other complexes have been tested via eight regular doses after initial arthritogen injection. The results are given in Table 7.2.

Table 7.2: *Biological Data For Female Dark Agouti Rats After Anti-arthritic Treatment.*

Complex	milligram dose	Δweight (g)	Δpaw swelling (mm)	incidence of disease	Rating
[Et$_3$PAu(6-MP)]	10	-09	0.45	0/3	+
[Cycl$_3$PAu(6-MP)]	10	-05	0.08	0/3	+
[(*m*-Tol)$_3$PAu(6-MP)]	10	-17	1.07	2/3	+3
Untreated	-	-19	1.69	-	+4

Incidence of disease indicates how many specimens of the three rats tested for each complex acquired the symptoms of arthritis. Thus it is evident from qualitative analysis of Table 7.2 that both [Et$_3$PAu(6-MP)] and [Cycl$_3$PAu(6-MP)] are very efficient at combatting the disease. However, the associated weight loss indicates that some side effects are present which are clearly detrimental to the health of the rats. The effectiveness of each complex was determined via a qualitative rating system[8], indicating severity of disease, compared simultaneously with the results obtained from the standard, aurothiomalate. A number of factors were assessed, including weight, overall health of the rat and the effect on the swelling. From the same testing protocol, Auranofin receives a rating of +, so [Et$_3$PAu(6-MP)] and [Cycl$_3$PAu(6-MP)] are comparable with this complex. [(m-Tol)$_3$PAu(6-MP)] evidently has little effect on swelling and produces a significant weight loss, hence a rating of +3, only slightly more effective than no treatment at all. On the same scale, [Ph$_3$PAu(6-MP)] would receive a rating of + or even 0.

Some interesting observations can hence be made in terms of a tentative structure/activity relationship. 6-mercaptopurine and its complexes appear to have a significant effect on arthritic swelling; possibly the solubility characteristics of this ligand provide for a comparatively large quantity of gold to be transferred to the site of action[8]. Comparisons with triorganophosphinegold(I) thiouracilates with the same phosphine show an improvement in activity with the change in thiolate e.g. [Ph$_3$PAu(2-TU)] and [Et$_3$PAu(2-TU)] have ratings of +2 and +3 respectively[8,9]. The triphenylphosphine ligand also appears to be the best phosphine in terms of both activity and toxicity (roughly associated with weight loss); the addition of a methyl group, as in [(m-Tol)$_3$PAu(6-MP)], gives a significant decrease in the efficiency of treatment. This difference might be related to the comparative solubilities of the phosphine ligands[8]. Generally, the effectiveness of the complexes is in the order of Ph$_3$P > Cycl$_3$P > Et$_3$P > (m-Tol)$_3$P, in accordance with earlier results[9,10].

The combination of Ph$_3$P and 6-MPH thus appears to possess suitable characteristics for an effective gold(I) complex which could be utilized in the treatment of rheumatoid arthritis. This is at variance with the structure of the Et$_3$P-containing drug Auranofin, but the effectiveness of

$[Ph_3PAu(6\text{-}MP)]$ is promising. Further work is continuing on the other complexes, to possibly result in an improved understanding of any structure/activity relationship that exists for triorganophosphinegold(I) thiolates.

CHAPTER 8

Conclusion

The aim of the work presented in this thesis was to synthesize a range of novel triorganophosphinegold(I) complexes containing the 6-mercaptopurinate ligand and a variety of phosphines, with possible applications in the treatment of rheumatoid arthritis. Complexes of the type [R_3PAu(6-MP)] (where R_3P = Et_3P, $Cycl_3$P, $PhMe_2$P, Ph_3P, (o-Tol)$_3$P, (m-Tol)$_3$P or (p-Tol)$_3$P), [(Ph_2P(CH_2)$_n$PPh_2)(AuCl)(Au(6-MP))] (where n = 2 or 3), and [(Ph_2P(CH_2)$_n$PPh_2)(Au(6-MP))$_2$] (where n = 1, 2 or 3) were prepared from the corresponding triorganophosphinegold(I) chloride precursors via the metathetical reaction with base and 6-mercaptopurine in the appropriate molar quantities, as described in Chapter 2. The composition and purity of the samples was determined from microanalytical and spectroscopic evidence.

The triorganophosphinegold(I) chloride and triorganophosphinegold(I) 6-mercaptopurinate complexes were characterized using the techniques of infrared and multinuclear nuclear magnetic resonance (nmr) spectroscopy (^{1}H and ^{13}C, and ^{31}P for the 6-MP complexes), and for the 6-mercaptopurinate complexes by Fast Atom Bombardment - mass spectroscopy (FAB-MS). Infrared data obtained for these complexes indicated complex formation via the appearance of both 6-mercaptopurine and phosphine absorption peaks in the spectra, and by alteration of the frequencies of the thioamide chromophore. Absorptions of the phosphine moieties were found to be independent of the presence of the purine moiety.

The resonances and integration found in the ^{1}H nmr spectra of the complexes are consistent with the proposed stoichiometries. The chemical shifts of the H^2 and H^8 proton resonances showed little variation with complexation. The ^{13}C nmr spectra revealed that the C^5 and C^8 nuclei were the most sensitive to, and thus the most indicative of, complexation. ^{31}P nmr spectra showed single signals in all the spectra, which suggested that, for the complexes with the general formula [(Ph$_2$P(CH$_2$)$_n$PPh$_2$)(AuCl)(Au(6-MP))] (where n = 2 or 3), the two independent phosphorus atoms possess the same resonance frequency. Low temperature nmr studies on one of these complexes revealed two signals, thus suggesting the ligands are fluctional at ambient temperature.

The FAB-MS studies of the complexes revealed the occurrence of high nuclearity phosphorus-gold(I)-sulphur clusters in most of the complexes, consistent with the observations for other triorganophosphinegold(I) thiolates. The molecular ion was more commonly observed for the complexes of the type [R$_3$PAu(6-MP)], but the aggregate containing two gold atoms to one 6-mercaptopurinate fragment was observed in high abundance for the complexes based on the dppm, dppe and dppp phosphines also. No otherwise significant trends were observed for the latter series. The combined spectroscopic evidence suggested product formation in all cases, with no significant differences between the complexes.

Single crystal X-ray structure determinations were performed on the complexes [PhMe$_2$PAuCl], [Ph$_3$PAu(6-MP)].C$_2$H$_5$OH, [(o-Tol)$_3$PAu(6-MP)].C$_2$H$_5$OH and [Cycl$_3$PAu(6p2-TU)]. The studies all revealed the near linear P–Au–Cl or S chromophore expected from analogous examples found in the literature. The results from the analysis of [PhMe$_2$PAuCl] were used in a study to compare the phosphine cone angle (θ) and a new quantity found in the literature, the ligand repulsive energy (E$_R$), with the P–Au and Au–Cl bond lengths for a variety of structurally characterized triorganophosphinegold(I) chloride complexes. The study revealed that the P–Au bond distance was independent of θ for complexes containing no significant gold to gold interactions in the lattice. As expected, the Au–Cl bond length was found to be unrelated to θ and probably dependent on electronic factors. The E$_R$ quantity appeared to be no better than θ in determining any steric effects of the

phosphine on the rest of the molecule, despite its more sophisticated calculation. The crystal structure determinations on [Ph₃PAu(6-MP)].C₂H₅OH and [(o-Tol)₃PAu(6-MP)].C₂H₅OH confirm the spectroscopic observations and reveal that the deprotonated 6-mercaptopurine molecule is coordinated in a monodentate mode to the gold(I) atom via the sulphur atom exclusively. The 6-mercaptopurine moiety is planar, and is oriented with the N(7) atom directed to the gold(I) atom; similar observations have been made for other triorganophosphinegold(I) thiolates. The six-membered ring system displays a general shortening of all the constituent bonds upon complexation when compared to the free ligand, an effect that is expected due to the changes in aromaticity. The observed alterations in intramolecular parameters are consistent with the spectroscopic data. The complex [Cycl₃PAu(6p2-TU)] possessed intramolecular characteristics consistent with analogous complexes. The phosphine and thiolate groups in triorganophosphinegold(I) thiolates have no discernable steric effects on the P–Au–S chromophore, the variations in the intramolecular parameters likely being due to electronic or packing factors.

The complexes that were assessed for their anti-arthritic activity were found to be generally effective, with activity ratings rivalling that of the clinically available drug Auranofin. The complex [Ph₃PAu(6-MP)] showed improved activity and less toxicity over Auranofin on a rating scheme based on the severity of rheumatoid arthritis experienced by Dark Agouti rats. The trend of Ph₃P being more active than Cycl₃P which was more active than Et₃P or (m-Tol)₃P for the same thiolate utilized was observed, consistent with earlier results. The 6-mercaptopurine ligand was found to be effective as the thiolate ligand, which is possibly related to its solubility in the bodily fluids.

This project also has further scope in the study of the anti-arthritic activity of these complexes. For instance, specially modified phosphines or 6-mercaptopurinates could be utilized, and the resultant gold(I) complexes investigated to determine what effects structural alterations have on the activity of these types of complexes, and possibly lead to a better understanding of the structure / activity relationships.

REFERENCES

1   E.R.T. Tiekink and M.W. Whitehouse, *Chem. Aust.*, **57**, 346-348 (1990).

2   C.K. Mirabelli, R.K.Johnson, L.F. Faucette, C-M. Sung, K. Muirhead and S.T. Crooke, *Can. Res.*, **45**, 32-39 (1985).

3   S.J. Berners-Price, C.K. Mirabelli, R.K.Johnson, M.R. Mattern, F.L. McCabe, L.F. Faucette, C-M. Sung, S-M. Mong, P.J. Sadler and S.T. Crooke, *Can. Res.*, **46**, 5486-5493 (1986).

4   R.V. Parish, *Interdisc. Sci. Rev.*, **17**, 221-228 (1992).

5   G.J. Higby, *Gold Bull.*, **15**, 130-140 (1982).

6   J. Reedijk, A-M.J. Fichtinger-Schepman, A.T. van Oosteron and P. van de Putte, *Struct. Bond.*, **67**, 53-87 (1987).

7   E.M. Kinsch and D.W. Stephan, *Inorg. Chim. Acta*, **91**, 263-267 (1984).

8   M.W. Whitehouse, personal communication.

9   C.S.W. Harker, E.R.T. Tiekink and M.W. Whitehouse, *Inorg. Chim. Acta*, **181**, 23-30 (1991).

10 P.D. Cookson, *Honours Report*, The University of Adelaide, 1991.

11 K.C. Agrawal, K.B. Bears, D. Marcus and H.B. Jonassen, *Proc. Am. Soc. Cancer Res.*, **19**, 23 (1978).

12 S.M. Skinner, J.M. Swatzell and R.W. Lewis, *Res. Comm. Chem. Path. Pharm.*, **19**, 165-168 (1978).

13 E. Dubler and E. Gyr, *Inorg. Chem.*, **27**, 1466-1473 (1988).

14 C. Périgaud, G. Gosselin and J.L. Imbach, *Nucleosides and Nucleotides*, **11**, 903-945 (1992).

15   G.L. Floersheim, K. Brune and K. Seiler, *Agents and Actions*, **3**, 24-27 (1973).

16   M.P. Arizti, A. Garcia-Orad, F. Sommer, L. Silvestro, P. Massiot, P. Chevallier, J.M. Gutiérrez-Zorrilla, E. Colacio, M. M. de Pancorbo and H. Tapiero, *Anticancer Res.*, **11**, 625-628 (1991).

17   M.P. Arizti, A. Garcia-Orad, J.M. Gutiérrez-Zorrilla, E. Còlacio and M. M. de Pancorbo, *Metal Ions in Biology and Medicine*, 385-389, P. Collery, L.A. Poirier, M. Manfait and J.C. Etienne (Eds.), John Libbey Eurotext, Paris, 1990.

18   H. Schmidbaur and K.C. Dash, *Adv. Inorg. Chem. Radiochem.*, **25**, 239-266 (1982).

19   B.F. Hoskins, L. Zhenrong and E.R.T. Tiekink, *Inorg. Chim. Acta*, **158**, 7-8 (1989).

20   A.K. Al-Sa'ady, C.A. McAuliffe, R.V. Parish and J.A. Sandbank, *Inorg. Synth.*, **23**, 191-195 (1985).

21   S.J. Berners-Price and P.J. Sadler, *Inorg. Chem.*, **25**, 3822-3827 (1986).

22   B.P. Block, *Inorg. Synth.*, **4**, 14-16 (1953).

23   *Aldrich Catalog Handbook of Fine Chemicals*, p.1224, 1992-1993.

24   L. Malatesta, L. Naldini, G. Simonetta and F. Cariati, *Coord. Chem. Rev.*, **1**, 255-262 (1966).

25   C.S.W. Harker and E.R.T. Tiekink, *Acta Cryst.*, **C46**, 1546-1547 (1990).

26   H. Schmidbaur, A. Wohlleben, F. Wagner, O. Orama and G. Huttner, *Chem. Ber.*, **110**, 1748-1754 (1977).

27   D.S. Eggleston, D.F. Chodosh, G.R. Girard and D.T. Hill, *Inorg. Chim. Acta*, **108**, 221-226 (1985).

28   C.K. Mirabelli, D.T. Hill, L.F. Faucette, F.L. McCabe, G.R. Girard, D.B. Bryan, B.M. Sutton, J.O. Bartus, S.T. Crooke and R.K. Johnson, *J. Med. Chem.*, **30**, 2181-2190 (1987).

29   G.M. Sheldrick, SHELXS86: Program for the Automatic Solution of Crystal Structures, Göttingen, Germany (1986).

30   teXsan, Crystal Structure Analysis Package of the Molecular Structure Corporation, Texas, U.S.A. (1992).

31   N. Walker and D. Stuart, *Acta Cryst.*, **A39**, 158-166 (1983).

32   S. Attar, W.H. Bearden, N.W. Alcock, E.C. Alyea and J.H. Nelson, *Inorg. Chem.*, **29**, 425-433 (1990).

33   C.A. McAuliffe, R.V. Parish and P.D. Randall, *J. Chem. Soc., Dalton Trans.*, 1730-1735 (1979).

34   D.H. Williams and I. Fleming, *Spectroscopic Methods in Organic Chemistry*, McGraw-Hill Book Co., 4th Ed., 1989.

35   A.D. Cross, *Introduction to Practical Infrared Spectroscopy*, Butterworths Publications Ltd., 1960.

36   C.J. Pouchert, *The Aldrich Library of Infrared Spectra*, Aldrich Chemical Co., 2nd Ed., 1975.

37   R. Cini, A. Cinquantini, M. Sabat and L.G. Marzilli, *Inorg. Chem.*, **24**, 3903-3908 (1985).

38   C.J. Pouchert and J.R. Campbell, *The Aldrich Library of ^1H NMR Spectra*, Aldrich Chemical Co., 1974.

39   M. Akhtar, P.D. Ellis, A.G. MacDiarmid and J.D. Odom, *Inorg. Chem.*, **11**, 2917-2921 (1972).

40   L.F. Johnson and W.C. Jankowski, *Carbon-13 NMR Spectra: A Collection of Assigned, Coded and Indexed Spectra*, Wiley-Interscience, 1972.

41   E. Cariati, L. Ganadu, L. Naldini and S. Seneci, *Gazz. Chim. Ital.*, **109**, 181-185, (1979).

42   B.E. Mann, *J. Chem. Soc., Perkin II*, 30-34 (1972).

43   J. Schrami, M. Capka and V. Blechta, *Mag. Res. Chem.*, **30**, 544-547 (1992).

44   T. Hahn (Ed.), *International Tables For Crystallography*, D. Reidel Pub. Co., 1983.

45   C.K. Johnson, ORTEP II, Report 5316, Oak Ridge National Laboratory, Tennessee, U.S.A. (1976).

46   H. Schmidbaur, *Gold Bull.*, **23**, 11-21 (1990).

47   N.C. Baenziger, W.E. Bennett and D.M. Soboroff, *Acta Cryst.*, **B32**, 962-963 (1976).

48   E.R.T. Tiekink, *Acta Cryst.*, **C45**, 1233-1234 (1989).

49   C.A. Tolman, *Chem. Rev.*, **77**, 313-348 (1977).

50   G. Wilkinson (Ed.), *Comprehensive Coordination Chemistry*, Ch.14, Pergamon Press, 1st Ed. (1987).

51   T.L. Brown, *Inorg. Chem.*, **31**, 1286-1294 (1992).

52   J.A. Muir, M.M. Muir, L.B. Pulgar, P.G. Jones and G.M. Sheldrick, *Acta Cryst.*, **C41**, 1174-1176 (1985).

53   M.M. Muir, S.I. Cuadrado and J.A. Muir, *Acta Cryst.*, **C47**, 1072-1074 (1991).

54   P.B. Hitchcock and P.L. Pye, *J. Chem. Soc., Dalton Trans.*, 1457-1460 (1977).

55   C.S.W. Harker and E.R.T. Tiekink, *Acta Cryst.*, **C46**, 1546-1547 (1990).

56   C.S.W. Harker and E.R.T. Tiekink, *Acta Cryst.*, **C47**, 878-879 (1991).

57   E. Sletten, J. Sletten and L.H. Jensen, *Acta Cryst.*, **B25**, 1330-1338 (1969).

58   G.M. Brown, *Acta Cryst.*, **B25**, 1338-1353 (1969).

59   D. Lichtenberg, F. Bergmann and Z. Neiman, *Isr. J. Chem.*, **10**, 805-817 (1972).

60   P.D. Cookson and E.R.T. Tiekink, *J. Coord. Chem.*, **26**, 313-320 (1992).

61   P.D. Cookson and E.R.T. Tiekink, *J. Cryst. Spectro. Res.*, **23**, 231-234 (1993).

62   P.D. Cookson and E.R.T. Tiekink, *J. Chem. Soc., Dalton Trans.*, 259-263 (1993).

63   B. Singh and K.P. Thakur, *J. Inorg. Nucl. Chem.*, **36**, 1735-1737 (1974).

64   J. Brigando, D. Colaitis and M. Morel, *Bull. Soc. Chim. Fr.*, **10**, 3440-3445 (1969).

65   R. Barbieri, E. Rivarola, F. Di Bianca and F. Huber, *Inorg. Chim. Acta*, **57**, 37-41 (1982).

66   C.N.R. Rao and R. Venkatarughavan, *Spectrochim. Acta*, **18**, 541-547 (1962).

67   L-M. Twanmoh, H-B. Wood, Jr. and J.S. Driscoll, *J. Heterocyclic Chem.*, **10**, 187-190 (1973).

68   N. Kottmair and W. Beck, *Inorg. Chim. Acta*, **34**, 137-144 (1979).

69   C.N. Banwell, *Fundamentals of Molecular Spectroscopy*, McGraw-Hill Book Co., 3rd Ed., 1983.

70   E. Breitmaier and W. Voetter, *Tetrahedron*, **30**, 3941-3943 (1974).

71   G.S. Reddy and R. Schmutzler, *Inorg. Chem.*, **6**, 823-830 (1967).

72   V. Parthasarathi, P.T. Beurskens and H.J.B. Slot, *Acta Cryst.*, **A39**, 860-864 (1983).

73   E. Shefter, *J. Pharmaceutical Sciences*, **57**, 1157-1162 (1968).

74   E. Sletten and A. Apeland, *Acta Cryst.*, **B31**, 2019-2022 (1975).

75   E.A.H. Griffith and E.L. Amma, *J. Chem. Soc., Chem. Comm.*, 1013-1014 (1979).

76   H.I. Heitner and S.J. Lippard, *Inorg. Chem.*, **13**, 815-822 (1974).

77   P.D. Cookson and E.R.T. Tiekink, in press

78   N. Okabe, T. Fujiwara, Y. Yamagata and K. Tomita, *Bull. Chem. Soc. Jpn.*, **56**, 1543 (1983).

79   E. Colacio, A. Romerosa, J. Ruiz, P. Román, J.M. Gutiérrez-Zorrilla, A. Vegas and M. Martinez-Ripoll, *Inorg. Chem.*, **30**, 3743 (1991).

80   M.M. Muir, S.I. Cuadrado and J.A. Muir, *Acta Cryst.*, **C45**, 1420, (1989).

81   M. Nakamoto, W. Hiller and H. Schmibaur, *Chem. Ber.*, **126**, 605-610 (1993).

82   F. Bonati, A. Burini, B.R. Pietroni, E. Giorgini and B. Bovio, *J. Organomet. Chem.*, **344**, 119-135 (1988).

APPENDIX

Structure Factor Tables

Table A1: *Observed And Calculated Structure Factors For The [PhMe$_2$PAuCl] Complex.*

10|F|o vs 10|F|c

Band 1

h k l Fo Fc sigF	h k l Fo Fc sigF	h k l Fo Fc sigF	h k l Fo Fc sigF	h k l Fo Fc sigF	h k l Fo Fc sigF
0 0 2 1198 1186 9	0 6 9 309 353 36	0 14 6 804 845 24	1 4 1 1274 1239 14	1 10 2 1909 1958 19	1 18 4 236 201 39
0 0 4 3571 3498 22	0 7 1 864 835 17	0 15 1 1283 1277 21	1 4 2 707 703 16	1 10 3 525 543 21	1 18 5 343 309 29
0 0 8 536 464 18	0 7 2 562 566 15	0 15 4 622 620 17	1 4 3 977 998 19	1 10 4 472 467 18	1 19 4 472 454 21
0 1 1 1824 1802 10	0 7 3 1690 1717 16	0 15 5 1063 1096 19	1 4 4 1978 1966 15	1 10 5 1442 1434 30	1 20 0 634 624 15
0 1 2 1600 1537 10	0 7 4 1344 1344 22	0 15 7 441 478 42	1 4 5 1194 1142 15	1 10 6 637 605 24	1 20 1 386 428 23
0 1 3 3772 3643 21	0 7 5 1608 1636 23	0 16 0 283 334 23	1 4 6 382 367 17	1 10 7 689 683 18	2 0 0 5003 4977 25
0 1 4 564 502 12	0 7 6 1302 1346 25	0 16 1 1228 1242 30	1 4 7 939 962 22	1 10 9 675 682 35	2 0 1 1935 1861 11
0 1 5 1328 1234 14	0 7 7 1150 1142 21	0 16 2 966 946 23	1 4 9 840 918 24	1 11 0 1083 1051 19	2 0 2 1159 1290 10
0 1 6 1697 1518 21	0 7 8 562 615 19	0 16 3 408 453 31	1 5 1 925 919 22	1 11 1 1411 1395 25	2 0 3 323 302 9
0 1 7 1987 1896 24	0 7 9 866 884 24	0 16 5 663 693 18	1 5 2 1204 1180 20	1 11 2 642 629 18	2 0 4 2529 2689 16
0 1 9 930 900 22	0 7 10 497 527 30	0 16 7 368 335 35	1 5 3 549 553 14	1 11 3 576 642 21	2 0 5 2120 2188 16
0 1 10 839 796 20	0 8 0 1790 1777 16	0 17 4 910 918 19	1 5 4 823 799 16	1 11 4 528 526 24	2 0 6 359 359 19
0 2 0 2059 2085 13	0 8 1 1079 1099 23	0 18 0 500 561 14	1 5 5 1343 1349 16	1 11 5 1466 1536 30	2 0 7 1134 1068 21
0 2 1 1465 1406 12	0 8 2 2887 2985 24	0 18 1 705 718 16	1 5 6 1959 2017 18	1 11 6 599 605 18	2 0 8 550 503 19
0 2 2 665 658 10	0 8 3 1896 1886 22	0 18 2 699 709 21	1 5 7 521 558 23	1 11 7 413 490 40	2 0 9 770 738 19
0 2 3 3659 3550 20	0 8 4 429 456 15	0 18 3 414 452 32	1 5 8 344 306 27	1 11 9 609 614 28	2 0 11 457 414 41
0 2 4 1952 1872 14	0 8 5 652 693 14	0 18 5 513 556 31	1 5 9 722 804 26	1 12 0 453 439 16	2 1 0 933 931 7
0 2 6 1009 956 17	0 8 6 1176 1172 20	0 19 1 752 750 16	1 5 10 977 996 21	1 12 1 637 627 14	2 1 1 1597 1569 11
0 2 7 1346 1350 19	0 8 7 798 841 19	0 20 2 796 804 20	1 6 0 640 626 13	1 12 2 2058 2025 20	2 1 2 3643 3877 21
0 2 9 1234 1235 26	0 8 9 459 525 40	1 0 1 1942 2226 11	1 6 1 2200 2185 21	1 12 3 784 810 18	2 1 3 2405 2443 15
0 3 1 779 758 15	0 9 1 1408 1376 17	1 0 2 1578 1588 10	1 6 2 2137 2191 21	1 12 4 579 533 16	2 1 4 252 257 16
0 3 2 741 756 14	0 9 2 899 931 20	1 0 3 2852 2878 16	1 6 3 1979 1978 21	1 12 5 484 498 20	2 1 5 992 900 16
0 3 3 1136 1135 14	0 9 3 1281 1321 25	1 0 4 734 738 14	1 6 4 953 966 17	1 12 6 768 787 17	2 1 6 1361 1342 18
0 3 4 262 249 13	0 9 4 682 661 17	1 0 6 295 307 21	1 6 5 859 856 22	1 13 0 304 267 23	2 1 7 1626 1582 20
0 3 5 351 342 13	0 9 5 1642 1676 19	1 0 7 1624 1545 19	1 6 7 1110 1125 22	1 13 1 1076 1041 21	2 1 9 643 565 21
0 3 6 2348 2366 17	0 9 6 1390 1339 29	1 0 8 850 788 20	1 6 8 725 682 18	1 13 2 269 247 28	2 1 10 506 522 32
0 3 9 397 450 29	0 9 7 399 386 25	1 0 9 1136 1097 29	1 6 9 471 498 27	1 13 3 414 405 21	2 1 11 478 505 40
0 3 10 1340 1422 29	0 9 8 581 623 21	1 1 1 2278 2156 16	1 7 0 607 555 14	1 13 4 1008 1034 24	2 2 0 1594 1581 10
0 4 0 3751 3809 21	0 9 9 733 748 28	1 1 2 2341 2240 13	1 7 1 2371 2338 18	1 13 5 750 743 18	2 2 1 1597 1612 12
0 4 1 1790 1772 13	0 9 10 575 600 41	1 1 3 1600 1537 12	1 7 2 961 1000 24	1 13 6 369 332 29	2 2 2 958 946 15
0 4 2 1413 1420 12	0 10 0 1400 1392 23	1 1 4 746 691 14	1 7 3 1828 1857 23	1 13 8 988 1021 22	2 2 3 2222 2230 15
0 4 3 1559 1561 12	0 10 1 1455 1422 24	1 1 5 851 791 16	1 7 4 1466 1487 23	1 14 1 1591 1507 20	2 2 4 1998 1977 15
0 4 4 1846 1873 18	0 10 2 1504 1599 24	1 1 6 2321 2204 18	1 7 5 1221 1224 19	1 14 2 257 204 30	2 2 5 806 785 17
0 4 5 355 379 18	0 10 3 1197 1264 26	1 1 7 1181 1102 20	1 7 6 1645 1639 19	1 14 3 593 591 16	2 2 6 431 440 16
0 4 6 700 689 15	0 10 4 796 820 19	1 1 10 1396 1347 30	1 7 7 607 565 23	1 14 5 1063 1096 27	2 2 7 1121 1096 22
0 4 7 1040 1032 20	0 10 5 1079 1101 22	1 2 0 4364 4311 22	1 7 8 1016 1054 19	1 14 6 530 459 22	2 2 8 1277 1198 23
0 4 8 542 522 18	0 10 6 1032 1042 24	1 2 1 2151 2156 14	1 7 10 693 740 35	1 14 7 359 368 36	2 2 9 1027 992 21
0 5 1 2143 2178 15	0 11 1 603 568 15	1 2 2 1423 1376 14	1 8 0 2062 2091 17	1 15 0 591 584 15	2 2 11 446 468 42
0 5 2 258 256 14	0 11 3 687 683 18	1 2 4 2451 2306 16	1 8 1 2530 2465 23	1 15 1 825 838 18	2 3 0 156 125 16
0 5 3 2366 2459 19	0 11 4 1314 1316 29	1 2 5 1009 918 15	1 8 2 892 926 19	1 15 3 392 369 22	2 3 1 1689 1667 13
0 5 4 1561 1563 14	0 11 8 1136 1172 25	1 2 6 819 759 19	1 8 3 1189 1198 25	1 15 4 1032 1016 25	2 3 2 1252 1234 15
0 5 5 416 397 12	0 12 0 538 556 19	1 2 7 816 731 19	1 8 4 1909 1857 18	1 15 5 683 713 18	2 3 3 1017 973 14
0 5 6 850 859 18	0 12 1 1182 1167 27	1 2 8 650 561 16	1 8 5 1608 1584 26	1 15 7 372 305 35	2 3 4 1346 1282 14
0 5 7 1211 1244 19	0 12 2 921 914 22	1 2 9 414 399 40	1 8 6 756 762 16	1 16 1 745 687 19	2 3 5 1292 1285 16
0 5 8 740 820 17	0 12 5 992 1025 25	1 3 0 423 379 9	1 9 0 556 580 17	1 16 2 1647 1630 21	2 3 6 1900 1809 18
0 5 9 544 575 21	0 12 6 538 349 27	1 3 1 1926 1969 17	1 9 2 742 743 16	1 16 3 605 593 16	2 3 7 510 530 17
0 5 11 476 470 35	0 12 7 623 635 20	1 3 2 1995 1941 17	1 9 3 1406 1457 25	1 16 5 469 521 24	2 3 9 457 439 28
0 6 0 4257 4290 24	0 12 8 382 428 57	1 3 3 2742 2812 16	1 9 4 1579 1559 19	1 16 6 531 543 23	2 3 10 983 1019 22
0 6 1 1765 1760 15	0 13 1 1145 1152 21	1 3 4 831 801 14	1 9 5 727 702 16	1 17 0 624 628 15	2 3 11 501 582 38
0 6 2 866 846 15	0 13 4 939 952 24	1 3 6 364 389 17	1 9 6 337 349 39	1 17 1 966 949 24	2 4 0 2588 2617 16
0 6 3 342 381 14	0 13 5 1111 1160 24	1 3 7 1586 1631 19	1 9 7 1025 1020 19	1 17 4 392 404 26	2 4 1 1265 1267 14
0 6 4 2517 2582 17	0 13 7 525 560 36	1 3 8 824 856 19	1 9 8 1220 1290 28	1 17 5 891 885 21	2 4 2 1517 1484 15
0 6 5 928 954 17	0 13 8 495 528 30	1 3 9 595 636 30	1 9 9 621 648 25	1 18 1 337 306 24	2 4 3 1877 1896 16
0 6 6 393 375 17	0 14 2 2345 2385 27	1 4 0 2436 2419 15	1 10 0 976 968 19	1 18 2 951 891 17	2 4 4 1542 1538 16
0 6 7 925 946 22	0 14 3 474 478 18		1 10 1 579 580 13	1 18 3 334 306 26	2 4 5 996 1014 17

Band 2

h k l Fo Fc sigF	h k l Fo Fc sigF	h k l Fo Fc sigF	h k l Fo Fc sigF
2 4 6 677 741 17	2 10 0 1214 1233 17	3 0 1 812 804 9	3 4 9 982 962 24
2 4 7 748 729 16	2 10 1 1271 1264 18	3 0 2 141 146 15	3 5 0 2088 2054 14
2 4 8 1120 1143 24	2 10 2 1689 1637 19	3 0 3 1480 1716 13	3 5 1 1536 1508 14
2 4 9 382 333 33	2 10 3 770 784 19	3 0 4 2709 3027 17	3 5 2 943 925 17
2 5 0 613 599 16	2 10 4 762 750 19	3 0 6 339 329 21	3 5 3 202 173 30
2 5 1 2308 2336 16	2 10 5 960 975 24	3 0 7 862 899 17	3 5 4 1239 1216 19
2 5 2 2133 2115 17	2 10 6 874 928 21	3 0 8 1798 1867 22	3 5 5 1637 1613 19
2 5 3 2311 2287 18	2 10 7 516 482 24	3 0 9 525 531 26	3 5 6 1075 1013 22
2 5 4 496 502 13	2 11 1 949 930 20	3 0 10 469 373 33	3 5 7 526 485 19
2 5 5 361 336 17	2 11 2 429 442 18	3 1 0 959 959 8	3 5 8 362 368 31
2 5 6 1151 1139 20	2 11 3 1257 1274 21	3 1 1 2761 2829 15	3 5 9 726 726 21
2 5 7 1013 1000 23	2 11 4 999 987 24	3 1 2 2543 2656 16	3 5 10 664 630 26
2 5 8 696 700 17	2 11 5 255 232 35	3 1 3 1740 1768 15	3 6 0 1079 1067 14
2 6 0 3026 3044 19	2 11 7 569 553 23	3 1 4 619 627 13	3 6 1 1255 1251 15
2 6 1 1641 1645 16	2 11 9 411 415 41	3 1 5 2168 2240 17	3 6 2 1374 1403 17
2 6 2 1006 966 17	2 12 1 1042 981 21	3 1 6 1352 1281 18	3 6 3 1951 1903 19
2 6 3 321 270 18	2 12 2 815 800 18	3 1 7 551 528 17	3 6 4 1812 1735 19
2 6 5 2033 1982 18	2 12 6 877 934 21	3 1 9 444 415 30	3 6 6 814 835 20
2 6 6 1324 1321 18	2 12 7 866 876 18	3 1 10 669 667 26	3 6 7 904 887 20
2 6 7 903 869 22	2 12 8 650 651 21	3 1 11 556 530 35	3 6 8 1406 1413 26
2 6 9 905 902 18	2 12 9 425 411 40	3 2 0 1579 1564 10	3 6 9 425 410 34
2 6 10 798 802 19	2 13 0 1546 1492 19	3 2 1 2669 2661 15	3 7 0 1758 1741 15
2 7 0 1531 1567 15	2 13 1 854 825 17	3 2 2 509 494 12	3 7 1 3042 3081 20
2 7 1 546 544 13	2 13 3 522 509 17	3 2 3 1222 1187 17	3 7 2 1707 1711 17
2 7 2 1778 1733 17	2 13 5 1038 1066 25	3 2 4 1455 1529 15	3 7 3 2062 2043 19
2 7 3 1478 1404 18	2 13 8 387 365 33	3 2 5 2141 2168 17	3 7 4 742 729 18
2 7 4 1362 1371 19	2 14 1 1085 1079 21	3 2 6 912 899 21	3 7 5 1039 1088 24
2 7 6 1302 1264 20	2 14 2 1728 1700 21	3 2 7 728 674 16	3 7 6 840 815 20
2 7 7 970 953 19	2 14 3 1038 1055 24	3 2 8 1032 991 20	3 7 7 366 360 28
2 7 8 593 555 21	2 14 5 327 351 31	3 2 9 693 682 21	3 7 8 497 479 26
2 7 9 845 844 19	2 14 6 594 593 21	3 2 10 460 395 34	3 7 10 361 353 49
2 7 10 728 555 28	2 14 7 650 645 24	3 3 0 222 234 12	3 8 0 1524 1547 16
2 8 0 414 429 14	2 15 0 1417 1387 20	3 3 1 1187 1197 12	3 8 1 1954 1989 17
2 8 1 1105 1061 17	2 15 1 421 399 19	3 3 2 3158 3245 20	3 8 2 1203 1211 19
2 8 2 2556 2454 20	2 15 3 379 380 23	3 3 3 1746 1668 17	3 8 3 473 416 17
2 8 3 1658 1648 19	2 15 4 442 463 21	3 3 4 226 248 24	3 8 4 1217 1208 21
2 8 4 1173 1113 20	2 15 5 1086 1055 25	3 3 5 621 587 16	3 8 5 1279 1290 23
2 8 5 633 637 15	2 15 8 823 827 18	3 3 6 1185 1151 19	3 8 6 1512 1477 23
2 8 6 780 770 20	2 16 1 910 914 18	3 3 7 1023 999 24	3 8 8 625 564 23
2 8 7 1222 1184 25	2 16 2 776 743 19	3 3 8 413 357 26	3 8 9 468 460 35
2 8 8 802 789 18	2 16 3 466 448 20	3 4 0 899 884 11	3 8 10 885 930 24
2 8 9 675 665 24	2 16 4 434 430 23	3 4 1 1330 1274 13	3 9 0 1210 1252 17
2 9 0 1851 1896 17	2 16 5 688 645 18	3 4 2 523 508 13	3 9 1 801 827 20
2 9 1 2117 2129 18	2 16 8 814 834 20	3 4 3 648 616 16	3 9 2 1735 1740 19
2 9 2 673 653 17	2 17 1 754 738 19	3 4 6 853 835 16	3 9 3 1715 1702 20
2 9 3 1195 1198 20	2 17 2 266 209 30	3 4 8 877 845 21	3 9 4 971 985 23
2 9 4 1367 1306 20	2 17 4 612 606 17		3 9 5 301 301 31
2 9 5 1238 1257 22	2 17 6 809 726 20		3 9 6 501 443 22
2 9 6 947 926 19	2 18 1 319 292 26		3 9 7 902 910 19
2 9 7 327 313 33	2 18 3 641 618 19		3 9 8 779 733 20
2 9 9 571 520 28	2 18 4 484 476 18		3 9 9 603 587 29
2 9 10 396 406 47	2 18 5 470 473 23		3 10 0 238 249 25
	2 19 0 521 516 17		3 10 1 401 402 17
	2 19 1 591 567 16		3 10 2 1001 1001 21
	2 19 3 328 319 27		3 10 3 948 932 17

Band 3

h k l Fo Fc sigF	h k l Fo Fc sigF	h k l Fo Fc sigF	h k l Fo Fc sigF	h k l Fo Fc sigF
3 10 4 375 382 24	4 0 0 623 587 11	4 6 1 1473 1478 15	4 12 5 382 369 27	5 2 6 546 606 17
3 10 5 820 817 17	4 0 1 2522 2452 15	4 6 2 696 724 15	4 12 6 1170 1208 28	5 2 8 948 927 22
3 10 6 703 708 18	4 0 2 1348 1323 11	4 6 3 224 208 30	4 12 7 733 750 21	5 2 9 538 562 30
3 10 7 1226 1203 29	4 0 3 889 820 12	4 6 4 324 248 24	4 13 0 1691 1709 19	5 3 0 391 408 10

```
 3 10  8  480  413 30    4  0  4  575  613 12    4  6  5 1720 1713 22    4 13  1  623  630 14    5  3  1  912  877 12
 3 10  9  688  695 28    4  0  5 2941 3335 20    4  6  6 1181 1173 25    4 13  2  384  399 21    5  3  2 3040 3041 19
 3 11  0 2221 2289 19    4  0  7 1024 1120 24    4  6  7  781  733 19    4 13  3  573  516 17    5  3  3  701  685 15
 3 11  1  965  922 20    4  0  9 1221 1203 29    4  6  8  430  397 29    4 13  4 1153 1173 25    5  3  4  459  437 20
 3 11  3  492  488 18    4  1  0 1553 1545 11    4  6  9  960  926 22    4 13  5  369  409 29    5  3  5  463  443 21
 3 11  4 1171 1201 23    4  1  1 1878 1874 12    4  6 10  523  573 36    4 13  7  441  433 31    5  3  6 1171 1152 23
 3 11  5  876  885 20    4  1  2 3629 3742 20    4  7  0 2473 2458 17    4 13  8  408  327 38    5  3  7  717  716 16
 3 11  6  350  370 32    4  1  3  656  651 15    4  7  1  341  310 15    4 14  1  585  584 15    5  4  0  229  159 14
 3 12  0  609  611 15    4  1  4  417  404 14    4  7  2 2100 2136 18    4 14  2  354  352 24    5  4  1 1176 1172 13
 3 12  1  948  938 21    4  1  5 1157 1199 18    4  7  3  447  452 18    4 14  3 1610 1594 22    5  4  2  975  921 15
 3 12  2  910  906 17    4  1  6 1498 1540 20    4  7  4 1489 1409 21    4 14  5  285  238 35    5  4  4 1252 1215 22
 3 12  3 1225 1252 22    4  1  7  796  788 20    4  7  5  788  773 17    4 14  7  980  953 20    5  4  5 1476 1444 23
 3 12  4  485  479 20    4  1  8  371  280 31    4  7  6  763  769 19    4 15  0 1807 1812 20    5  4  6  783  775 18
 3 12  6  600  605 21    4  1  9  315  204 43    4  7  7  748  729 18    4 15  1  541  597 17    5  4  7  592  606 20
 3 12  7  780  753 20    4  2  0  554  552 11    4  7  9  860  820 22    4 15  2  476  483 18    5  4  8  978  966 22
 3 13  0  984 1019 21    4  2  1  311  305  9    4  8  0  311  314 17    4 15  3  833  828 20    5  4  9  730  689 23
 3 13  1 1001  995 22    4  2  2  754  686 13    4  8  1  741  728 14    4 15  4 1174 1177 25    5  4 10  422  356 42
 3 13  2  367  355 22    4  2  3  470  448 15    4  8  2  418  371 15    4 16  2  632  647 15    5  5  0 1590 1609 14
 3 13  3 1321 1325 20    4  2  4 2703 2670 21    4  8  3 1779 1752 20    4 16  3  485  460 20    5  5  1 1637 1583 15
 3 13  4  921  925 19    4  2  5 1349 1327 18    4  8  4 1182 1228 23    4 16  6 1078 1059 25    5  5  2  944  904 17
 3 13  5  343  348 30    4  2  6  284  210 26    4  8  5  850  801 20    4 17  1  771  765 19    5  5  3  430  422 17
 3 13  7  419  448 32    4  2  7  624  626 17    4  8  7 1322 1284 28    4 17  2  400  379 22    5  5  5 1146 1107 23
 3 13  8  433  432 37    4  2  8 1569 1580 25    4  8  8 1147 1078 23    4 17  3  957  993 19    5  5  6 1586 1580 24
 3 14  1  602  593 15    4  2  9  683  686 23    4  8  9  708  655 26    4 18  1  376  374 23    5  5  7  716  701 19
 3 14  2  670  650 15    4  3  0 1202 1202 11    4  9  0 3006 3017 20    4 18  2  301  328 30    5  5  9  711  690 24
 3 14  4  304  327 31    4  3  1 2381 2391 15    4  9  1 1744 1813 18    4 18  3  649  643 16    5  6  0  390  365 12
 3 14  5  528  498 21    4  3  2  739  720 16    4  9  2  276  258 24    4 19  0  745  749 17    5  6  1 1756 1706 16
 3 14  6 1221 1227 28    4  3  3  453  466 15    4  9  3 1078 1048 21    4 19  1  379  377 23    5  6  2  525  513 12
 3 14  7  409  380 32    4  3  4 1150 1165 21    4  9  4 1519 1549 22    5  0  0  670  639 12    5  6  3 1605 1667 19
 3 15  0 1094 1055 21    4  3  5 1825 1821 19    4  9  5  576  557 19    5  0  2  163  144 19    5  6  4 1687 1663 22
 3 15  1 1030 1021 22    4  3  6  318  326 25    4  9  7  404  361 30    5  0  3 1258 1181 13    5  6  5  248  223 40
 3 15  2  234  176 34    4  3  7  753  796 17    4  9  8  509  479 30    5  0  4 2340 2484 16    5  6  6  644  615 19
 3 15  3 1100 1055 23    4  3  9  502  452 29    4 10  0  347  367 18    5  0  5  479  587 16    5  6  7  738  754 19
 3 15  4  856  832 20    4  4  0  328  314 10    4 10  1 1502 1593 18    5  0  6  250  229 32    5  6  8 1460 1434 30
 3 15  5  458  408 24    4  4  1 2071 2023 14    4 10  2 1072 1050 20    5  0  8 1809 1978 24    5  7  0 1841 1835 16
 3 15  7  553  556 26    4  4  2 1007  997 16    4 10  3 1090 1081 23    5  1  0  183  212 14    5  7  1 2278 2279 18
 3 16  1  388  449 22    4  4  3 1640 1651 18    4 10  4  659  683 16    5  1  1 2401 2445 14    5  7  2 1893 1934 18
 3 16  2  701  690 16    4  4  4 1489 1437 20    4 10  5  501  488 22    5  1  2 2239 2193 14    5  7  3 1369 1381 20
 3 16  3 1082 1076 25    4  4  5 1369 1363 21    4 10  6 1066 1102 20    5  1  3  896  881 15    5  7  4 1097 1071 23
 3 16  5  349  355 32    4  4  6  736  733 16    4 10  7  415  479 32    5  1  4  775  728 19    5  7  5  984  961 20
 3 16  6  648  612 21    4  4  8 1285 1314 26    4 10  8  493  482 33    5  1  5 1963 2091 19    5  7  7  875  897 19
 3 17  0 1283 1271 21    4  4  9  431  327 33    4 11  0  526  536 14    5  1  6  507  553 16    5  7  8  389  381 33
 3 17  1  468  422 18    4  5  0 1135 1129 13    4 11  1  668  705 14    5  1  7  500  544 22    5  7  9  472  535 32
 3 17  3  234  254 38    4  5  1 1730 1703 14    4 11  2  851  864 17    5  1  8  473  475 27    5  8  0  418  429 14
 3 17  4  984  947 19    4  5  2 2763 2819 19    4 11  3 1439 1375 21    5  1  9  461  469 33    5  8  1 1905 1917 17
 3 17  5  578  576 20    4  5  3  933  946 21    4 11  4  342  312 28    5  2  0  569  612 12    5  8  2  909  934 20
 3 18  2  429  438 21    4  5  4  360  328 23    4 11  7  764  792 20    5  2  1 2574 2579 15    5  8  3  917  955 17
 3 18  3  549  521 18    4  5  5  453  428 20    4 11  9  534  568 36    5  2  2 1200 1170 13    5  8  4  566  566 18
 3 19  0  425  409 20    4  5  6 1312 1283 23    4 12  2  463  450 18    5  2  3 1157 1187 16    5  8  5 1186 1233 27
 3 19  2  389  411 23    4  5  7  465  467 23    4 12  3  272  221 31    5  2  4  972  961 18    5  8  6 1428 1445 27
 3 19  3  437  467 21    4  6  0  913  890 14    4 12  4  338  217 26    5  2  5 2038 1988 21    5  8  8  511  457 31
 5  9  0  926  916 19    6  0  2 1509 1446 13    6  6  2 1020 1022 18    6 12  6  889  890 25    7  3  3 1552 1533 23
 5  9  1  733  788 16    6  0  3  720  697 16    6  6  3  627  612 15    6 13  0 1467 1416 28    7  3  4  679  716 19
 5  9  2 1615 1648 19    6  0  4 1005  970 16    6  6  4 1115 1158 23    6 13  1  370  312 28    7  3  5  533  538 30
 5  9  3 1524 1524 20    6  0  5 2014 2016 25    6  6  5 1336 1321 27    6 13  3  493  478 27    7  3  6  507  515 41
 5  9  4  539  502 19    6  0  7  482  587 24    6  6  6  980  945 23    6 13  4  972  997 22    7  3  7  952  975 26
 5  9  5  551  570 20    6  0  9  682  758 25    6  6  7  575  562 25    6 13  5  668  687 26    7  3  8  411  463 54
 5  9  6  320  292 36    6  1  1 1032 1005 12    6  6  8  425  426 34    6 13  7  515  459 38    7  3  9  630  670 41
 5  9  7 1026 1041 24    6  1  2 2950 3069 18    6  6  9  639  535 29    6 14  0  787  815 19    7  4  0 1394 1409 18
 5  9  9  558  533 33    6  1  3  968  943 14    6  7  0 1314 1314 16    6 14  1  683  724 20    7  4  1 1049 1018 20
 5 10  0  761  758 15    6  1  4  597  569 13    6  7  1  742  730 14    6 14  2  871  863 21    7  4  2  869  808 18
 5 10  1  307  274 22    6  1  5 1018  968 21    6  7  2 1467 1460 18    6 14  3 1117 1109 24    7  4  3  810  790 17
 5 10  2  812  827 16    6  1  6 1040 1170 23    6  7  3 1025 1062 22    6 15  0 1377 1410 30    7  4  4 1421 1441 29
 5 10  3  955 1006 24    6  1  7 1097 1152 20    6  7  4  849  821 19    6 15  1  481  490 28    7  4  5  655  675 26
 5 10  4  578  533 18    6  1  9  591  670 30    6  7  5 1286 1277 26    6 15  3  493  541 30    7  4  6  627  631 34
 5 10  5  525  489 21    6  2  0  480  492 11    6  7  6  495  484 26    6 15  4  857  887 21    7  4  7  437  481 48
 5 10  6  818  856 18    6  2  1 1212 1226 12    6  7  7  999  962 25    6 15  5  479  483 33    7  4  8  526  603 44
 5 10  7  969 1011 25    6  2  2  769  766 14    6  7  9  801  810 26    6 16  1  710  716 21    7  4  9  545  378 43
 5 10  8  460  475 35    6  2  3 1374 1343 15    6  8  0  924  939 18    6 16  2  513  516 27    7  5  0  748  716 16
 5 10  9  435  479 45    6  2  4 1819 1743 19    6  8  1  880  919 21    6 16  3  424  439 32    7  5  1  816  804 17
 5 11  0 2140 2162 19    6  2  5  730  755 18    6  8  2 1312 1334 19    6 16  5  320  287 47    7  5  2  545  495 17
 5 11  4 1352 1410 24    6  2  6  341  415 31    6  8  3 1447 1474 20    6 17  1  433  460 32    7  5  3  573  574 18
 5 11  5  532  509 21    6  2  7  465  468 24    6  8  4 1216 1198 24    6 17  3  613  575 24    7  5  5 1176 1195 27
 5 11  7  526  503 27    6  2  8 1205 1288 22    6  8  6  486  511 26    6 17  4  445  457 34    7  5  6 1074 1063 23
 5 12  0  400  390 19    6  3  0  801  810 13    6  8  7  933  954 22    6 18  1  563  560 26    7  5  7  741  826 33
 5 12  1 1170 1238 21    6  3  1 1562 1520 13    6  8  8  794  806 24    6 18  2  284  285 44    7  5  9  615  662 45
 5 12  2  392  401 21    6  3  2  758  706 16    6  8  9  385  383 48    7  0  1 2118 2030 19    7  6  0  270  231 26
 5 12  3 1249 1260 23    6  3  3  423  383 14    6  9  0 2084 2072 18    7  0  2  202  182 30    7  6  1 1626 1675 21
 5 12  4  522  522 20    6  3  4  869  862 17    6  9  1 1074 1074 19    7  0  3 2229 2139 21    7  6  2 1229 1194 24
 5 12  5  383  383 28    6  3  5 1153 1164 28    6  9  2  649  650 15    7  0  4 1164 1141 23    7  6  3 1503 1514 27
 5 12  6  509  469 24    6  3  6  973 1002 22    6  9  3  352  386 24    7  0  7  682  696 16    7  6  4  924  927 21
 5 12  7  716  767 22    6  3  7  795  812 19    6  9  4 1588 1604 23    7  0  8 1204 1013 26    7  6  5  695  677 25
 5 13  0  940  928 22    6  3  8  588  595 24    6  9  5  739  729 17    7  0  9  687  506 35    7  6  7  768  770 32
 5 13  1  919  976 17    6  3  9  576  569 29    6  9  6  674  683 20    7  1  0 1174 1156 17    7  6  8  716  699 36
 5 13  2  359  386 23    6  3 10  546  587 36    6  9  7  564  539 25    7  1  2 1477 1447 18    7  7  0  925  915 23
 5 13  3 1144 1135 24    6  4  0  715  703 14    6  9  8  471  467 36    7  1  3  987  954 21    7  7  1  801  784 20
 5 13  4  767  748 18    6  4  1 1753 1725 14    6 10  1 1205 1267 20    7  1  4  814  828 19    7  7  2 1311 1294 26
 5 13  7  467  467 30    6  4  2  303  245 16    6 10  2  551  575 15    7  1  5  890  871 20    7  7  3  928  857 23
 5 14  1  607  659 15    6  4  3 1466 1497 18    6 10  3 1068 1096 23    7  1  6 1468 1500 30    7  7  4 1330 1401 32
 5 14  2  799  829 19    6  4  4  940  903 24    6 10  4  393  321 24    7  1  7  836  807 23    7  7  5  669  662 26
 5 14  3  353  347 25    6  4  5 1107 1134 20    6 10  5  914  885 22    7  1  8  633  518 34    7  7  6 1239 1237 25
 5 14  5  300  263 35    6  4  7  434  440 29    6 10  6  725  746 20    7  1  9  724  585 38    7  7  8  832  840 32
 5 14  6 1288 1239 28    6  4  8  926  950 22    6 10  7  424  467 34    7  1 10  849  831 39    7  8  0 1152 1154 24
 5 15  0 1022 1032 23    6  5  0 1085 1081 14    6 11  0  303  263 23    7  2  1 1973 2084 18    7  8  1 1817 1814 24
 5 15  1  862  861 18    6  5  1  611  606 13    6 11  1  558  563 15    7  2  2  466  416 14    7  8  2  487  470 23
 5 15  3 1072 1066 25    6  5  2 2318 2239 18    6 11  2  589  616 15    7  2  3 1231 1230 22    7  8  3 1204 1209 30
 5 15  4  809  783 17    6  5  3 1076  988 19    6 11  3  856  930 18    7  2  4 1270 1240 26    7  8  4  922  939 23
 5 16  0  499  515 18    6  5  4  905  831 18    6 11  4  677  702 17    7  2  5  806  797 21    7  8  5 1151 1180 27
 5 16  1  561  559 17    6  5  5  305  188 35    6 11  7  586  640 37    7  2  7  429  419 41    7  8  6  729  712 28
 5 16  2  373  355 24    6  5  6 1248 1264 29    6 11  8  563  631 43    7  2  8  522  503 40    7  9  1  426  334 23
 5 16  3 1085 1052 25    6  5  7  407  456 32    6 12  0  569  521 21    7  3  0 1261 1272 17    7  9  2  682  613 18
 5 17  0 1347 1331 22    6  5  8  547  590 28    6 12  1  461  501 26    7  3  1  742  739 15    7  9  3 1264 1216 30
 5 17  4  949  909 19    6  5  9  498  445 34    6 12  2  604  593 21    7  3  2 1770 1771 20    7  9  4  799  825 21
 5 18  3  458  464 22    6  6  0 1445 1423 15    6 12  3  567  524 24    9  2  4 1496 1469 26    7  9  5  878  857 22
 6  0  0 2765 2631 17    6  6  1 1492 1440 15    6 12  4  401  332 35    9  3  1  938  940 21    7  9  7  947  947 27
 6  0  1 2487 2375 16    8  1  6  965  923 22    6 12  5  497  462 33    9  3  3 1410 1404 25    7  9  8  578  661 44
 7 10  0 1044 1018 20    8  1  7 1055 1051 28    8  9  0  590  564 19    9  3  4  767  790 19    9 12  1  696  678 22
 7 10  1  361  334 29    8  1  9  834  713 35    8  9  1  809  749 20    9  3  9  452  433 61    9 12  2 1142 1122 25
 7 10  2 1424 1382 28    8  2  0 1362 1380 18    8  9  2  826  841 21    9  4  0 1639 1683 20    9 12  3  396  393 37
 7 10  3  573  652 24    8  2  1 1008 1016 19    8  9  3  475  485 29    9  4  1  279  250 28    9 12  5  447  441 36
 7 10  4  625  648 25    8  2  2  749  750 17    8  9  4  819  805 21    9  4  2  453  398 20    9 12  6  398  388 45
 7 10  5  560  626 30    8  2  3 1401 1359 21    8  9  6  863  837 25    9  4  3  857  840 18    9 13  1  555  525 27
 7 10  6  774  708 27    8  2  4  881  902 22    8 10  0  387  428 29    9  4  4  982  963 24    9 13  2  412  423 37
 7 10  7  371  359 58    8  2  6  592  776 28    8 10  1 1086 1081 22    9  4  5  584  586 27    9 13  4  537  560 30
 7 11  0 1332 1364 27    8  2  7  574  606 44    8 10  2  946  878 20    9  4  7  641  658 38    9 13  5  459  496 38
 7 11  1  517  509 23    8  2  9  741  749 37    8 10  3  956  929 21    9  5  1  344  358 25    9 14  1  847  846 21
 7 11  2  570  561 23    8  3  0  752  772 15    8 10  4  303  277 46    9  5  2  883  913 21    9 14  4  509  429 30
 7 11  3  549  474 24    8  3  1 1384 1382 18    8 10  5  699  755 26    9  5  3  440  420 27    9 15  1  570  575 29
 7 11  4  805  847 21    8  3  2  675  633 16    8 11  0  472  459 25                               9 15  2  364  244 36
 7 11  5  854  905 24    8  3  3  555  579 18    8 11  3  378  330 34                               9 16  1  418  476 38
 7 11  7  545  584 40    8  3  4  398  368 28    8 11  4  822  837 21                               9 16  2  957  942 23
 7 12  1  802  808 19    8  3  5  584  584 27                                                      10  0  0 2542 2385 23
 7 12  2  887  950 22                                                                              10  0  3  785  769 19
```

```
7 12 3  993 1026 24      8  3 6 1461 1444 30      8 11 7  374  308 54      9  5 4  429  407 31     10  0 4 1573 1436 27
7 12 5  489  465 33      8  3 7  602  558 42      8 12 0  366  317 33      9  5 5  659  711 27     10  0 5  596  545 23
7 12 6  513  510 37      8  4 0 1348 1350 19      8 12 1  913  883 20      9  5 6 1066 1127 26     10  0 7  790  859 24
7 13 0  626  678 22      8  4 1 1577 1541 20      8 12 2  587  652 25      9  5 7  548  583 45     10  1 0  984 1053 17
7 13 1  510  515 25      8  4 2  843  786 19      8 12 4  331  330 44      9  6 0  306  339 28     10  1 1  719  703 16
7 13 2  538  543 25      8  4 3 1078 1120 27      8 12 5  640  642 28      9  6 1 1321 1328 24     10  1 2  951  961 19
7 13 3  457  479 30      8  4 4  819  812 18      8 13 1  637  611 23      9  6 2 1218 1153 27     10  1 3 1425 1453 24
7 13 4  702  693 23      8  4 5  608  608 26      8 13 2  399  377 33      9  6 3 1321 1331 28     10  1 4  646  704 20
7 13 6  436  317 40      8  4 7  498  582 49      8 13 4  588  616 28      9  6 4  491  427 28     10  1 5  283  327 43
7 14 1 1003 1067 21      8  5 0  704  738 15      8 13 5  810  817 24      9  6 6  760  708 28     10  1 6  787  776 22
7 14 3  568  579 25      8  5 1  994  927 23      8 14 0  302  285 43      9  6 7  695  684 36     10  1 7  794  804 28
7 14 5  613  630 28      8  5 2  946  942 19      8 14 1  528  542 29      9  7 0  432  449 24     10  2 0  766  807 19
7 14 6  582  561 31      8  5 3 1191 1158 26      8 14 2 1496 1495 32      9  7 1 1336 1288 26     10  2 1  383  404 23
7 15 0  709  722 22      8  5 4 1148 1143 23      8 14 4  317  265 46      9  7 2  760  748 18     10  2 2  660  646 15
7 15 1  394  402 34      8  5 6  639  656 32      8 15 0  423  399 34      9  7 3  992  974 24     10  2 3 1013 1041 20
7 15 3  498  494 30      8  5 7  710  738 34      8 15 1  609  619 25      9  7 4  802  848 22     10  2 4  760  788 18
7 15 4  720  757 24      8  5 8  540  620 49      8 15 2  464  472 31      9  7 6  843  845 27     10  2 5  573  574 25
7 15 5  508  455 31      8  6 0 2052 2042 22      8 15 4  409  425 38      9  7 8  501  626 54     10  2 6  579  578 30
7 16 1  763  777 21      8  6 1  994  969 24      8 16 1  749  796 23      9  8 0 1341 1325 26     10  2 7  582  663 42
7 16 2 1015  988 21      8  6 2  780  768 18      8 16 2  512  564 31      9  8 1 1323 1295 27     10  3 1  908  936 18
7 16 3  541  569 29      8  6 3  627  592 20      8 16 3  471  413 31      9  8 2  315  343 37     10  3 2  645  637 17
7 17 0  821  847 21      8  6 4 1431 1388 30      9  0 1 1730 1633 21      9  8 3 1045  991 24     10  3 3  918  885 21
7 17 1  521  485 28      8  6 5  796  780 23      9  0 2  837  779 19      9  8 4 1043 1039 22     10  3 5  518  561 29
7 17 2  281  228 45      8  6 8  418  349 60      9  0 3 1844 1800 24      9  8 5  740  808 27     10  3 6 1030 1071 26
7 18 1  366  330 36      8  7 1  328  335 29      9  0 6  611  592 24      9  9 0  727  750 18     10  4 0 1160 1186 23
8  0 0 4134 3987 26      8  7 2  469  428 23      9  0 7  968 1069 23      9  9 3  631  617 23     10  4 1  419  416 21
8  0 1 1253 1164 20      8  7 3  928  939 20      9  0 9  560  484 52      9  9 4  918  908 21     10  4 2  863  876 21
8  0 2  588  598 15      8  7 4  621  587 24      9  1 0 1009 1007 22      9  9 7  565  588 32     10  4 3  911  878 22
8  0 3  756  702 19      8  7 5 1277 1292 26      9  1 1  693  708 15      9 10 0  551  571 23     10  4 4  852  820 22
8  0 4 1826 1770 23      8  7 6  647  723 32      9  1 2  763  786 19      9 10 2 1156 1147 24     10  4 6  732  668 27
8  0 5  536  502 21      8  7 7  895  885 30      9  1 3 1096 1107 24      9 10 4  340  286 41     10  4 7  397  381 58
8  0 7  540  548 34      8  8 0 1044 1064 19      9  1 4  450  428 22      9 10 5  748  816 26     10  5 0  485  490 19
8  1 0  932  975 21      8  8 1  775  773 19      9  1 6 1366 1352 24      9 11 1  939  902 20     10  5 1 1216 1247 26
8  1 1  832  818 21      8  8 2 1723 1779 27      9  1 7  623  613 39      9 11 2  631  601 23     10  5 2  435  387 24
8  1 2 1118 1138 20      8  8 3 1055 1036 24      9  2 0 2074 2137 20      9 11 5  803  877 25     10  5 3 1238 1231 29
8  1 3 1667 1707 21      8  8 4  568  495 26      9  2 1 1035 1083 21      9 11 6  452  443 41     10  5 4  720  692 22
8  1 4  646  625 16      8  8 5  419  424 38      9  2 2  439  435 19                              10  5 7  646  636 38
8  1 5  886  855 19      8  8 6  784  769 29      9  2 3 1138 1139 24                              10  6 0 1628 1721 24
10  6 1  401  323 25     11  1 5  765  791 20     11 12 0  535  486 29     12 10 4  408  439 44     14  5 2  759  829 22
10  6 2  329  271 34     11  1 6  743  747 25     11 12 1  367  302 41     12 11 1  469  504 36     14  5 3  370  338 41
10  6 3  562  562 24     11  2 0  876  931 19     11 12 2  646  672 28     12 11 2  364  298 45     14  6 1  428  405 31
10  6 4  867  828 21     11  2 1  482  470 19     11 12 4  335  345 50     12 11 3  601  605 30     14  6 2  575  623 28
10  6 5  504  466 34     11  2 2  700  718 17     11 13 0  359  294 40     13  0 0  434  446 30     14  7 0  475  478 29
10  7 0  901  938 22     11  2 3  580  615 21     11 13 1  551  612 32     13  0 4  920  853 21     14  7 2  538  522 30
10  7 1  254  262 41     11  2 4  980  966 23     11 13 3  609  640 29     13  0 5  413  416 41     14  8 0  525  568 28
10  7 2  938  916 23     11  2 5  629  662 26     12  0 0  713  648 18     13  1 1  951  947 23     15  0 1  637  672 26
10  7 3  546  514 26     11  2 6  516  519 35     12  0 1  618  589 20     13  1 2  664  648 21     15  1 0  416  466 35
10  7 4  788  777 23     11  2 7  474  469 45     12  0 2  771  788 19     13  1 5  511  459 27     15  1 1  393  336 36
10  7 5  504  543 36     11  3 0  613  677 16     12  0 4  879  777 20     13  2 1  755  768 18     15  2 0  368  412 37
10  7 6  563  610 39     11  3 1  739  803 18     12  0 5 1007  966 23     13  2 2  854  887 21     15  2 1  671  697 24
10  7 7  525  545 45     11  3 2  767  743 18     12  0 7  536  536 37     13  2 4  320  429 47     15  3 0  351  352 38
10  8 2 1343 1312 30     11  3 3  985 1056 22     12  1 0  906  889 21     13  2 5  633  661 27
10  8 3  837  798 20     11  3 4  523  537 26     12  1 1  878  880 22     13  3 1  583  558 21
10  8 4  309  316 49     11  3 7  482  500 48     12  1 2 1132 1150 29     13  3 3  956  951 23
10  8 5  547  576 33     11  4 0  725  786 18     12  1 3  627  598 21     13  4 1  273  301 42
10  8 6  640  620 33     11  4 3  498  491 26     12  1 4  568  598 25     13  4 2  548  541 25
10  8 7  544  564 42     11  4 4  433  458 34     12  1 5  380  451 40     13  4 5  589  621 32
10  9 0  333  351 35     11  4 5  741  749 25     12  1 6  575  590 30     13  5 0  594  653 22
10  9 1 1310 1280 30     11  4 7  600  607 40     12  2 0  383  381 26     13  5 1  497  493 26
10  9 2  620  612 24     11  5 0  834  850 21     12  2 4  770  824 20     13  5 2  391  355 34
10  9 3  699  674 24     11  5 1  529  553 21     12  2 5  756  737 23     13  5 3  337  356 43
10  9 4  318  319 49     11  5 2  755  777 18     12  3 0  478  509 22     13  5 5  452  543 43
10  9 5  733  742 27     11  5 3  398  416 33     12  3 1  954 1003 21     13  6 0  498  586 25
10  9 6  565  549 35     11  5 4  572  574 28     12  3 3  572  554 22     13  6 1  509  502 26
10 10 0  779  745 19     11  5 5  462  497 38     12  3 5  622  647 28     13  6 3  482  447 33
10 10 1  628  616 24     11  5 6  708  690 31     12  4 0  636  672 18     13  6 4  719  719 28
10 10 2 1041 1012 24     11  6 0  861  894 21     12  4 1  479  502 23     13  7 0  379  366 33
10 10 4  507  461 32     11  6 2  730  708 20     12  4 2  673  692 20     13  7 1  899  852 21
10 10 5  380  389 45     11  6 3  802  779 22     12  4 4  849  842 21     13  7 2  479  542 34
10 10 6  416  550 49     11  6 4  694  698 25     12  4 5  414  358 40     13  7 3  694  743 26
10 11 0  408  343 32     11  6 6  576  597 38     12  4 6  472  451 43     13  7 4  436  388 40
10 11 1  549  548 28     11  7 1 1510 1568 28     12  5 2  881  866 21     13  8 1  514  525 28
10 11 3  596  584 29     11  7 2  289  238 42     12  5 3  759  745 21     13  8 2  587  557 27
10 11 4  558  614 33     11  7 3 1060 1040 22     12  5 5  406  394 45     13  8 3  353  356 47
10 12 1  465  468 33     11  7 5  569  563 34     12  5 6  392  426 53     13  9 0  380  424 37
10 12 2  413  373 36     11  8 0  931  969 23     12  6 0  611  600 20     13  9 1  471  489 32
10 12 5  516  544 34     11  8 1  500  482 27     12  6 2  410  446 32     13  9 2  536  575 33
10 13 0  473  495 33     11  8 2  615  634 25     12  6 3  355  365 42     13  9 3  487  511 37
10 13 1  576  632 29     11  8 4  715  706 27     12  6 5  745  695 28     13 10 0  430  425 36
10 14 2  982  964 24     11  8 5  574  579 33     12  7 0 1094 1088 22     14  0 1  740  756 23
10 15 0  461  439 34     11  8 6  624  611 34     12  7 2  927  916 22     14  0 2  941  947 23
10 15 1  550  556 30     11  9 0  731  744 20     12  7 4  624  690 32     14  1 1  499  450 27
11  0 1  339  240 30     11  9 1  468  499 30     12  8 0  403  448 31     14  1 2  906  967 23
11  0 2  574  562 20     11  9 2  695  682 24     12  8 2  382  334 38     14  1 4  388  341 40
11  0 3  859  762 20     11  9 3  541  585 32     12  8 3  688  621 26     14  2 1  511  543 26
11  0 4 1006  986 21     11  9 4  625  635 29     12  8 5  417  452 46     14  2 2  412  343 31
11  0 6  672  572 25     11 10 1  358  333 38     12  9 0  881  905 19     14  2 4  451  487 35
11  0 7  741  757 27     11 10 2  404  459 39     12  9 1  912  931 23     14  3 1  450  484 29
11  1 0  359  428 27     11 10 3  460  420 35     12  9 3  621  572 28     14  3 4  395  416 41
11  1 1 1271 1302 25     11 10 5  563  592 35     12  9 5  541  540 35     14  4 1  634  647 22
11  1 2  740  740 17     11 11 0  769  740 22     12 10 2  644  618 27     14  4 3  447  426 33
11  1 3  944  928 21     11 11 1  690  655 24     12 10 3  411  287 40     14  5 1  325  335 40
11  1 4  397  387 30     11 11 4  401  435 44
```

Table A2: *Observed And Calculated Structure Factors For The [Ph₃PAu(6-MP)].C₂H₅OH Complex.*

$10|F|o$ vs $10|F|c$

h	k	l	Fo	Fc	sigF	h	k	l	Fo	Fc	sigF	h	k	l	Fo	Fc	sigF	h	k	l	Fo	Fc	sigF	h	k	l	Fo	Fc	sigF
0	0	1	1554	1614	8	0	3	5	295	300	7	0	6	1	830	839	7	0	9	4	440	440	9	0	16	-1	191	153	14
0	0	2	1202	1182	7	0	3	6	140	142	14	0	6	2	969	987	8	0	9	5	427	420	10	0	16	0	131	108	20
0	0	3	762	798	7	0	3	7	166	145	14	0	6	3	894	853	9	0	9	6	459	488	11	0	17	-2	138	155	20
0	0	4	1342	1331	9	0	3	8	155	101	17	0	6	4	398	406	8	0	9	7	308	302	11	0	17	2	207	202	15
0	0	5	1310	1313	10	0	3	9	146	119	21	0	6	5	268	266	8	0	9	8	262	250	13	0	17	3	144	144	20
0	0	6	627	636	10	0	4	-10	167	191	20	0	6	6	687	680	11	0	9	9	160	182	22	1	-17	-3	168	178	18
0	0	7	503	511	12	0	4	-9	239	207	13	0	6	7	379	376	10	0	10	-4	158	173	14	1	-17	-2	164	160	18
0	0	8	396	406	9	0	4	-8	255	256	11	0	6	8	322	324	10	0	10	-2	135	138	13	1	-17	-1	145	115	19
0	0	9	382	393	10	0	4	-7	494	479	13	0	7	-9	155	148	20	0	10	-1	194	202	9	1	-17	1	142	165	22
0	0	10	272	262	13	0	4	-6	595	611	11	0	7	-8	304	285	10	0	10	0	191	184	9	1	-17	3	186	151	20
0	1	-6	252	227	8	0	4	-5	677	670	9	0	7	-7	320	293	9	0	10	1	255	263	8	1	-15	-5	164	184	19
0	1	-5	98	105	15	0	4	-4	848	839	8	0	7	-6	218	222	10	0	10	2	153	144	12	1	-15	-4	285	294	12
0	1	-4	116	102	9	0	4	-3	612	626	7	0	7	-5	237	218	8	0	10	4	224	232	10	1	-15	-3	263	274	12
0	1	-3	193	189	5	0	4	-2	1409	1429	9	0	7	-4	555	559	10	0	10	5	249	254	11	1	-15	-2	175	153	15
0	1	-2	626	632	5	0	4	-1	1097	1082	7	0	7	-3	887	864	9	0	10	6	188	166	15	1	-15	0	223	229	12
0	1	-1	316	319	4	0	4	0	1023	1021	7	0	7	-2	724	722	8	0	11	-7	165	170	18	1	-15	1	309	290	10
0	1	1	329	310	4	0	4	1	659	683	6	0	7	-1	607	601	8	0	11	-6	306	317	10	1	-15	2	206	191	15
0	1	2	574	573	5	0	4	2	1029	1018	7	0	7	0	456	457	8	0	11	-5	449	447	11	1	-15	5	140	104	23
0	1	3	197	202	5	0	4	3	1104	1084	8	0	7	1	693	696	8	0	11	-4	494	492	10	1	-15	6	138	119	22
0	1	4	241	226	6	0	4	4	708	710	8	0	7	2	618	613	8	0	11	-3	436	420	9	1	-14	-2	130	117	18
0	1	5	205	192	9	0	4	5	411	412	8	0	7	3	575	579	9	0	11	-2	366	357	9	1	-14	1	198	182	13
0	1	7	189	200	12	0	4	6	356	363	8	0	7	4	520	527	10	0	11	-1	638	631	10	1	-14	2	147	144	20
0	2	-10	302	323	12	0	4	7	459	452	10	0	7	5	366	350	8	0	11	0	579	572	10	1	-14	3	139	81	23
0	2	-9	274	282	12	0	4	8	448	460	11	0	7	6	606	598	12	0	11	1	568	570	11	1	-13	-7	172	160	18
0	2	-8	256	266	11	0	4	9	266	304	13	0	7	7	348	356	9	0	11	2	481	488	9	1	-13	-6	220	201	14
0	2	-7	449	450	9	0	5	-8	247	254	12	0	7	8	231	262	14	0	11	3	393	397	8	1	-13	-5	228	241	14
0	2	-6	752	773	10	0	5	-7	492	499	10	0	7	9	170	169	20	0	11	4	470	456	10	1	-13	-4	313	324	10
0	2	-5	835	839	9	0	5	-6	336	340	8	0	8	-7	173	205	16	0	11	5	409	426	10	1	-13	-3	270	268	10
0	2	-4	720	725	8	0	5	-5	195	187	9	0	8	-6	326	335	8	0	11	6	370	368	10	1	-13	-2	212	223	11
0	2	-3	799	802	7	0	5	-4	321	311	8	0	8	-5	204	205	10	0	11	7	190	205	17	1	-13	-1	281	291	9
0	2	-2	955	1000	7	0	5	-3	644	646	8	0	8	-4	339	346	8	0	11	8	208	224	17	1	-13	0	367	370	9
0	2	-1	1399	1364	8	0	5	-2	769	753	7	0	8	-3	341	341	9	0	13	-6	201	192	16	1	-13	1	365	363	9
0	2	0	992	971	6	0	5	-1	594	591	7	0	8	-2	498	498	10	0	13	-5	254	245	12	1	-13	2	181	173	15
0	2	1	772	773	5	0	5	0	689	684	6	0	8	-1	503	494	9	0	13	-4	250	265	12	1	-13	3	233	187	13
0	2	2	1149	1140	7	0	5	1	438	432	7	0	8	0	480	460	9	0	13	-3	220	213	15	1	-13	4	256	229	12
0	2	3	1199	1224	8	0	5	2	1122	1104	8	0	8	1	607	621	9	0	13	-2	361	370	9	1	-13	5	253	217	13
0	2	4	1478	1494	10	0	5	3	566	564	8	0	8	2	418	407	10	0	13	-1	468	469	10	1	-13	6	146	137	20
0	2	5	819	811	9	0	5	4	560	550	9	0	8	3	233	234	8	0	13	0	469	469	9	1	-12	-6	162	187	19
0	2	6	608	603	10	0	5	5	339	336	7	0	8	4	148	134	13	0	13	1	298	294	9	1	-12	-5	303	285	10
0	2	7	498	513	12	0	5	6	446	434	9	0	8	5	394	389	10	0	13	2	316	303	8	1	-12	-4	217	216	12
0	2	8	540	536	10	0	5	7	429	446	11	0	8	6	383	369	10	0	13	3	425	439	9	1	-12	-3	211	197	11
0	2	9	366	393	10	0	5	8	227	227	14	0	8	7	209	224	14	0	13	4	427	432	10	1	-12	-2	197	203	11
0	2	10	275	275	13	0	5	9	161	165	20	0	9	-9	189	210	18	0	13	5	295	306	11	1	-12	0	241	238	9
0	3	-7	244	226	10	0	5	10	155	167	23	0	9	-8	266	266	13	0	13	6	186	169	17	1	-12	3	167	167	16
0	3	-6	386	392	9	0	6	-10	166	153	19	0	9	-7	181	177	15	0	13	7	199	207	17	1	-12	4	219	217	13
0	3	-5	349	342	8	0	6	-9	193	162	16	0	9	-6	207	202	12	0	15	-5	155	106	19	1	-12	6	170	142	17
0	3	-4	542	514	8	0	6	-8	268	280	11	0	9	-5	465	473	9	0	15	-3	228	222	12	1	-11	-8	142	136	23
0	3	-3	403	399	7	0	6	-7	260	263	10	0	9	-4	602	594	11	0	15	-2	287	292	10	1	-11	-7	180	206	18
0	3	-2	967	961	7	0	6	-6	229	233	10	0	9	-3	496	481	11	0	15	-1	197	206	14	1	-11	-6	269	295	12
0	3	-1	365	369	5	0	6	-5	351	357	7	0	9	-2	304	278	9	0	15	0	126	146	20	1	-11	-5	285	298	10
0	3	0	626	622	5	0	6	-4	441	435	10	0	9	-1	441	433	10	0	15	1	261	255	11	1	-11	-4	228	227	10
0	3	1	541	550	5	0	6	-3	783	782	8	0	9	0	831	826	9	0	15	2	271	280	12	1	2	-1	1166	1140	7
0	3	2	727	710	6	0	6	-2	632	627	8	0	9	1	833	818	9	0	15	4	217	220	14	1	2	0	161	160	4
0	3	3	781	763	7	0	6	-1	582	567	7	0	9	2	724	735	9	0	16	-2	177	156	16	1	2	1	1266	1231	8
0	3	4	442	445	9	0	6	0	283	311	6	0	9	3	427	415	8	1	-1	9	171	171	18	1	2	2	1166	1156	8
1	-11	-3	222	231	10	1	-7	-5	336	337	8	1	-3	-8	158	126	16	1	-1	10	143	85	22	1	2	3	831	822	7
1	-11	-2	359	375	8	1	-7	-4	147	126	11	1	-3	-5	258	259	7	1	0	-11	190	168	18	1	2	4	584	601	8
1	-11	-1	493	497	11	1	-7	-3	116	121	13	1	-3	-4	539	529	8	1	0	-10	175	201	20	1	2	5	399	395	8
1	-11	0	431	434	9	1	-7	-2	135	130	9	1	-3	-3	545	539	7	1	0	-9	327	331	10	1	2	6	356	353	8
1	-11	1	304	287	8	1	-7	-1	271	270	6	1	-3	-2	425	420	6	1	0	-8	341	358	9	1	2	7	449	427	10
1	-11	2	259	242	11	1	-7	0	274	272	6	1	-3	-1	1013	985	7	1	0	-7	507	496	12	1	2	8	400	410	10
1	-11	3	259	248	10	1	-7	1	140	145	11	1	-3	0	500	475	6	1	0	-6	635	639	10	1	2	9	256	253	13
1	-11	4	337	313	8	1	-7	2	527	518	10	1	-3	1	718	687	6	1	0	-5	780	762	8	1	2	10	159	105	21
1	-11	5	233	239	12	1	-7	3	139	134	12	1	-3	2	149	166	6	1	0	-4	766	783	7	1	3	-11	185	200	18
1	-11	6	181	181	15	1	-7	6	188	177	12	1	-3	3	226	223	5	1	0	-3	908	913	7	1	3	-10	172	153	19
1	-11	8	155	116	19	1	-7	7	241	238	11	1	-3	4	360	349	7	1	0	-2	1625	1599	9	1	3	-9	155	192	19
1	-10	-9	141	132	22	1	-6	-9	284	311	12	1	-3	6	205	205	10	1	0	-1	1727	1757	9	1	3	-8	440	447	11
1	-10	-7	256	255	12	1	-6	-8	497	511	11	1	-3	7	181	186	13	1	0	0	1170	1260	7	1	3	-7	579	586	12
1	-10	-6	385	387	10	1	-6	-7	506	533	9	1	-2	-11	154	160	21	1	0	1	929	925	6	1	3	-6	703	694	10
1	-10	-5	421	418	10	1	-6	-6	385	391	10	1	-2	-10	243	221	14	1	0	2	336	340	6	1	3	-5	641	645	9
1	-10	-4	350	359	9	1	-6	-5	387	388	8	1	-2	-9	327	337	10	1	0	3	1153	1171	8	1	3	-4	733	730	8
1	-10	-3	241	251	9	1	-6	-4	977	961	9	1	-2	-8	423	435	11	1	0	4	1004	972	8	1	3	-3	867	863	7
1	-10	-2	397	402	9	1	-6	-3	1322	1310	9	1	-2	-7	496	499	12	1	0	5	856	838	9	1	3	-2	1090	1100	7
1	-10	-1	543	545	10	1	-6	-2	942	936	8	1	-2	-6	613	601	10	1	0	6	394	385	9	1	3	-1	2249	2256	13
1	-10	0	556	553	10	1	-6	-1	765	757	7	1	-2	-5	1045	1034	9	1	0	7	278	281	9	1	3	0	727	737	6
1	-10	1	394	384	9	1	-6	1	1194	1187	10	1	-2	-4	791	797	8	1	0	9	290	309	12	1	3	1	847	858	6
1	-10	2	289	281	9	1	-6	2	994	997	9	1	-2	-3	776	788	7	1	0	10	193	173	17	1	3	2	1078	1076	8
1	-10	3	447	440	9	1	-6	3	843	851	9	1	-2	-2	177	169	4	1	1	-11	195	128	18	1	3	3	1338	1323	9
1	-10	4	287	280	9	1	-6	4	559	549	9	1	-2	-1	1277	1238	8	1	1	-10	231	257	15	1	3	4	910	894	9
1	-10	5	169	185	14	1	-6	5	512	483	11	1	-2	0	1553	1517	9	1	1	-9	171	186	17	1	3	5	442	452	11
1	-10	7	199	185	14	1	-6	6	476	478	9	1	-2	1	1225	1192	8	1	1	-8	146	128	17	1	3	6	321	313	8
1	-9	-5	251	263	10	1	-6	7	508	509	10	1	-2	2	1009	1012	7	1	1	-7	359	377	9	1	3	7	484	496	10
1	-9	-4	289	301	8	1	-6	8	333	346	10	1	-2	3	690	686	7	1	1	-6	552	570	10	1	3	8	376	364	9
1	-9	-3	311	312	8	1	-6	9	207	209	15	1	-2	4	666	692	8	1	1	-5	958	957	9	1	3	9	270	289	13
1	-9	-2	272	274	7	1	-5	-6	195	225	11	1	-2	5	842	831	9	1	1	-4	243	248	6	1	4	-9	199	208	16
1	-9	-1	480	475	10	1	-5	-2	192	187	6	1	-2	6	611	621	11	1	1	-3	973	949	7	1	4	-8	189	216	14
1	-9	0	262	262	7	1	-5	3	105	111	12	1	-2	7	298	304	9	1	1	-2	927	924	6	1	4	-7	126	84	17
1	-9	1	151	137	12	1	-4	-10	228	242	15	1	-2	8	315	314	9	1	1	-1	991	966	6	1	4	-6	291	279	7
1	-9	2	314	312	8	1	-4	-9	412	431	9	1	-2	9	335	349	11	1	1	0	744	740	5	1	4	-5	339	341	8
1	-9	3	439	428	9	1	-4	-8	443	468	11	1	-2	10	244	275	15	1	1	1	325	293	5	1	4	-4	438	445	9
1	-9	4	340	323	8	1	-4	-7	573	597	12	1	-1	-11	158	119	21	1	1	2	854	879	8	1	4	-3	469	456	7
1	-9	5	161	171	14	1	-4	-6	270	270	8	1	-1	-10	216	214	15	1	1	3	884	878	7	1	4	-2	522	516	7
1	-8	-8	262	277	12	1	-4	-5	778	786	9	1	-1	-9	196	205	15	1	1	4	770	776	8	1	4	-1	926	902	8
1	-8	-7	545	551	10	1	-4	-4	1090	1092	9	1	-1	-7	201	212	11	1	1	5	531	523	9	1	4	0	82	64	9
1	-8	-6	576	591	13	1	-4	-3	1244	1217	9	1	-1	-6	477	466	10	1	1	6	427	431	9	1	4	1	425	433	6
1	-8	-5	476	458	12	1	-4	-2	1374	1379	9	1	-1	-5	513	521	9	1	1	7	336	336	8	1	4	2	371	379	8
1	-8	-4	465	487	11	1	-4	-1	741	740	9	1	-1	-4	462	467	7	1	1	9	263	252	13	1	4	3	698	700	8
1	-8	-3	901	885	9	1	-4	0	1123	1127	8	1	-1	-3	212	203	5	1	2	-10	192	179	17	1	4	4	288	283	7
1	-8	-2	974	967	9	1	-4	1	1239	1229	9	1	-1	-2	160	151	4	1	2	-9	206	193	14	1	4	7	183	176	14
1	-8	-1	809	808	8	1	-4	2	1162	1163	8	1	-1	-1	759	741	5	1	2	-7	346	334	8	1	4	8	257	253	12
1	-8	0	683	661	8	1	-4	3	822	821	8	1	-1	0	1181	1199	7	1	2	-5	572	559	9	1	5	-9	239	232	14
1	-8	1	579	567	10	1	-4	4	673	668	9	1	-1	1	848	836	6	1	2	-4	439	442	9	1	5	-8	470	479	11
1	-8	2	904	901	10	1	-4	5	831	823	10	1	-1	2	339	347	6	1	2	-2	1098	1092	7	1	5	-7	685	676	11
1	-8	3	910	903	10	1	-4	6	670	684	11	1	-1	3	624	636	7	2	-12	-5	391	388	10	1	5	-6	434	436	9
1	-8	4	563	541	11	1	-4	7	369	372	9	1	-1	4	473	472	8	2	-12	-4	331	323	8	1	5	-5	494	509	10
1	-8	5	348	367	9	1	-4	8	181	167	15	1	-1	5	423	427	8	2	-12	-3	202	220	12	2	-7	1	323	322	8
1	-8	6	333	325	8	1	-4	10	253	244	14	1	-1	6	289	289	8	2	-12	-2	384	397	8	2	-7	2	460	453	10
1	-8	7	400	401	10	1	9	-4	590	598	10	1	-1	8	188	192	15							2	-7	3	230	233	8
1	-8	8	225	243	14	1	9	-3	435	431	9	1	13	-4	141	154	18							2	-7	4	226	231	9
1	-7	-6	199	213	12	1	9	-2	500	489	11	1	13	-3	206	203	14												
1	5	-4	750	745	8	1	9	-1	597	611	9	1	13	-2	320	321	9												
1	5	-3	1355	1334	9							1	13	-1	272	273	10												
1	5	-2	1505	1486	10																								
1	5	-1	1223	1200	9																								

```
1  5   0   965  976  7     1  9   0   905  890  9     1 13   0   282  296  9    2 -12  -1   472  486 10    2  -7   5   129  123 16
1  5   1  1230 1255  8     1  9   1   838  831  9     1 13   1   203  209 11    2 -12   0   472  479 10    2  -7   6   153  170 16
1  5   2  1382 1361  9     1  9   2   547  539 10     1 13   2   265  257 10    2 -12   1   283  286 10    2  -6  -9   300  323 11
1  5   3   980  982  9     1  9   3   360  350  9     1 13   3   379  381  9    2 -12   2   264  265 11    2  -6  -8   354  359  9
1  5   4   565  584  9     1  9   4   591  571 11     1 13   4   270  287 12    2 -12   3   331  326  9    2  -6  -7   297  285  9
1  5   5   684  683 10     1  9   5   737  744 12     1 13   5   141  178 21    2 -12   4   334  334 10    2  -6  -6   283  284  8
1  5   6   823  819 11     1  9   6   397  411  9     1 14  -7   156  153 20    2 -12   5   236  220 13    2  -6  -5   520  530 11
1  5   7   568  592 14     1  9   7   255  267 13     1 14  -6   179  165 16    2 -11  -2   130  127 16    2  -6  -4   712  697  9
1  5   8   341  311 10     1  9   8   214  206 16     1 14  -5   158  121 16    2 -11   1   147  166 17    2  -6  -3   820  830  8
1  5   9   217  241 16     1 10  -6   126   98 19     1 14  -3   205  220 14    2 -10  -8   278  244 12    2  -6  -2   816  809  8
1  6  -6   198  225 11     1 10  -5   221  207 10     1 14  -2   330  318  9    2 -10  -7   362  365 10    2  -6  -1   611  616  8
1  6  -2   200  211  8     1 10  -4   205  187 10     1 14  -1   207  204 12    2 -10  -6   385  394 10    2  -6   0   854  830  8
1  6  -1   179  169  6     1 10  -3   138  113 15     1 14   1   243  244 11    2 -10  -5   374  384  9    2  -6   1  1083 1085  9
1  6   0   121  126  8     1 10  -2   157  172 12     1 14   2   296  298 10    2 -10  -4   357  335  8    2  -6   2   879  874  9
1  6   1   227  227  6     1 10  -1   329  316  8     1 14   3   239  254 13    2 -10  -3   462  454 12    2  -6   3   434  434 10
1  6   2   388  367  9     1 10   0   183  193 10     1 14   4   172  179 17    2 -10  -2   591  593 10    2  -6   4   559  538 10
1  6   3   248  239  6     1 10   1   208  204  9     1 15  -4   168  108 20    2 -10  -1   591  581 10    2  -6   5   555  561 12
1  6   5   144  115 14     1 10   2   173  167 11     1 15  -3   190  179 14    2 -10   0   430  425  9    2  -6   6   542  537 13
1  6   6   234  236 11     1 10   3   242  235  9     1 15  -2   147  130 18    2 -10   1   338  341  8    2  -6   7   286  278 10
1  6   7   191  150 14     1 10   5   170  150 15     1 15   2   159  159 18    2 -10   2   483  484  9    2  -6   8   171  158 17
1  7 -10   162  149 20     1 10   6   176  184 17     1 15   3   132  118 21    2 -10   3   465  482 10    2  -5  -9   297  323 11
1  7  -9   240  234 14     1 10   7   159  139 19     1 16  -3   221  205 14    2 -10   4   351  350  8    2  -5  -8   425  426 11
1  7  -8   363  373  9     1 11  -7   189  213 16     1 16  -2   215  187 14    2 -10   5   233  221 11    2  -5  -7   269  270  9
1  7  -7   288  286  9     1 11  -6   294  295 10     1 16  -1   216  179 13    2 -10   6   260  260 12    2  -5  -6   263  265  8
1  7  -6   358  368  8     1 11  -5   368  378  9     1 16   0   204  180 14    2 -10   7   194  195 16    2  -5  -5   425  413 11
1  7  -5   626  614 10     1 11  -4   306  304  8     1 16   1   242  232 12    2  -9  -3   195  191 10    2  -5  -4   692  667  8
1  7  -4   742  743  9     1 11  -3   352  336  9     1 16   2   241  225 13    2  -9  -2   287  279  7    2  -5  -3   487  483  8
1  7  -3   984  974  9     1 11  -2   461  462  8     1 16   3   180  191 17    2  -8  -8   347  350 10    2  -5  -2   488  476  7
1  7  -2   525  506 11     1 11  -1   607  604 11     1 18   0   145  153 20    2  -8  -7   448  431 11    2  -5  -1   508  506  7
1  7  -1   714  704  8     1 11   0   566  554 11     1 18   1   177  186 17    2  -8  -6   564  576 13    2  -5   0   446  470  8
1  7   0  1044 1033  8     1 11   1   452  465  9     2 -16  -4   195  189 16    2  -8  -5   376  372 10    2  -5   1   526  522  8
1  7   1  1331 1335 10     1 11   2   359  366  8     2 -16   0   168  208 19    2  -8  -4   666  656 10    2  -5   2   609  608  8
1  7   2   713  728  8     1 11   3   435  447 10     2 -15  -3   144  137 20    2  -8  -3   772  761  9    2  -5   3   324  323  7
1  7   3   632  631  9     1 11   4   486  465 10     2 -15  -1   182  168 15    2  -8  -2   856  847  9    2  -5   4   282  284  7
1  7   4   603  590 10     1 11   5   364  362  9     2 -15   0   191  186 15    2  -8  -1   628  614  9    2  -5   5   321  315  7
1  7   5   792  800 11     1 11   6   209  210 15     2 -15   2   153  109 21    2  -8   0   499  517 10    2  -5   6   361  372  9
1  7   6   592  579 12     1 11   7   202  198 17     2 -14  -5   210  234 15    2  -8   1   787  780 11    2  -5   7   228  214 12
1  7   7   345  339  9     1 11   8   226  240 16     2 -14  -4   238  226 12    2  -8   2   801  802 10    2  -4 -10   218  219 15
1  7   8   261  270 13     1 12  -6   220  202 13     2 -14  -3   157  196 17    2  -8   3   568  578 11    2  -4  -9   267  249 11
1  7   9   212  234 17     1 12  -5   189  165 13     2 -14  -2   226  227 12    2  -8   4   259  246  9    2  -4  -8   309  318  9
1  8  -5   275  261  8     1 12  -4   155  158 15     2 -14  -1   286  286 10    2  -8   5   268  260  9    2  -4  -7   363  368  8
1  8  -4   262  245  7     1 12  -2   302  292  8     2 -14   0   335  339  9    2  -8   6   344  348  9    2  -4  -6   670  682 10
1  8   0   163  163  8     1 12  -1   399  398 10     2 -14   1   223  213 13    2  -8   7   320  321 10    2  -4  -5   707  688  9
1  8   1   413  405 10     1 12   0   213  224 11     2 -14   2   138  174 23    2  -7  -8   233  230 13    2  -4  -4   941  926  8
1  8   2   275  267  7     1 12   1   210  207 11     2 -14   3   196  157 16    2  -7  -4   330  328  7    2  -4  -3   617  622  7
1  8   3   207  191  9     1 12   2   165  183 13     2 -14   4   205  211 16    2  -7  -3   479  466  9    2  -4  -2   941  933  7
1  9  -9   218  238 15     1 12   3   289  309 10     2 -14   6   144  147 23    2  -7  -2   125   87 10    2  -4  -1   613  616  7
1  9  -8   179  192 17     1 12   4   278  286 10     2 -13  -1   130  146 19    2  -7  -1   350  344  7    2  -4   1  1069 1035  8
1  9  -7   254  240 11     1 12   5   240  252 13     2 -13   3   163  135 18    2  -7   0   158  144  9    2  -4   2   643  647  7
1  9  -6   401  398 10     1 13  -7   133  129 22     2 -12  -7   225  227 14    2   6   1   617  633  8    2  -4   3   516  513  8
1  9  -5   567  570 11     1 13  -5   172  156 14     2 -12  -6   334  342 10    2   6   2   429  420  9    2   9   4   361  374  9
2 -4   4   388  376  8     2 -1   1   418  410  6     2  3  -4   844  840  8    2   6   3   399  389  8    2   9   5   301  305 10
2 -4   5   592  585 11     2 -1   2  1126 1150  6     2  3  -3  1360 1359  9    2   6   4   445  412 11    2   9   6   187  216 16
2 -4   6   411  417 10     2 -1   3  1064 1049  8     2  3  -2  1578 1607 10    2   6   5   288  275  8    2  10  -7   215  201 13
2 -4   7   155  136 16     2 -1   4   923  921  9     2  3  -1   483  479  7    2   6   6   318  321  9    2  10  -6   334  331  8
2 -4   9   173  200 19     2 -1   5   809  804 10     2  3   0   967  966  7    2   6   7   144  155 20    2  10  -5   376  371  8
2 -3 -10   265  286 13     2 -1   6   467  471  9     2  3   1  1298 1313  8    2   6   8   221  224 15    2  10  -4   344  330  9
2 -3  -9   328  324 10     2 -1   7   452  460 10     2  3   2  1907 1868 11    2   7  -9   249  246 13    2  10  -3   386  360  8
2 -3  -8   312  330  9     2 -1   8   443  454 10     2  3   3  1105 1096  9    2   7  -8   267  251 10    2  10  -2   475  471  9
2 -3  -7   299  301  8     2 -1   9   263  281 13     2  3   5   536  557 11    2   7  -7   233  254 11    2  10  -1   821  832 10
2 -3  -6   546  544 10     2  0  -8   148  129 15     2  3   6   669  669 11    2   7  -6   330  327  7    2  10   0   694  685 10
2 -3  -5  1286 1288 10     2  0  -6   235  219  8     2  3   7   605  633 14    2   7  -5   540  528 10    2  10   1   388  399  9
2 -3  -4  1280 1269  9     2  0  -4   131  135  8     2  3   8   396  398  9    2   7  -4   612  625 10    2  10   2   442  426  8
2 -3  -3   598  611  7     2  0  -2   457  434  6     2  4  -8   156  152 16    2   7  -3   592  580 10    2  10   3   497  502 13
2 -3  -2   415  427  6     2  0  -1   272  245  7     2  4  -7   245  248  9    2   7  -2   573  570 10    2  10   4   708  727 12
2 -3  -1  1499 1482  9     2  0   0   197  165  5     2  4  -6   136  146 13    2   7  -1   749  728  8    2  10   5   324  318  9
2 -3   0  2188 2193 12     2  0   1   492  505  6     2  4  -4   263  277  6    2   7   0  1060 1068  9    2  10   6   249  256 13
2 -3   1  1381 1354  9     2  0   3   200  202  6     2  4  -3   101  113 11    2   7   1   842  837  9    2  10   7   237  244 15
2 -3   2   713  699  7     2  0   4   422  403 10     2  4  -2   940  913  8    2   7   2   536  534  9    2  10   8   212  267 17
2 -3   3   662  660  8     2  0   7   215  216 12     2  4  -1   346  361  8    2   7   3   439  442 11    2  11  -5   179  152 16
2 -3   4   898  875  9     2  0   8   175  172 17     2  4   0   371  373  7    2   7   4   640  645 11    2  11  -4   247  259 11
2 -3   5   606  597 10     2  1 -11   236  258 15     2  4   1   182  197  6    2   7   5   504  509 13    2  11  -3   186  162 15
2 -3   6   432  434  9     2  1 -10   232  257 15     2  4   2   311  298  6    2   7   6   368  405  9    2  11  -2   238  237  9
2 -3   7   286  294 10     2  1  -9   293  294 10     2  4   3   123  139 11    2   7   7   231  232 13    2  11  -1   290  286  8
2 -3   8   274  295 12     2  1  -8   348  356  8     2  4   4   250  257  7    2   7   8   208  230 17    2  11   0   293  297  8
2 -3   9   215  206 15     2  1  -7   703  696 11     2  4   5   294  276  8    2   8  -9   218  203 14    2  11   1   166  168 12
2 -2  -9   207  217 14     2  1  -6   924  901  9     2  5 -11   159  150 19    2   8  -8   203  211 14    2  11   2   232  246 10
2 -2  -8   242  250 11     2  1  -5   884  873  8     2  5 -10   203  196 16    2   8  -7   211  207 12    2  11   3   370  367  9
2 -2  -7   253  264  9     2  1  -4  1017 1001  8     2  5  -9   241  262 13    2   8  -6   479  480  9    2  11   4   226  222 12
2 -2  -6   276  266  7     2  1  -3  1087 1102  8     2  5  -8   404  411  9    2   8  -5   531  538 11    2  12  -7   290  294 11
2 -2  -5   581  560  9     2  1  -2  2160 2144 12     2  5  -7   494  482 12    2   8  -4   523  509 10    2  12  -6   314  319 10
2 -2  -4   445  449  8     2  1  -1   835  852  6     2  5  -6   567  571 11    2   8  -3   467  447 12    2  12  -5   208  202 12
2 -2  -3   430  436  7     2  1   0  1008  979  7     2  5  -5   479  497 10    2   8  -2   609  571 11    2  12  -4   253  236 11
2 -2  -2   654  650  6     2  1   1  1036 1064  7     2  5  -4  1004 1012  9    2   8  -1   680  673  9    2  12  -3   450  428 10
2 -2  -1  1134 1122  7     2  1   2  1541 1538  9     2  5  -3  1282 1269  9    2   8   0   778  770  9    2  12  -2   510  516 13
2 -2   0  2416 2356 13     2  1   3  1243 1230  9     2  5  -2  1110 1095  9    2   8   1   572  589  9    2  12  -1   400  398 10
2 -2   1   236  248  5     2  1   4   856  851  9     2  5  -1   627  630  8    2   8   2   437  448 11    2  12   0   265  274  9
2 -2   2   366  356  7     2  1   5   510  493 10     2  5   0   972  999  8    2   8   3   358  342  9    2  12   1   286  280  8
2 -2   3   295  293  7     2  1   6   368  366  8     2  5   1  1186 1225  9    2   8   4   414  400  9    2  12   2   405  398 10
2 -2   4   691  682  9     2  1   7   521  509 13     2  5   2   847  849  8    2   8   5   407  400  9    2  12   3   539  517 13
2 -2   5   558  536 11     2  1   8   464  468 12     2  5   3   616  620  9    2   8   6   270  271 11    2  12   4   411  424 10
2 -2   6   179  177 13     2  1   9   279  304 13     2  5   4   569  578 10    2   8   7   193  193 16    2  12   5   198  225 15
2 -2   7   161  166 15     2  2  -7   118  103 17     2  5   5   732  730 11    2   8   8   187  209 19    2  14  -5   189  183 16
2 -2   8   158  176 19     2  2  -5   154  148  9     2  5   6   788  763 11    2   9  -7   260  261 10    2  14  -4   272  250 14
2 -2   9   192  192 17     2  2  -4   236  226  5     2  5   7   394  414 10    2   9  -6   356  370  9    2  14  -3   387  383  9
2 -1 -10   357  364 11     2  2  -3   176  169  5     2  5   8   249  237 13    2   9  -5   295  315  8    2  14  -2   384  391 10
2 -1  -9   327  333 10     2  2  -1   119   92  8     2  6  -9   231  221 14    2   9  -4   366  370  8    2  14  -1   318  309  9
2 -1  -8   328  331  8     2  2   0   184  163  5     2  6  -8   137  155 19    2   9  -3   317  313  8    2  14   0   349  351  9
2 -1  -7   474  454 12     2  2   3   119   70 10     2  6  -6   139  120 13    2   9  -2   399  393  9    2  14   1   369  372  9
2 -1  -6   897  894 10     2  3 -10   218  218 15     2  6  -5   485  489 10    2   9  -1   542  535 10    2  14   2   417  402 10
2 -1  -5   859  856  9     2  3  -9   300  335 11     2  6  -4   474  483 10    2   9   0   363  370  8    2  14   3   287  297 11
2 -1  -4   457  489  8     2  3  -8   588  581 13     2  6  -3   259  265  6    2   9   1   449  455 11    2  14   4   216  224 14
2 -1  -3  1129 1125  8     2  3  -7   704  697 11     2  6  -2   124   97 12    2   9   2   346  342  7    2  14   5   213  219 15
2 -1  -2  1629 1631  9     2  3  -6   482  462 10     2  6  -1   193  195  7    2   9   3   403  387  9    2  16  -3   165  181 17
2 -1  -1  1391 1358  8     2  3  -5   428  431  9     2  6   0   430  446  8    3  -2  -2   157  141  6    3   1   0   433  449  7
2 -1   0  1498 1483  9     3 -9  -6   214  194 12     3 -6   4   342  328  8    3  -2  -1    95  103 11    3   1   1   993 1028  7
2 16  -2   168  152 16     3 -9  -5   191  213 12     3 -6   5   255  228 10    3  -2   0   483  456  7    3   1   2   907  930  8
2 16  -1   194  185 15     3 -9  -4   441  437  9     3 -6   6   156  142 16    3  -2   1   206  190  5    3   1   3  1084 1099  9
2 16   0   261  249 12     3 -9  -3   631  625 10     3 -5 -10   286  290 12    3  -2   2   127  134  9    3   1   4   617  601 10
2 16   1   263  269 12     3 -9  -2   498  480 11     3 -5  -9   313  326 10    3  -2   4   104   84 16    3   1   5   287  283  8
2 16   2   247  252 13     3 -9  -1   371  362  9     3 -5  -8   281  287 10    3  -2   5   119   84 17    3   1   6   367  382  9
2 18   0   151  162 18     3 -9   0   297  307  8     3 -5  -7   365  384  9    3  -1   7   127   76 20    3   1   7   477  461 10
3 -14 -6   230  229 15     3 -9   1   473  478  9     3 -5  -6   517  506 11    3  -1 -11   252  272 14    3   1   8   310  312 11
3 -14 -5   230  240 14     3 -9   2   397  421  8     3 -5  -5   958  952 10    3  -1 -10   311  323 11    3   1   9   176  170 19
3 -14 -4   177  162 16     3 -9   3   399  405 10     3 -5  -4   832  825  9    3  -1  -9   292  290 10    3   2  -9   177  214 16
3 -14 -3   217  194 13     3 -9   4   235  263 11     3 -5  -3   702  709  8    3  -1  -8   258  229  9    3   2  -8   387  405  9
3 -14 -2   240  252 12     3 -9   5   264  275 11     3 -5  -2   657  653  8    3  -1  -7   690  700 11    3   2  -7   602  627 11
3 -14 -1   311  291 10     3 -8  -8   199  190 15     3 -5  -1   872  900  8    3  -1  -6   783  781  9    3   2  -6   258  266  7
3 -14  0   165  162 16     3 -8  -7   194  191 14     3 -5   0  1092 1114  9    3  -1  -5   991  992  9    3   2  -5   279  271  7
3 -14  1   211  187 14     3 -8  -6   247  236 10     3 -5   1   983  994  9    3  -1  -4   484  502  8    3   2  -4   531  548  8
3 -14  3   213  192 16     3 -8  -5   175  180 12     3 -5   2   465  486  9    3  -1  -3  1460 1478  9    3   2  -3  1103 1105  8
3 -14  4   216  194 15     3 -8  -4   430  437  9
3 -13 -5   144  151 20
```

h	k	l	Fo	Fc	σ
3	-12	-6	264	284	12
3	-12	-5	266	233	10
3	-12	-4	252	244	10
3	-12	-3	281	293	10
3	-12	-2	462	458	10
3	-12	-1	432	448	10
3	-12	0	265	281	10
3	-12	1	240	259	12
3	-12	2	256	248	12
3	-12	3	311	310	10
3	-12	4	230	208	13
3	-11	-7	236	229	13
3	-11	-6	243	247	12
3	-11	-5	168	164	15
3	-11	-3	269	258	9
3	-11	-2	330	343	8
3	-11	-1	353	360	8
3	-11	0	213	215	11
3	-11	1	225	206	11
3	-11	2	232	219	12
3	-11	3	200	199	13
3	-10	-8	169	186	19
3	-10	-7	277	288	12
3	-10	-6	331	339	9
3	-10	-5	304	303	9
3	-10	-4	305	317	8
3	-10	-3	469	465	9
3	-10	-2	424	410	9
3	-10	-1	323	337	7
3	-10	0	255	261	9
3	-10	1	400	407	9
3	-10	2	547	554	12
3	-10	3	377	395	9
3	-10	4	202	199	13
3	-10	6	199	184	15
3	-10	7	225	208	14
3	-9	-8	293	287	11
3	-9	-7	259	243	11
3	4	-1	612	618	8
3	4	0	1091	1090	8
3	4	1	1092	1110	8
3	4	2	468	496	8
3	4	3	355	365	8
3	4	4	546	520	10
3	4	5	572	540	11
3	4	6	457	428	10
3	4	7	314	323	10
3	4	8	238	235	14
3	4	9	171	171	20
3	5	-11	140	97	22
3	5	-8	274	280	10
3	5	-7	174	159	12
3	5	-6	315	314	7
3	5	-5	190	196	9
3	5	-4	292	297	7
3	5	-3	508	498	9
3	5	-2	128	125	10
3	5	-1	792	792	8
3	5	0	546	543	8
3	5	1	611	627	8
3	5	2	129	135	10
3	5	3	500	477	10
3	5	4	398	372	9
3	5	5	456	458	10
3	5	6	304	307	10
3	6	-10	255	253	13
3	6	-9	331	321	10
3	6	-8	311	310	9
3	6	-7	257	267	9
3	6	-6	521	539	11
3	6	-5	877	887	10
3	6	-4	774	778	9
3	6	-3	715	713	9
3	6	-2	227	250	7
3	6	-1	934	962	9
3	6	0	1293	1304	9
3	6	1	1249	1237	9
3	6	2	716	708	9
3	6	3	627	597	10
3	6	4	710	699	10
3	6	5	677	670	12
3	6	6	455	475	11
3	6	7	291	269	11
3	6	8	245	255	15
3	7	-6	169	158	12
3	7	-5	224	218	9
3	7	-4	308	306	8
3	7	-2	114	104	13
3	7	-1	251	243	7
3	7	0	366	376	7
3	7	1	265	255	6
3	7	2	193	180	9
3	7	4	255	262	9
4	-2	-7	603	602	11
4	-2	-6	540	546	10
4	-2	-5	576	571	9
4	-2	-4	413	434	8
4	-2	-3	1023	1018	8
4	-2	-2	995	1009	8
4	-2	-1	662	674	8
4	-2	0	725	754	8
4	-2	1	225	230	6
4	-2	2	892	909	8
4	-2	3	619	616	9
4	-2	4	532	543	11
4	-2	5	265	257	9
4	-2	6	253	242	11
4	-2	7	221	236	14
4	-2	8	250	238	14
4	-1	-10	159	158	19
4	-1	-9	178	198	15
4	-1	-8	237	210	10
4	-1	-7	300	308	8
4	-1	-6	442	460	11
4	-1	-5	519	509	9
4	-1	-4	752	730	9
4	-1	-3	626	659	7
4	-1	-2	920	938	8
4	-1	-1	743	757	7
4	-1	0	260	269	6
4	-1	1	661	669	8
4	-1	2	693	689	8
4	-1	3	593	571	9
3	-8	-3	468	462	11
3	-8	-2	340	348	8
3	-8	-1	335	320	8
3	-8	0	363	369	9
3	-8	1	439	450	9
3	-8	2	293	292	8
3	-8	3	182	197	12
3	-8	4	201	188	11
3	-8	5	186	173	13
3	-8	6	228	196	12
3	-8	7	196	210	16
3	-7	-9	348	349	10
3	-7	-8	392	409	10
3	-7	-7	308	331	9
3	-7	-6	402	403	10
3	-7	-5	474	461	11
3	-7	-4	686	695	10
3	-7	-3	692	699	9
3	-7	-2	621	606	9
3	-7	-1	534	526	9
3	-7	0	685	683	10
3	-7	1	786	777	10
3	-7	2	557	578	10
3	-7	3	356	373	8
3	-7	4	370	362	8
3	-7	5	515	509	13
3	-7	6	269	285	11
3	-7	7	209	198	14
3	-6	-8	124	43	20
3	-6	-7	234	204	10
3	-6	-5	298	288	7
3	-6	-4	159	168	11
3	-6	-3	337	346	8
3	-6	-2	314	311	7
3	-6	0	346	344	8
3	-6	2	274	268	7
3	-6	3	170	164	10
3	7	5	290	282	9
3	8	-9	203	209	14
3	8	-8	249	244	11
3	8	-7	366	369	9
3	8	-6	520	535	12
3	8	-5	655	668	11
3	8	-4	565	565	11
3	8	-3	635	613	11
3	8	-1	1065	1055	10
3	8	0	734	760	9
3	8	1	672	674	9
3	8	2	573	564	10
3	8	3	758	741	11
3	8	4	634	635	12
3	8	5	458	471	11
3	8	6	369	351	9
3	8	7	300	331	12
3	8	8	321	344	12
3	10	-8	200	207	14
3	10	-7	298	298	9
3	10	-6	357	357	9
3	10	-5	375	371	9
3	10	-4	420	435	9
3	10	-3	531	537	10
3	10	-2	776	754	11
3	10	-1	779	776	10
3	10	0	479	487	11
3	10	1	407	412	9
3	10	2	620	603	11
3	10	3	802	812	12
3	10	4	506	519	10
3	10	5	333	350	10
3	10	6	237	243	14
3	10	7	225	339	12
3	11	-7	165	160	16
3	11	-6	163	132	15
3	11	-3	238	232	12
3	11	-2	180	160	12
3	11	-1	164	168	12
3	11	1	145	153	14
3	11	2	126	115	17
3	11	3	163	151	15
3	12	-7	233	257	13
3	12	-6	200	202	13
3	12	-5	217	217	13
3	12	-4	285	276	12
3	12	-3	469	448	11
3	12	-2	475	491	10
3	12	-1	252	237	9
3	12	0	268	260	9
3	12	1	401	400	9
3	12	2	517	513	10
3	12	3	385	381	10
3	12	4	176	163	16
4	1	-10	160	166	19
4	1	-9	146	147	18
4	1	-8	296	273	9
4	1	-6	166	160	10
4	1	-5	234	238	6
4	1	-4	421	426	9
4	1	-3	252	264	6
4	1	-2	292	305	7
4	1	-1	252	301	6
4	1	0	167	185	7
4	1	1	674	669	8
4	1	2	611	606	8
4	1	3	399	383	8
4	1	4	133	116	14
4	1	5	156	148	14
4	1	6	239	222	11
4	1	7	218	205	14
4	2	-10	230	227	14
4	2	-9	357	359	9
4	2	-8	561	545	12
4	2	-7	620	612	10
4	2	-6	421	434	11
4	2	-5	581	575	9
4	2	-4	1150	1157	9
4	2	-3	1134	1152	9
4	2	-2	1293	1285	9
4	2	-1	922	940	8
4	2	0	1396	1416	9
4	2	1	1257	1264	9
4	2	2	1049	1066	9
3	-5	3	523	518	10
3	-5	4	601	602	10
3	-5	5	618	629	12
3	-5	6	372	375	9
3	-5	7	254	252	12
3	-5	8	195	210	17
3	-5	9	220	226	15
3	-4	-8	205	196	12
3	-4	-7	218	208	10
3	-4	-4	127	108	10
3	-4	-3	328	318	6
3	-4	-1	294	297	7
3	-4	0	154	130	8
3	-4	1	160	137	8
3	-4	4	108	86	16
3	-3	-10	272	309	13
3	-3	-9	343	363	9
3	-3	-8	278	295	10
3	-3	-7	662	649	11
3	-3	-6	847	840	10
3	-3	-5	821	824	9
3	-3	-4	601	633	8
3	-3	-3	494	511	7
3	-3	-2	1207	1216	8
3	-3	-1	1579	1573	10
3	-3	0	1861	1871	11
3	-3	1	842	858	8
3	-3	2	510	514	8
3	-3	3	842	833	9
3	-3	4	904	882	10
3	-3	5	707	716	11
3	-3	6	329	321	8
3	-3	7	348	343	9
3	-3	8	323	327	11
3	-3	9	248	264	14
3	-2	-6	249	236	8
3	-2	-4	174	163	7
3	-2	-3	129	100	8
3	12	5	210	223	15
3	12	6	271	280	13
3	13	-4	173	167	19
3	13	-2	238	221	10
3	13	-1	230	225	10
3	13	0	227	233	11
3	13	1	237	224	11
3	13	2	134	147	20
3	13	3	206	220	14
3	13	4	141	79	19
3	14	-5	229	218	15
3	14	-4	222	244	17
3	14	-3	231	230	13
3	14	-2	256	266	10
3	14	-1	252	258	10
3	14	0	287	285	10
3	14	1	330	327	9
3	14	2	287	303	11
3	14	3	213	230	14
3	15	-4	257	213	15
3	15	-3	210	196	14
3	15	0	151	158	18
3	15	1	234	215	13
3	16	-1	174	138	15
3	16	0	186	187	15
3	17	-1	168	171	17
3	17	0	198	197	15
3	17	1	179	158	16
3	-15	0	140	122	21
4	-14	-5	137	96	21
4	-14	-2	166	159	17
4	-13	-6	202	211	16
4	-13	-4	162	145	16
4	-13	-2	255	245	11
4	-13	-1	200	190	13
4	-13	0	194	216	14
4	-13	1	207	213	15
4	-13	2	212	205	15
4	-13	3	186	180	17
4	-12	-5	130	142	20
4	-12	-4	150	158	17
4	-12	-3	124	165	20
4	-12	0	144	115	17
4	-12	2	149	157	19
4	-11	-9	147	145	22
4	-11	-7	299	300	11
4	-11	-6	224	285	13
4	-11	-5	222	201	12
4	-11	-4	318	334	9
4	-11	-3	457	493	10
4	-11	-2	443	468	10
4	-11	-1	191	168	12
4	-11	0	269	267	10
4	-11	1	289	282	10
4	-11	2	374	362	9
4	4	0	1214	1191	9
4	4	1	984	995	9
4	4	2	566	583	9
4	4	3	720	721	10
4	4	4	770	749	11
4	4	5	710	720	12
4	4	6	507	501	10
4	4	7	229	225	14
4	5	-6	234	238	9
4	5	-5	277	273	7
4	5	-1	173	169	8
4	5	1	188	184	9
4	5	3	174	146	11
4	6	-11	179	201	18
4	6	-10	235	235	14
4	6	-9	265	274	11
4	6	-8	330	343	9
4	6	-6	840	851	11
4	6	-5	801	793	10
4	6	-4	703	699	10
4	6	-3	507	497	10
4	6	-1	977	993	9
4	6	0	1065	1049	9
4	6	1	729	710	9
4	6	2	667	655	10
3	-1	-2	1344	1375	9
3	-1	-1	836	838	7
3	-1	0	1000	1027	8
3	-1	1	838	842	7
3	-1	2	1305	1320	9
3	-1	3	1115	1108	9
3	-1	4	834	835	9
3	-1	5	507	515	12
3	-1	6	451	454	10
3	-1	7	464	466	11
3	-1	8	419	414	11
3	-1	9	233	232	15
3	0	-9	143	164	19
3	0	-8	212	214	11
3	0	-7	310	303	8
3	0	-5	373	346	9
3	0	-4	335	338	8
3	0	-3	479	484	7
3	0	-2	701	695	7
3	0	-1	711	744	7
3	0	0	838	804	7
3	0	1	131	130	7
3	0	2	573	560	7
3	0	3	549	556	8
3	0	4	329	321	7
3	0	5	206	205	10
3	0	7	177	151	15
3	1	-10	226	236	14
3	1	-9	330	335	10
3	1	-8	461	479	10
3	1	-7	569	572	11
3	1	-6	728	722	9
3	1	-5	718	700	8
3	1	-4	1042	1048	8
3	1	-3	898	932	7
3	1	-2	1154	1163	8
3	1	-1	1496	1541	9
4	-11	3	241	253	12
4	-11	-1	156	174	18
4	-10	-7	159	134	18
4	-10	-6	155	145	16
4	-10	-4	169	147	13
4	-10	-1	130	135	16
4	-10	0	188	208	13
4	-10	1	196	171	13
4	-10	2	130	126	19
4	-9	-9	272	271	11
4	-9	-8	296	282	11
4	-9	-7	245	225	11
4	-9	-6	260	249	10
4	-9	-5	309	305	8
4	-9	-4	608	599	11
4	-9	-3	581	599	11
4	-9	-2	408	419	9
4	-9	-1	358	369	8
4	-9	0	498	528	13
4	-9	1	598	631	13
4	-9	2	479	495	10
4	-9	3	295	304	9
4	-9	4	299	308	9
4	-9	5	275	293	11
4	-9	6	230	269	14
4	-7	-10	243	261	14
4	-7	-9	358	357	10
4	-7	-8	346	342	9
4	-7	-7	388	379	9
4	-7	-5	637	625	11
4	-7	-4	775	749	10
4	-7	-3	600	602	10
4	-7	-2	710	687	9
4	-7	-1	522	539	10
4	-7	0	662	659	10
4	-7	1	611	601	10
4	-7	2	503	504	11
4	-7	3	344	364	8
4	-7	4	418	411	10
4	-7	5	374	378	10
4	-7	6	323	329	10
4	-6	-6	114	96	18
4	-6	-5	338	323	8
4	-6	-3	197	198	8
4	-6	-1	428	430	10
4	-6	0	632	602	10
4	-6	1	135	156	13
4	-6	2	103	119	17
4	-6	3	263	280	9
4	-6	6	146	99	18
4	-6	7	138	121	21
4	-5	-11	167	130	18
4	-5	-10	228	228	15
4	8	-3	444	452	9
4	8	-2	815	817	10
4	8	-1	941	925	10
4	8	0	585	606	10
4	8	1	425	448	8
4	8	2	648	639	11
4	8	3	669	662	11
4	8	4	638	637	13
4	8	5	299	301	10
4	8	6	283	264	12
4	8	7	300	310	12
4	9	-7	198	189	13
4	9	-6	292	283	9
4	9	-5	121	113	17
4	9	-3	238	244	10
4	9	-2	529	517	12
4	9	-1	434	438	8
4	9	1	217	215	9
4	9	2	277	278	9
4	9	3	395	388	9
4	9	5	230	217	13
4	10	-7	219	237	12
4	10	-6	271	290	10
4	10	-5	235	254	11
4	10	-4	344	342	9
4	10	-3	375	366	8
4	10	-2	523	516	12
3	2	-2	768	782	7
3	2	-1	451	452	7
3	2	0	502	519	7
3	2	1	989	966	8
3	2	2	919	933	8
3	2	3	459	463	9
3	2	4	569	531	10
3	2	5	451	433	8
3	2	6	510	513	10
3	2	7	397	397	10
3	2	8	160	155	19
3	3	-10	200	198	16
3	3	-9	250	240	11
3	3	-8	325	310	8
3	3	-7	481	470	12
3	3	-6	361	365	9
3	3	-5	595	591	9
3	3	-4	769	773	8
3	3	-3	967	981	8
3	3	-2	827	830	8
3	3	-1	1169	1160	9
3	3	0	769	774	7
3	3	1	1139	1146	8
3	3	2	908	920	8
3	3	3	666	646	8
3	3	4	364	365	8
3	3	5	459	458	9
3	3	6	722	730	12
3	3	7	361	371	9
3	4	-10	237	221	13
3	4	-9	344	340	9
3	4	-8	383	401	9
3	4	-7	348	329	8
3	4	-6	232	244	8
3	4	-5	655	661	9
3	4	-4	1077	1082	9
3	4	-3	1265	1259	9
3	4	-2	430	435	9
4	-5	-9	247	242	12
4	-5	-8	345	358	9
4	-5	-7	472	480	9
4	-5	-6	555	562	11
4	-5	-4	894	888	10
4	-5	-4	740	725	9
4	-5	-3	494	491	9
4	-5	-2	704	694	8
4	-5	-1	1269	1294	10
4	-5	0	1289	1260	10
4	-5	1	727	725	9
4	-5	2	464	483	10
4	-5	3	661	634	10
4	-5	4	650	647	11
4	-5	5	359	363	8
4	-5	6	272	292	11
4	-5	7	190	181	16
4	-4	-10	219	222	15
4	-4	-7	325	344	8
4	-4	-6	559	543	10
4	-4	-5	378	368	8
4	-4	-4	245	252	6
4	-4	-3	339	328	7
4	-4	-2	583	595	8
4	-4	-1	535	540	9
4	-4	0	507	470	9
4	-4	1	401	421	10
4	-4	2	338	329	8
4	-4	3	408	420	8
4	-4	4	445	425	9
4	-4	5	210	192	11
4	-4	6	198	185	13
4	-4	7	193	150	15
4	-3	-11	198	171	16
4	-3	-10	220	220	14
4	-3	-9	273	263	10
4	-3	-8	351	350	8
4	-3	-7	356	345	8
4	-3	-6	553	532	10
4	-3	-5	377	396	8
4	-3	-4	487	496	9
4	-3	-3	698	710	8
4	-3	-2	685	704	8
4	-3	-1	878	883	8
4	-3	0	527	521	8
4	-3	1	273	282	6
4	-3	2	611	637	9
4	-3	3	763	780	10
4	-3	4	567	557	11
4	-3	5	343	336	9
4	-3	6	263	275	11
4	-3	7	317	329	11
4	-3	8	273	287	13
4	-2	-10	194	172	16
4	-2	-8	254	245	10
4	12	-2	246	252	10
4	12	-1	142	160	15
4	12	0	288	264	9
4	12	1	255	253	10
4	12	2	235	237	11
4	12	3	131	131	20
4	12	4	168	176	17
4	13	-5	260	257	13
4	13	-4	343	337	11
4	13	-3	375	362	9
4	13	-2	300	298	9
4	13	-1	270	267	9
4	13	0	356	371	8
4	13	1	424	426	9
4	13	2	390	387	10
4	13	3	225	230	13
4	13	4	234	251	13
4	13	5	286	294	12
4	14	-1	175	147	14
4	14	0	148	108	17
4	14	1	151	119	17
4	15	-4	277	271	13
4	15	-3	209	218	14
4	15	-2	168	179	16
4	15	-1	210	209	13
4	15	0	361	355	9
4	15	2	226	233	13
4	15	4	196	201	15
4	17	-2	150	162	18

h	k	l	Fo	Fc	σ
4	-1	4	333	322	8
4	-1	5	170	140	12
4	-1	6	242	231	11
4	-1	7	298	294	11
4	-1	9	141	112	23
4	0	-10	150	145	20
4	0	-9	274	254	10
4	0	-8	656	642	12
4	0	-7	656	661	10
4	0	-6	434	424	10
4	0	-5	429	433	9
4	0	-4	773	770	8
4	0	-3	1376	1385	9
4	0	-2	1075	1093	8
4	0	-1	917	904	8
4	0	0	767	758	8
4	0	1	935	941	8
4	0	2	1065	1048	9
4	0	3	846	841	9
4	0	4	507	511	11
4	0	5	407	407	10
4	0	6	486	476	10
4	0	7	363	356	9
4	0	8	252	251	14
4	0	9	144	154	24
5	-11	-3	360	369	9
5	-11	-2	241	235	10
5	-11	-1	288	297	9
5	-11	0	277	281	10
5	-11	1	340	340	9
5	-11	2	245	255	12
5	-11	3	172	193	16
5	-11	4	165	135	17
5	-11	5	150	149	20
5	-11	6	147	157	21
5	-10	-5	188	195	13
5	-10	-4	189	185	12
5	-10	-3	241	240	10
5	-10	0	184	165	13
5	-10	1	170	173	15
5	-10	2	139	160	18
5	-9	-9	171	213	20
5	-9	-8	205	194	15
5	-9	-6	253	228	10
5	-9	-5	297	313	9
5	-9	-4	398	399	10
5	-9	-3	308	307	8
5	-9	-2	276	277	8
5	-9	-1	384	404	8
5	-9	0	382	383	9
5	-9	1	397	395	9
5	-9	2	256	258	10
5	-9	3	211	218	12
5	-9	4	266	262	11
5	-9	5	264	257	12
5	-9	6	168	166	19
5	-8	-9	215	195	15
5	-8	-8	167	193	18
5	-8	-7	137	137	18
5	-8	-6	299	289	9
5	-8	-5	319	322	8
5	-8	-4	418	422	9
5	-8	-3	269	265	8
5	-8	-2	178	176	11
5	-8	-1	430	453	9
5	-8	0	404	409	10
5	-8	1	344	356	8
5	-8	2	190	182	12
5	-8	3	171	172	13
5	-8	4	135	144	18
5	-8	5	149	175	19
5	-7	-10	146	121	22
5	-7	-8	204	217	14
5	-7	-7	278	264	10
5	-7	-6	343	320	8
5	-7	-5	474	478	9
5	-7	-4	288	288	8
5	-7	-3	266	272	7
5	-7	-2	304	316	7
5	-7	-1	421	443	8
5	7	-10	176	169	17
5	7	-9	170	186	16
5	7	-8	236	235	11
5	7	-7	429	432	10
5	7	-6	523	489	12
5	7	-5	414	403	9
5	7	-4	266	277	8
5	7	-3	671	705	11
5	7	-2	993	984	10
5	7	-1	931	919	10
5	7	0	573	572	10
5	7	1	395	384	9
5	7	2	680	672	11
5	7	3	678	682	12
5	7	4	578	579	13
5	7	5	348	334	9
5	7	6	242	244	13
5	7	7	288	298	13
5	8	-5	223	233	10
5	8	-4	274	292	9
5	8	-3	221	228	10
5	8	-2	222	199	9
5	8	-1	247	243	8
5	8	0	233	249	9
5	8	1	234	229	9
5	8	2	322	311	8
5	8	3	355	379	8
5	8	4	210	201	13
5	8	7	190	183	18
5	9	-10	155	122	18
5	9	-9	143	140	19
5	9	-8	320	299	9
5	9	-7	434	444	10
5	9	-6	369	370	9
5	9	-5	239	250	10
5	9	-4	383	395	9
5	9	-3	769	804	12
5	9	-2	559	573	11
5	9	-1	343	365	8
5	9	0	201	192	10
5	9	1	666	672	11
5	9	2	690	684	11
5	9	3	473	502	11
4	2	3	542	555	9
4	2	4	604	602	10
4	2	5	752	724	11
4	2	6	628	650	13
4	2	7	403	399	9
4	2	9	219	225	16
4	3	-8	153	140	15
4	3	-7	220	215	9
4	3	-6	342	332	8
4	3	-4	115	103	11
4	3	-3	442	431	9
4	3	-2	361	351	9
4	3	-1	187	156	7
4	3	5	246	253	10
4	3	6	148	102	17
4	4	-10	299	295	11
4	4	-9	367	372	9
4	4	-8	385	397	9
4	4	-7	289	296	8
4	4	-6	624	623	10
4	4	-5	992	979	9
4	4	-4	939	953	9
4	4	-3	583	587	9
4	4	-2	573	595	9
4	4	-1	1051	1065	9
5	-7	0	363	374	8
5	-7	1	296	305	8
5	-7	2	207	219	10
5	-7	3	243	259	10
5	-7	4	281	282	10
5	-7	5	261	256	11
5	-7	6	143	139	21
5	-6	-10	235	222	14
5	-6	-9	183	158	16
5	-6	-8	135	131	19
5	-6	-7	316	325	9
5	-6	-6	420	401	9
5	-6	-5	630	628	11
5	-6	-4	358	365	9
5	-6	-3	287	285	7
5	-6	-2	471	470	10
5	-6	-1	703	707	10
5	-6	0	723	741	10
5	-6	1	433	431	8
5	-6	2	316	319	7
5	-6	3	473	468	12
5	-6	4	400	411	9
5	-6	5	327	330	9
5	-6	6	202	205	14
5	-6	7	179	185	18
5	-5	-9	195	199	15
5	-5	-8	210	226	13
5	-5	-7	254	240	10
5	-5	-6	286	269	8
5	-5	-5	279	280	7
5	-5	-4	340	342	9
5	-5	-3	306	305	7
5	-5	-2	499	501	10
5	-5	-1	699	673	9
5	-5	0	626	637	10
5	-5	1	212	213	9
5	-5	2	212	235	9
5	-5	3	280	272	8
5	-5	4	288	295	9
5	-5	5	184	190	14
5	-5	8	145	119	22
5	-4	-11	207	231	16
5	-4	-10	270	273	12
5	-4	-9	175	187	16
5	-4	-8	319	303	9
5	-4	-7	506	512	12
5	-4	-6	641	632	10
5	-4	-5	523	520	10
5	-4	-4	461	465	10
5	-4	-3	834	849	9
5	-4	-2	963	964	9
5	-4	-1	678	665	9
5	-4	0	305	320	7
5	-4	1	581	605	10
5	-4	2	654	668	10
5	11	-2	531	530	12
5	11	-1	409	421	10
5	11	0	594	603	12
5	11	1	545	528	12
5	11	2	387	387	9
5	11	3	309	325	10
5	11	4	258	253	12
5	11	5	354	357	10
5	11	6	286	306	12
5	13	-7	156	159	18
5	13	-6	181	182	16
5	13	-5	328	298	10
5	13	-4	321	323	11
5	13	-3	312	306	10
5	13	-2	213	219	12
5	13	-1	324	328	9
5	13	0	455	446	10
5	13	1	407	412	9
5	13	2	309	305	10
5	13	3	245	263	13
5	13	4	245	266	14
5	14	0	149	150	18
5	14	1	164	155	17
5	15	-6	173	160	18
5	15	-5	184	175	18
5	15	-4	187	209	17
5	15	-3	172	164	16
5	15	-2	235	216	12
5	15	-1	280	286	11
5	15	0	266	276	12
5	15	1	158	170	18
5	15	2	132	125	22
5	15	3	214	210	14
5	16	-1	181	177	16
5	16	0	187	172	15
5	16	1	136	118	20
6	-13	-4	181	187	16
6	-13	-3	147	192	19
6	-13	-2	148	144	18
6	-13	1	190	166	16
6	-13	3	135	79	22
6	-12	-8	144	124	22
4	6	3	643	624	10
4	6	4	586	578	12
4	6	5	615	615	13
4	6	6	317	315	10
4	6	7	243	253	14
4	6	8	286	279	13
4	7	-6	231	220	9
4	7	-5	278	285	8
4	7	-4	264	262	8
4	7	-3	164	148	12
4	7	-2	160	181	11
4	7	-1	621	592	10
4	7	0	423	437	10
4	7	1	175	185	9
4	7	2	210	200	9
4	7	3	351	348	8
4	7	4	301	293	9
4	7	5	163	134	16
4	7	6	182	171	16
4	8	-9	238	220	12
4	8	-8	198	198	14
4	8	-7	289	290	9
4	8	-6	371	380	8
4	8	-5	457	466	9
4	8	-4	462	479	9
5	-4	3	687	689	10
5	-4	4	330	331	8
5	-4	5	371	349	9
5	-4	6	273	274	11
5	-4	7	286	286	12
5	-4	8	200	226	17
5	-3	-7	121	101	16
5	-3	-6	108	114	16
5	-3	-5	185	193	9
5	-3	-3	337	346	7
5	-3	-1	116	87	12
5	-3	0	154	176	10
5	-3	1	245	235	7
5	-3	2	296	314	7
5	-3	4	142	149	15
5	-3	6	150	127	18
5	-2	-11	161	210	21
5	-2	-10	179	179	16
5	-2	-9	404	416	10
5	-2	-8	468	461	9
5	-2	-7	603	595	11
5	-2	-6	550	564	10
5	-2	-5	752	723	9
5	-2	-4	757	768	8
5	-2	-3	1065	1073	9
5	-2	-2	1191	1197	9
5	-2	-1	871	877	8
5	-2	0	703	732	8
5	-2	1	729	743	9
5	-2	2	1068	1078	10
5	-2	3	801	795	10
5	-2	4	343	343	9
5	-2	5	365	361	8
5	-2	6	288	302	11
5	-2	7	356	351	10
5	-2	8	208	211	17
5	-1	-8	149	107	15
5	-1	-6	201	203	9
5	-1	-5	199	196	8
5	-1	-4	111	96	11
5	-1	-3	294	291	6
5	-1	3	112	76	16
5	0	-11	149	153	21
5	0	-10	245	248	12
5	0	-9	441	451	9
5	0	-8	582	576	12
5	0	-7	588	600	11
5	0	-6	442	443	8
5	0	-5	700	697	9
5	0	-4	1017	1029	9
5	0	-3	1032	1054	9
5	0	-2	936	939	8
5	0	-1	685	696	8
5	0	0	666	689	8
6	-10	-7	182	181	16
6	-10	-6	275	271	10
6	-10	-5	280	284	10
6	-10	-4	311	318	9
6	-10	-3	187	185	12
6	-10	-2	260	279	10
6	-10	-1	252	253	10
6	-10	0	289	289	10
6	-10	1	261	266	10
6	-10	2	218	235	13
6	-10	3	161	162	16
6	-10	4	167	159	17
6	-10	5	203	180	15
6	-9	-7	136	143	20
6	-9	-6	147	113	17
6	-9	-3	175	183	12
6	-9	-2	191	204	12
6	-8	-9	201	182	16
6	-8	-8	211	198	15
6	-8	-7	287	266	10
6	-8	-6	429	440	10
6	-8	-5	515	535	13
6	-8	-4	412	412	10
6	-8	-3	268	274	8
6	-8	-2	486	522	12
6	-8	0	613	631	12
6	-8	1	302	302	9
6	-8	2	226	240	11
6	-8	3	269	278	10
6	-8	4	308	306	10
6	-8	5	212	210	14
6	-7	-1	126	100	16
6	-6	-10	224	208	14
6	-6	-9	172	194	17
6	-6	-8	269	271	11
6	-6	-7	432	429	10
6	-6	-6	511	496	12
6	-6	-5	393	392	9
6	-6	-4	329	330	7
6	-6	-3	432	440	8
6	-6	-2	752	779	10
4	10	-1	315	323	7
4	10	0	337	338	8
4	10	1	398	379	9
4	10	2	434	445	10
4	10	3	467	476	10
4	10	4	294	285	10
4	10	5	165	186	18
4	10	7	198	224	17
4	11	-7	280	276	10
4	11	-6	270	256	10
4	11	-5	242	249	11
4	11	-4	346	357	9
4	11	-3	469	462	10
4	11	-2	484	481	9
4	11	-1	313	311	9
4	11	0	420	428	9
4	11	1	535	534	12
4	11	2	578	583	13
4	11	3	250	270	12
4	11	4	159	185	18
4	11	5	216	224	14
4	11	6	242	256	14
4	12	-5	177	182	16
4	12	-4	170	184	18
4	12	-3	266	278	11
5	0	1	1326	1322	16
5	0	2	1037	1038	9
5	0	3	613	609	10
5	0	4	426	417	9
5	0	5	534	532	13
5	0	6	578	600	14
5	0	7	385	380	10
5	0	8	158	178	22
5	1	-9	195	189	14
5	1	-8	247	253	10
5	1	-5	137	153	11
5	1	-4	451	485	9
5	1	-3	155	164	8
5	1	0	194	206	7
5	1	1	278	276	7
5	1	3	161	164	12
5	1	5	125	109	19
5	2	-10	255	243	12
5	2	-9	357	347	9
5	2	-8	382	387	9
5	2	-7	402	406	9
5	2	-6	507	498	10
5	2	-5	752	750	9
5	2	-4	1004	1014	9
5	2	-3	986	961	9
5	2	-2	917	940	9
5	2	-1	920	907	9
5	2	0	1099	1114	9
5	2	1	914	916	9
5	2	2	467	463	10
5	2	3	511	500	11
5	2	4	610	609	12
5	2	5	657	654	13
5	2	6	441	435	9
5	2	7	248	227	13
5	2	8	225	183	15
5	3	-10	216	196	14
5	3	-9	266	269	11
5	3	-8	161	167	12
5	3	-6	300	289	7
5	3	-4	512	537	9
5	3	-3	225	242	7
5	3	-2	321	320	8
5	3	-1	555	563	9
5	3	0	723	717	8
5	3	1	569	549	9
5	3	2	437	425	10
5	3	3	220	215	9
5	3	4	398	389	10
5	3	5	347	329	9
5	3	6	235	215	12
5	3	7	157	153	20
5	4	-10	180	190	17
5	4	-9	295	300	10
6	-5	2	138	118	14
6	-4	-11	180	179	18
6	-4	-10	152	199	21
6	-4	-9	239	256	12
6	-4	-8	287	283	10
6	-4	-7	514	494	12
6	-4	-6	531	534	11
6	-4	-5	494	488	11
6	-4	-4	550	543	10
6	-4	-3	809	825	9
6	-4	-2	729	760	9
6	-4	-1	552	535	10
6	-4	0	442	468	11
6	-4	1	490	510	11
6	-4	2	669	700	11
6	-4	3	463	451	9
6	-4	4	363	370	9
6	-4	5	205	212	14
6	-4	6	263	254	12
6	-4	7	246	245	14
6	-3	-9	146	161	19
6	-3	-8	318	316	9
6	-3	-7	256	247	9
6	-3	-6	133	140	14
6	-3	-4	218	230	8
6	-3	-3	374	388	8
6	-3	-2	220	228	8
6	-3	0	314	308	7
6	-3	1	240	228	8
6	-3	2	357	374	8
6	-3	4	168	160	14
6	-3	5	149	169	18
6	-2	-10	206	205	14
6	-2	-9	292	294	10
6	-2	-8	416	413	10
6	-2	-7	373	372	8
6	-2	-5	508	507	10
6	-2	-4	762	785	9
6	-2	-3	777	784	9
6	-2	-2	615	614	9
4	17	-1	200	205	15
4	17	0	177	191	16
5	-15	-5	139	155	22
5	-15	-2	160	161	19
5	-15	-1	185	173	16
5	-15	2	157	111	20
5	-13	-8	188	172	17
5	-13	-7	187	205	18
5	-13	-6	177	190	18
5	-13	-5	162	173	17
5	-13	-4	184	211	15
5	-13	-3	285	293	10
5	-13	-2	255	281	12
5	-13	-1	224	258	13
5	-13	0	174	181	16
5	-13	1	249	226	12
5	-13	3	186	207	17
5	-12	-5	159	143	15
5	-11	-9	168	155	19
5	-11	-8	198	193	17
5	-11	-7	197	189	16
5	-11	-6	182	190	16
5	-11	-5	250	267	11
5	-11	-4	355	362	8
5	4	-8	272	292	10
5	4	-7	262	260	8
5	4	-6	596	600	10
5	4	-5	686	667	10
5	4	-4	597	595	9
5	4	-3	615	635	9
5	4	-2	317	340	8
5	4	-1	948	929	9
5	4	0	1002	1006	9
5	4	1	856	852	9
5	4	2	519	510	10
5	4	3	503	500	11
5	4	4	663	642	12
5	4	5	464	460	10
5	4	6	239	256	13
5	4	7	209	180	16
5	4	8	211	252	18
5	5	-11	150	168	21
5	5	-10	220	214	14
5	5	-9	147	160	18
5	5	-8	242	235	10
5	5	-7	285	269	8
5	5	-6	615	641	11
5	5	-5	521	520	10
5	5	-3	360	372	8
5	5	-2	678	679	9
5	5	-1	960	934	9
5	5	0	517	513	9
5	5	1	564	534	9
5	5	2	479	468	11
5	5	3	610	598	11
5	5	4	430	419	10
5	5	5	322	335	10
5	5	6	187	211	17
5	5	7	167	203	21
5	6	-10	142	131	20
5	6	-9	178	191	15
5	6	-8	246	250	10
5	6	-7	319	336	8
5	6	-6	355	351	8
5	6	-5	353	342	9
5	6	-4	433	432	8
5	6	-3	522	525	11
5	6	-2	543	534	10
5	6	-1	603	608	10
5	6	0	345	346	8
5	6	1	492	497	10
5	6	2	346	339	8
5	6	3	418	415	10
5	6	4	410	396	9
5	6	5	195	189	14
5	6	6	138	161	23
5	6	7	181	197	19
6	-1	-7	350	354	8
6	-1	-6	270	247	7
6	-1	-5	481	468	10
6	-1	-4	638	651	9
6	-1	-3	861	857	9
6	-1	-2	482	486	10
6	-1	-1	303	317	7
6	-1	0	675	667	9
6	-1	1	595	594	10
6	-1	2	550	560	10
6	-1	3	172	167	12
6	-1	4	371	367	9
6	-1	5	351	343	9
6	-1	6	279	286	12
6	-1	7	157	146	21
6	0	-11	162	179	19
6	0	-10	225	186	13
6	0	-9	172	160	15
6	0	-8	359	345	9
6	0	-7	408	420	9
6	0	-6	382	386	9
6	0	-5	316	326	7
6	0	-4	568	570	9
6	0	-3	624	621	9
6	0	-2	583	570	9
6	0	-1	625	645	9
6	0	0	786	768	9
6	0	1	634	641	9
6	0	2	312	317	9
6	0	3	216	213	10
6	0	4	406	400	8
6	0	5	446	435	11
6	0	6	371	364	10
6	0	7	191	158	17
6	1	-10	326	338	10
6	1	-9	330	331	9
6	1	-8	220	215	11
6	1	-7	172	163	12
6	1	-6	420	392	11
6	1	-5	765	774	9
6	1	-4	639	648	9
6	1	-3	412	415	10
6	1	-2	415	427	10

```
 5   9   4   360  348   9     6 -12  -5   154  130  17     6  -6  -1   641  626  10     6  -2  -1   592  603   9     6   1  -1   661  663   9
 5   9   5   267  266  12     6 -12  -4   221  211  13     6  -6   0   526  511  11     6  -2   0   553  577  10     6   1   0   918  922   9
 5   9   6   305  308  12     6 -12  -3   237  214  11     6  -6   1   363  377   8     6  -2   1   817  830  10     6   1   1   741  740   9
 5   9   7   250  271  14     6 -12  -2   149  167  17     6  -6   2   415  442  10     6  -2   2   634  651  10     6   1   2   355  373   9
 5  10  -3   189  188  13     6 -12   0   196  158  14     6  -6   3   528  519  13     6  -2   4   354  360   9     6   1   3   324  299   8
 5  11  -9   211  198  14     6 -12   2   177  160  17     6  -6   4   389  409   9     6  -2   5   262  262  11     6   1   4   529  505  13
 5  11  -8   223  243  13     6 -11  -4   166  178  15     6  -6   5   218  232  13     6  -2   7   212  222  16     6   1   5   393  379  10
 5  11  -7   264  277  11     6 -11  -3   181  173  14     6  -6   6   193  186  16     6  -2   8   138  147  23     6   1   6   304  305  11
 5  11  -6   245  256  12     6 -11   0   197  194  14     6  -7   7   205  183  15     6  -1  -9   297  276  10     6   1   7   201  189  16
 5  11  -5   381  356   9     6 -11   1   131  177  21     6  -5  -6   132  119  16     6  -1  -8   298  281   9     6   2  -8   221  225  10
 5  11  -4   422  426  10     6 -10  -9   195  201  17     6  -5  -5   109  138  17     6  16  -3   207  178  13     6   2  -7   148  154  13
 5  11  -3   479  487  10     6   5   2   709  672  11     6  -5  -2   235  230   8     6  16  -2   267  268  11     6   2  -6   329  331   8
 6   2  -5   239  216   7     6   5   3   747  770  11     6  10  -5   132  115  18     6  16  -1   242  232  12     7  -6  -7   254  258  10
 6   2  -4   376  369   8     6   5   4   577  557  13     6  10  -4   316  341   9     6  16   0   138  164  20     7  -6  -6   280  280   9
 6   2  -3   366  358   8     6   5   5   308  316  10     6  10  -3   267  266  10     7 -14  -4   169  162  17     7  -6  -5   198  194  11
 6   2  -1   553  556   9     6   5   6   287  310  12     6  10  -2   228  230  10     7 -14  -3   132  162  22     7  -6  -4   348  350   8
 6   2   0   392  393   8     6   5   7   335  354  12     6  10  -1   284  291   9     7 -14  -2   131  133  22     7  -6  -3   502  509  11
 6   2   1   315  322   7     6   6  -6   122  115  16     6  10   0   298  309   9     7 -12  -5   209  217  15     7  -6  -2   331  334   8
 6   2   2   137  130  13     6   6  -5   231  227   9     6  10   1   374  378   9     7 -12  -4   197  205  14     7  -6  -1   274  268   8
 6   2   3   384  365   9     6   6  -4   171  157  11     6  10   2   205  197  13     7 -12  -3   183  187  15     7  -6   0   217  212  10
 6   2   4   377  364   9     6   6   2   123  107  17     6  10   3   190  174  14     7 -12  -2   134  116  19     7  -6   1   332  335   8
 6   2   5   233  246  13     6   7 -10   219  209  13     6  10   4   157  139  19     7 -12  -1   151  162  18     7  -6   2   317  320   8
 6   3 -11   252  227  13     6   7  -9   228  237  12     6  10   5   147  154  22     7 -12   0   200  186  14     7  -6   3   269  276  10
 6   3 -10   316  332  11     6   7  -8   351  351   8     6  11  -8   198  185  13     7 -12   1   210  189  14     7  -6   4   151  162  18
 6   3  -9   301  283   9     6   7  -7   469  464   9     6  11  -7   147  163  18     7 -12   3   143  102  20     7  -6   5   162  138  17
 6   3  -8   263  267   9     6   7  -6   436  429   9     6  11  -6   185  210  15     7 -10  -9   177  151  18     7  -6   6   172  157  19
 6   3  -7   457  468   9     6   7  -5   403  390   9     6  11  -5   287  297  10     7 -10  -8   142  139  21     7  -5 -10   138   91  21
 6   3  -6   842  841  10     6   7  -4   745  756  11     6  11  -4   330  345   9     7 -10  -7   194  186  15     7  -5  -9   156  171  18
 6   3  -5   865  851  10     6   7  -3   699  733  11     6  11  -3   267  255  10     7 -10  -6   261  264  12     7  -5  -8   294  289  10
 6   3  -4   612  617  10     6   7  -2   856  851  10     6  11  -2   258  276  10     7 -10  -5   274  268  10     7  -5  -7   331  348   9
 6   3  -3   561  554   9     6   7  -1   512  528  11     6  11  -1   310  316   8     7 -10  -4   276  267   9     7  -5  -6   307  296   8
 6   3  -2   775  774   9     6   7   0   375  389  10     6  11   0   423  415   8     7 -10  -3   224  216  11     7  -5  -5   289  280   8
 6   3  -1   804  811   9     6   7   1   555  540  11     6  11   1   349  353   9     7 -10  -2   224  242  11     7  -5  -4   336  338   8
 6   3   0   904  915  10     6   7   2   644  644  12     6  11   2   325  313   9     7 -10   0   289  281  10     7  -5  -3   534  540  11
 6   3   1   684  668   9     6   7   3   737  702  12     6  11   3   234  246  13     7 -10   1   252  244  11     7  -5  -2   539  543  11
 6   3   2   557  568  11     6   7   4   399  403  10     6  11   4   227  244  15     7 -10   2   147  146  18     7  -5  -1   378  363   9
 6   3   3   552  547  11     6   7   5   257  262  13     6  11   5   280  282  13     7 -10   3   160  162  17     7  -5   0   300  296   8
 6   3   4   514  528  10     6   7   6   297  299  12     6  12  -8   128   92  20     7 -10   4   154  175  20     7  -5   1   345  356   8
 6   3   5   421  427  10     6   7   7   282  318  13     6  12  -5   281  286  11     7  -9  -1   190  192  13     7  -5   2   378  383   8
 6   3   6   269  266  12     6   8  -8   155  133  16     6  12  -4   339  351  10     7  -9   0   183  172  14     7  -5   3   301  309   9
 6   3   7   169  187  21     6   8  -7   157  164  15     6  12  -3   238  245  12     7  -8  -8   188  206  16     7  -5   4   144  137  18
 6   4  -8   188  190  12     6   8  -4   203  208  11     6  12  -2   174  154  14     7  -8  -7   307  291  10     7  -4 -10   169  140  17
 6   4  -7   204  188  10     6   8  -3   383  392   8     6  12  -1   191  172  12     7  -8  -6   273  259  10     7  -4  -9   171  184  16
 6   4  -6   286  282   8     6   8  -2   171  141  11     6  12   0   377  388   9     7  -8  -5   330  338   8     7  -4  -8   159  137  15
 6   4  -5   135  127  13     6   8   1   271  275   9     6  12   1   290  284  10     7  -8  -4   245  236   9     7  -4  -7   192  192  12
 6   4  -4   198  184   9     6   8   2   204  191  12     6  12   2   204  222  14     7  -8  -3   318  337   8     7  -4  -6   250  241   9
 6   4  -3   157  163  11     6   8   4   129  116  21     6  12   3   201  198  15     7  -8  -2   324  348   8     7  -4  -5   349  345   8
 6   4  -2   269  257   7     6   9 -10   136  127  19     6  12   4   177  215  19     7  -8  -1   462  471  10     7  -4  -4   364  383   9
 6   4  -1   184  174   9     6   9  -9   188  187  14     6  13  -5   152  154  19     7  -8   0   373  374   9     7  -4  -3   423  419   8
 6   4   0   298  293   7     6   9  -8   289  285  10     6  13  -4   215  215  14     7  -8   1   241  239  10     7  -4  -2   290  286   7
 6   4   1   187  179  10     6   9  -7   348  345   8     6  13  -3   170  157  15     7  -8   3   223  223  11     7  -4  -1   238  246   9
 6   4   2   161  152  12     6   9  -6   297  287   9     6  13  -2   200  180  13     7  -8   4   225  262  13     7  -4   0   266  256   8
 6   4   5   180  179  15     6   9  -5   339  369   9     6  13  -1   201  214  13     7  -7  -6   231  220  10     7  -4   1   295  291   8
 6   4   7   148   76  22     6   9  -4   546  555  13     6  13   0   247  257  11     7  -7  -3   304  305   8     7  -4   2   337  362   8
 6   5 -11   182  193  17     6   9  -3   552  587  13     6  13   1   215  209  13     7  -7  -2   280  276   8     7  -4   3   201  202  12
 6   5 -10   205  237  15     6   9  -2   553  556  12     6  13   2   181  160  16     7  -7  -1   129  114  17     7  -4   4   135  114  18
 6   5  -9   212  217  12     6   9  -1   386  407  10     6  13   4   142  172  22     7  -7   1   158  165  14     7  -4   5   153  101  18
 6   5  -8   332  332   8     6   9   0   671  675  11     6  14  -6   186  213  18     7  -7   2   181  205  13     7  -4   6   162  110  19
 6   5  -7   387  381  10     6   9   1   641  649  12     6  14  -5   195  213  17     7  -7   3   207  189  12     7  -3  -9   311  312  10
 6   5  -6   631  639  11     6   9   2   572  564  13     6  14  -4   166  160  17     7  -6  -9   143  133  21     7  -3  -8   388  383   9
 6   5  -5   498  507  11     6   9   3   341  322   9     6  14  -2   221  228  13     7  -6  -8   249  225  11     7  -3  -7   364  369   8
 6   5  -4   501  510  11     6   9   4   196  217  15     6  14  -1   317  328  10     7   8   4   216  206  14     7  -3  -6   190  188  11
 6   5  -3   692  692  10     6   9   5   314  316  11     6  14   0   284  274  11     7   8   5   294  269  12     7  -3  -5   362  363   7
 6   5  -2   813  831  10     6   9   6   299  339  13     6  14   2   170  194  17     7   8   6   246  258  14     7  -3  -4   570  560  10
 6   5  -1  1054 1055  10     6  10  -9   162  152  17     6  14   3   238  242  13     7   9  -8   137   95  17     7  -3  -3   774  789  10
 6   5   0   712  718  10     6  10  -8   240  215  11     6  15  -1   146   84  18     7   9  -7   191  203  13     7  -3  -2   409  416   9
 6   5   1   528  529  11     7   1  -3   499  498  10     7   5  -5   418  432   9     7   9  -6   238  243  11     7  -3  -1   467  450  11
 7  -3   0   420  446   9     7   1  -2   641  626  10     7   5  -4   482  487  12     7   9  -5   266  284  10     7  16  -2   191  206  15
 7  -3   1   560  567  11     7   1  -1   947  953  10     7   5  -3   610  611  11     7   9  -4   233  209  10     7  16  -1   142  167  19
 7  -3   2   504  495  12     7   1   0   906  920  10     7   5  -2   799  814  11     7   9  -3   313  303   8     8 -14  -4   135  127  20
 7  -3   3   375  368   8     7   1   1   599  599  10     7   5  -1   665  671  10     7   9  -2   367  371   8     8 -14  -1   134  105  21
 7  -3   4   257  266  11     7   1   2   438  443   9     7   5   0   494  462  11     7   9  -1   278  284   9     8 -12  -7   138  116  20
 7  -3   5   316  325  11     7   1   3   618  624  12     7   5   1   407  406   9     7   9   0   367  350   9     8 -12  -5   135  117  20
 7  -3   6   268  274  13     7   1   4   599  590  13     7   5   2   660  652  12     7   9   1   235  227  11     8 -12  -2   126  102  21
 7  -3   7   154  188  22     7   1   5   440  422  10     7   5   3   593  579  13     7   9   2   176  190  15     8 -12  -1   144  117  19
 7  -2  -8   186  202  13     7   1   6   205  227  16     7   5   4   391  397   9     7   9   4   164  181  19     8 -12   0   140  109  20
 7  -2  -7   189  182  11     7   2  -7   175  148  11     7   5   5   202  216  16     7   9   5   198  210  17     8 -11  -7   137   91  20
 7  -2  -6   222  211   9     7   2  -5   151  142  11     7   5   6   250  250  14     7  10  -9   208  220  13     8 -11  -6   160  150  18
 7  -2  -5   208  215   9     7   2  -4   121  116  13     7   6  -8   313  312   9     7  10  -8   229  193  11     8 -11  -5   172  152  15
 7  -2  -4   247  238   7     7   2  -3   124  105  13     7   6  -7   318  316   8     7  10  -6   186  188  14     8 -11  -1   174  192  16
 7  -2  -3   174  184  10     7   2  -2   235  227   8     7   6  -4   398  392  10     7  10  -5   470  478  11     8 -11   1   135   94  19
 7  -2  -2   294  300   7     7   2  -1   184  161  10     7   6  -3   653  668  11     7  10  -4   419  426  11     8 -10  -7   161  136  18
 7  -2  -1   285  282   7     7   2   1   106  115  17     7   6  -2   416  447   9     7  10  -3   343  356   8     8 -10  -6   145  159  19
 7  -2   0   236  260   8     7   2   2   170  147  13     7   6  -1   252  255   8     7  10  -2   266  264   9     8 -10  -4   147  137  16
 7  -2   1   351  371   8     7   3 -11   209  217  15     7   6   0   164  154  12     7  10  -1   354  359   8     8 -10  -3   157  142  15
 7  -2   2   273  267   8     7   3 -10   207  179  13     7   6   1   383  374   8     7  10   0   499  497  10     8 -10  -2   201  214  13
 7  -2   3   130  136  17     7   3  -9   247  244  11     7   6   2   388  392   9     7  10   1   380  378   9     8 -10  -1   224  207  12
 7  -1 -10   244  254  13     7   3  -8   399  407   8     7   6   3   283  275  10     7  10   2   347  334   9     8 -10   0   146  147  18
 7  -1  -9   349  340   9     7   3  -7   482  490  12     7   6   4   211  182  13     7  10   3   257  249  12     8  -9  -8   154  100  18
 7  -1  -8   391  390   9     7   3  -6   771  765  11     7   6   5   223  205  14     7  10   4   287  279  12     8  -9  -7   188  188  15
 7  -1  -7   387  383  10     7   3  -5   484  490  11     7   7 -10   140  129  19     7  10   5   286  336  13     8  -9  -6   224  222  12
 7  -1  -6   453  459   8     7   3  -4   604  600  10     7   7  -9   149  136  17     7  11  -1   142  170  17     8  -9  -5   152  165  17
 7  -1  -5   603  626  10     7   3  -3   588  588  10     7   7  -8   249  236  10     7  11   4   141  106  21     8  -9  -4   164  178  14
 7  -1  -4   814  816   9     7   3  -2   827  828  10     7   7  -7   305  311   9     7  12  -7   183  182  15     8  -9  -3   180  173  13
 7  -1  -3   546  551  10     7   3  -1   942  942  10     7   7  -6   268  270   9     7  12  -6   291  303  11     8  -9  -2   227  277  10
 7  -1  -2   596  573  10     7   3   0   575  583  10     7   7  -5   238  231  10     7  12  -5   354  395  10     8  -9  -1   227  228  12
 7  -1  -1   740  741  10     7   3   1   510  506  11     7   7  -4   306  311   8     7  12  -4   310  305  10     8  -9   0   174  178  15
 7  -1   0   821  837  10     7   3   2   500  495  12     7   7  -3   407  426  10     7  12  -3   230  237  12     8  -9   1   145  112  17
 7  -1   1   676  687  11     7   3   3   633  621  12     7   7  -2   303  295   8     7  12  -1   475  446  10     8  -9   2   142  141  18
 7  -1   2   283  281   8     7   3   4   413  397   9     7   7  -1   252  227   9     7  12   0   434  433  11     8  -9   3   203  190  14
 7  -1   3   409  407  10     7   3   5   297  308  11     7   7   0   213  201  10     7  12   1   279  285  11     8  -9   4   159  147  18
 7  -1   4   368  372   8     7   3   6   202  209  17     7   7   1   500  491  13     7  12   2   219  234  14     8  -8  -6   144   80  16
 7  -1   5   408  393  10     7   3   7   227  250  16     7   7   2   446  419  10     7  12   3   247  267  14     8  -8  -5   139  111  16
 7  -1   6   268  254  13     7   4  -8   132  118  16     7   7   3   230  250  13     7  12   4   285  290  12     8  -8  -2   174  177  13
 7  -1   7   168  190  20     7   4  -7   222  221  10     7   7   4   192  193  15     7  14  -6   191  192  16     8  -8  -1   150  155  16
 7   0  -8   136  106  16     7   4  -6   338  351   9     7   7   5   164  199  20     7  14  -5   180  223  17     8  -8   0   155  161  16
 7   0  -7   127  119  16     7   4  -5   168  149  11     7   8  -9   183  211  16     7  14  -4   140  174  20     8  -8   2   150  150  17
 7   0  -4   128  119  12     7   4  -3   308  314   7     7   8  -8   280  270  10     7  14  -3   225  229  13     8  -8   3   136  130  19
 7   0  -3   225  231   8     7   4  -2   322  314   8     7   8  -7   261  253  10     7  14  -2   317  320  10     8  -7 -10   152  119  20
 7   0  -2   365  342   8     7   4  -1   464  470   8     7   8  -6   229  233  10     7  14  -1   309  308  10     8  -7  -8   225  228  14
 7   0   1   135  113  13     7   4   1   162  146  12     7   8  -5   366  383   9     7  14   0   231  236  13     8  -7  -7   292  276  10
 7   0   2   140  110  14     7   4   2   216  242  11     7   8  -4   435  449  10     7  14   1   228  212  13     8  -7  -6   262  256  10
 7   0   3   144  114  15     7   4   3   332  327   9     7   8  -3   293  323   9     7  14   2   237  253  13     8  -7  -5   258  255   9
 7   0   4   126   82  19     7   4   4   208  186  13     7   8  -2   328  343   9     7  16  -3   174  200  16     8  -7  -4   302  318   9
 7   1 -11   215  206  15     7   5 -10   192  167  14     7   8  -1   428  432   9     8   6   1   683  683  12     8  -7  -3   356  375   9
 7   1 -10   306  290  11     7   5  -9   237  244  11     7   8   1   545  549  12                                  8  -7  -2   370  372   9
 7   1  -9   316  299   9     7   5  -8   260  241  10     7   8   1   579  581  13                                  8  -7  -1   227  222  11
 7   1  -8   272  276   9     7   5  -7   302  312   8     7   8   2   406  412   9                                  8  -7   0   215  228  11
 7   1  -7   411  405   9     7   5  -6   298  279   8     7   8   3   240  238  12                                  8  -7   1   268  280  10
 7   1  -6   603  590  10                                                                                           8  -7   2   297  306  10
 7   1  -5   878  890  10                                                                                           8  -7   3   263  248  11
 7   1  -4   665  657  10                                                                                           8  -7   4   131  122  21
 8  -6  -5   131  135  16     8  -1  -1   555  570  11     8   3 -10   154  159  18     8   6   1   683  683  12     8  13   0   134  152  20
```

h	k	l	Fo	Fc	σ
8	-6	-4	119	93	17
8	-6	2	124	91	18
8	-5	-10	192	151	16
8	-5	-9	298	297	11
8	-5	-8	362	354	9
8	-5	-7	253	263	11
8	-5	-6	280	267	9
8	-5	-5	340	345	9
8	-5	-4	600	597	11
8	-5	-3	489	486	12
8	-5	-2	488	457	12
8	-5	-1	387	384	8
8	-5	0	418	425	9
8	-5	1	422	430	10
8	-5	2	387	410	9
8	-5	3	252	265	11
8	-5	4	177	179	16
8	-5	5	176	194	17
8	-4	-3	201	191	10
8	-3	-10	177	175	17
8	-3	-9	273	276	11
8	-3	-8	316	309	9
8	-3	-7	328	335	8
8	-3	-6	330	325	7
8	-3	-5	499	504	12
8	-3	-4	628	627	11
8	-3	-3	475	485	12
8	-3	-2	373	383	9
8	-3	-1	475	479	12
8	-3	0	605	617	11
8	-3	1	547	569	12
8	-3	2	386	396	8
8	-3	3	215	226	12
8	-3	4	294	309	11
8	-3	5	329	316	11
8	-3	6	240	262	14
8	-2	-6	130	142	15
8	-2	-5	242	243	9
8	-2	-4	233	235	8
8	-2	-1	171	165	11
8	-2	0	241	245	9
8	-2	1	203	190	11
8	-2	2	152	161	14
8	-2	3	134	102	18
8	-1	-11	139	161	22
8	-1	-10	194	227	16
8	-1	-9	252	227	11
8	-1	-8	270	259	9
8	-1	-7	211	210	11
8	-1	-6	409	395	9
8	-1	-5	493	484	11
8	-1	-4	495	508	11
8	-1	-3	355	362	9
8	-1	-2	463	472	12
9	-4	-4	300	292	8
9	-4	-3	202	207	11
9	-4	-2	118	113	18
9	-4	-1	216	203	11
9	-4	0	262	254	9
9	-4	1	184	178	13
9	-4	2	170	154	14
9	-4	3	141	112	18
9	-4	4	155	141	19
9	-3	-8	202	203	12
9	-3	-7	243	241	10
9	-3	-6	255	254	9
9	-3	-5	212	228	10
9	-3	-4	244	263	9
9	-3	-3	333	331	7
9	-3	-2	399	404	10
9	-3	-1	388	385	10
9	-3	0	312	326	8
9	-3	1	207	221	12
9	-3	2	130	117	18
9	-3	3	157	168	17
9	-3	4	225	214	14
9	-3	5	192	175	16
9	-2	-10	223	226	14
9	-2	-9	198	205	14
9	-2	-8	120	131	19
9	-2	-7	186	198	12
9	-2	-6	390	400	10
9	-2	-5	490	497	12
9	-2	-4	279	278	8
9	-2	-3	219	213	10
9	-2	-2	357	351	8
9	-2	-1	522	536	12
9	-2	0	437	441	9
9	-2	1	311	322	8
9	-2	2	176	171	14
9	-2	3	229	232	12
9	-2	4	232	240	13
9	-2	5	164	180	20
9	-1	-8	128	120	18
9	-1	-6	181	189	12
9	-1	-5	217	228	10
9	-1	-4	139	131	13
9	-1	-3	196	191	10
9	-1	-2	153	146	13
9	-1	-1	195	212	11
9	-1	0	241	227	10
9	-1	1	147	150	15
9	-1	2	170	168	14
9	-1	3	207	211	13
9	-1	4	184	174	17
9	0	-11	194	198	15
9	0	-10	200	195	14
9	0	-9	167	163	15
9	0	-8	258	245	10
10	1	0	139	130	15
10	1	2	151	163	18
10	2	-10	133	156	21
10	2	-9	239	226	11
10	2	-8	223	225	11
10	2	-7	211	220	11
10	2	-6	248	260	10
10	2	-5	267	252	9
10	2	-4	431	425	10
10	2	-3	402	410	10
10	2	-2	380	378	8
10	2	-1	300	302	8
10	2	0	228	247	11
10	2	1	259	275	10

h	k	l	Fo	Fc	σ
8	-1	0	527	523	11
8	-1	1	346	350	8
8	-1	2	218	221	11
8	-1	3	310	307	9
8	-1	4	409	398	10
8	-1	5	300	279	11
8	-1	6	172	175	19
8	0	-10	176	179	16
8	0	-7	222	225	10
8	0	-6	326	334	7
8	0	-5	400	417	9
8	0	-4	215	222	9
8	0	-3	181	173	10
8	0	-2	443	423	8
8	0	-1	322	330	8
8	0	0	318	339	7
8	0	1	164	163	13
8	0	2	242	244	10
8	0	3	181	172	14
8	0	4	224	208	13
8	0	5	146	154	21
8	1	-11	195	141	15
8	1	-10	196	167	14
8	1	-9	229	216	12
8	1	-8	259	248	9
8	1	-7	380	367	8
8	1	-6	525	536	11
8	1	-5	474	468	12
8	1	-4	366	361	9
8	1	-3	435	440	8
8	1	-2	509	507	11
8	1	-1	513	511	11
8	1	0	489	498	12
8	1	1	436	435	9
8	1	2	420	424	10
8	1	3	313	300	9
8	1	4	303	298	10
8	1	5	186	208	17
8	2	-10	152	137	18
8	2	-8	201	199	12
8	2	-7	304	294	8
8	2	-6	359	374	8
8	2	-5	343	354	8
8	2	-4	265	259	8
8	2	-3	425	415	9
8	2	-2	615	620	11
8	2	-1	581	585	11
8	2	0	325	329	8
8	2	1	241	236	9
8	2	2	460	467	10
8	2	3	410	415	9
8	2	4	229	255	13
8	2	5	142	134	22
8	2	6	190	169	18
9	0	-7	422	421	10
9	0	-6	500	501	12
9	0	-5	463	467	9
9	0	-4	319	328	8
9	0	-3	431	433	9
9	0	-2	587	593	11
9	0	-1	520	503	12
9	0	0	387	397	8
9	0	1	365	371	8
9	0	2	329	339	9
9	0	3	391	389	9
9	0	4	265	265	13
9	0	5	220	200	15
9	1	-9	131	110	19
9	1	-8	128	114	17
9	1	-6	144	161	15
9	1	-4	189	177	10
9	1	-3	109	102	17
9	1	-2	117	108	16
9	1	-1	115	108	17
9	1	0	142	129	14
9	1	3	128	52	20
9	2	-11	136	151	21
9	2	-10	155	165	18
9	2	-9	233	227	12
9	2	-8	310	305	9
9	2	-7	358	365	9
9	2	-6	420	412	9
9	2	-5	305	310	8
9	2	-4	427	434	9
9	2	-3	635	623	11
9	2	-2	623	612	11
9	2	-1	532	557	12
9	2	0	360	360	8
9	2	1	421	422	10
9	2	2	460	455	10
9	2	3	448	444	11
9	2	4	256	260	13
9	2	5	210	205	16
9	3	-8	160	154	15
9	3	-5	168	162	12
9	3	-3	140	144	15
9	3	0	112	110	18
9	4	-10	160	158	16
9	4	-9	182	209	14
9	4	-8	329	299	9
9	4	-7	320	320	8
9	4	-6	303	303	8
9	4	-5	303	291	8
9	4	-4	595	605	12
9	4	-3	630	634	11
9	4	-2	387	400	8
9	4	-1	249	242	9
9	4	0	364	347	9
9	4	1	543	560	13
10	5	3	171	171	18
10	6	-8	133	125	18
10	6	-7	140	135	16
10	6	-6	186	162	12
10	6	-5	162	162	14
10	6	-4	156	116	13
10	6	-3	158	163	14
10	6	-2	252	244	10
10	6	-1	260	252	10
10	6	0	216	184	12
10	7	-9	135	140	18
10	7	-8	138	135	17
10	7	-7	191	176	12
10	7	-6	252	256	10

h	k	l	Fo	Fc	σ
8	3	-9	214	213	12
8	3	-8	245	233	10
8	3	-7	134	128	16
8	3	-6	315	311	8
8	3	-5	258	258	8
8	3	-4	332	329	8
8	3	-3	493	487	12
8	3	-2	392	398	9
8	3	-1	421	429	9
8	3	0	263	237	8
8	3	1	354	360	8
8	3	2	403	393	8
8	3	3	256	283	11
8	3	4	210	204	14
8	4	-11	153	165	19
8	4	-9	260	251	10
8	4	-8	399	400	8
8	4	-7	400	381	10
8	4	-6	365	369	8
8	4	-5	198	184	10
8	4	-4	415	428	9
8	4	-3	624	635	11
8	4	-2	722	714	11
8	4	-1	425	448	9
8	4	0	313	306	8
8	4	1	356	332	9
8	4	2	567	566	13
8	4	3	450	448	11
8	4	4	314	295	10
8	4	5	208	215	16
8	5	-10	147	142	18
8	5	-9	139	104	17
8	5	-7	129	139	17
8	5	-6	196	186	11
8	5	-5	296	305	8
8	5	-4	256	267	9
8	5	-3	188	185	11
8	5	-2	251	243	9
8	5	-1	145	152	14
8	5	0	149	152	14
8	5	1	232	221	10
8	5	2	221	214	12
8	5	3	218	205	13
8	6	-10	156	139	17
8	6	-9	238	234	11
8	6	-8	399	375	9
8	6	-7	418	410	10
8	6	-6	337	342	7
8	6	-5	484	489	9
8	6	-4	598	622	12
8	6	-3	652	696	12
8	6	-2	470	487	9
8	6	-1	325	334	8
8	6	0	483	480	9
9	4	2	425	418	9
9	4	3	288	309	11
9	4	4	238	223	13
9	4	5	214	245	17
9	5	-5	150	150	14
9	5	-4	200	210	11
9	5	-3	207	218	11
9	5	-2	124	105	16
9	5	-1	117	124	18
9	5	0	177	159	13
9	5	1	242	228	11
9	5	2	153	147	17
9	6	-10	186	168	14
9	6	-9	236	218	11
9	6	-8	248	243	11
9	6	-7	319	329	9
9	6	-6	309	300	9
9	6	-5	389	394	8
9	6	-4	446	449	10
9	6	-3	395	389	10
9	6	-2	407	397	10
9	6	-1	426	435	10
9	6	0	563	571	12
9	6	1	518	506	10
9	6	2	273	263	10
9	6	3	213	200	14
9	6	4	240	237	14
9	7	-10	154	141	16
9	7	-9	161	155	15
9	7	-8	143	133	16
9	7	-7	204	205	12
9	7	-4	236	234	10
9	7	-3	146	151	14
9	7	-1	221	213	11
9	7	0	219	214	12
9	7	1	247	269	11
9	7	4	176	131	18
9	8	-9	180	156	14
9	8	-8	154	166	16
9	8	-7	198	195	12
9	8	-6	236	242	11
9	8	-5	346	335	8
9	8	-4	286	292	9
9	8	-3	276	283	9
9	8	-2	268	258	9
9	8	-1	357	348	8
9	8	0	401	392	9
9	8	1	258	271	11
9	8	2	244	243	12
9	8	3	235	224	13
9	9	-7	153	157	16
9	9	-6	256	271	11
9	9	-5	320	331	9
9	9	-4	264	262	10
9	9	-3	192	197	12
11	-6	-5	200	231	14
11	-6	-4	196	206	13
11	-6	-2	176	164	14
11	-6	0	193	199	14
11	-6	1	149	138	17
11	-6	-6	153	119	15
11	-5	-5	134	124	15
11	-4	-7	175	151	14
11	-4	-6	136	46	16
11	-4	-5	223	235	11
11	-4	-3	196	194	12

h	k	l	Fo	Fc	σ
8	6	2	555	541	14
8	6	3	300	281	10
8	6	4	270	262	12
8	6	5	272	266	13
8	7	-3	148	153	14
8	8	-10	185	178	14
8	8	-9	277	273	10
8	8	-8	301	279	9
8	8	-7	205	223	12
8	8	-6	307	315	9
8	8	-5	430	407	10
8	8	-4	482	501	10
8	8	-3	423	422	10
8	8	-2	484	496	9
8	8	-1	514	513	13
8	8	0	573	588	13
8	8	1	539	511	13
8	8	2	319	314	10
8	8	3	293	288	11
8	8	4	311	317	12
8	9	-5	139	127	17
8	10	-9	152	150	16
8	10	-8	143	139	17
8	10	-7	223	225	12
8	10	-6	275	271	10
8	10	-5	360	373	9
8	10	-4	325	345	9
8	10	-3	295	303	9
8	10	-2	299	306	9
8	10	-1	371	355	9
8	10	0	520	500	10
8	10	1	356	348	9
8	10	2	216	249	14
8	10	3	262	259	12
8	11	-5	193	177	13
8	11	-1	213	206	13
8	11	0	144	133	19
8	11	3	147	131	20
8	12	-7	166	171	17
8	12	-6	195	219	15
8	12	-5	178	171	15
8	12	-4	175	206	16
8	12	-3	220	226	13
8	12	-2	312	303	9
8	12	-1	313	310	9
8	12	0	233	228	13
8	12	1	183	182	16
8	12	2	205	209	15
8	13	-7	152	150	17
8	13	-6	181	177	15
8	13	-3	161	152	16
8	13	-2	274	264	11
8	13	-1	215	222	13
9	9	-2	222	241	12
9	9	-1	312	302	9
9	9	0	343	356	9
9	9	1	150	184	19
9	9	2	149	164	19
9	9	3	238	222	13
9	10	-7	156	152	16
9	10	-6	138	152	18
9	10	-5	185	199	14
9	10	-4	205	227	13
9	10	-3	210	197	12
9	10	-2	201	188	12
9	10	-1	249	243	11
9	10	0	225	203	12
9	10	2	150	160	20
9	11	-7	233	230	12
9	11	-6	238	238	11
9	11	-5	180	208	14
9	11	-3	231	255	12
9	11	-2	317	312	10
9	11	-1	309	306	10
9	11	0	207	225	12
9	11	1	176	165	16
9	11	2	265	252	12
9	12	-5	159	131	15
9	13	-4	195	222	14
9	13	-3	308	308	10
9	13	-2	312	322	10
9	13	-1	232	223	12
9	13	0	193	185	14
10	-11	-4	123	101	20
10	-11	-3	131	135	21
10	-9	-7	139	96	19
10	-9	-6	140	118	19
10	-9	-4	124	130	21
10	-9	-3	169	164	15
10	-8	-6	189	165	15
10	-8	-5	123	133	20
10	-8	-4	170	160	15
10	-8	-3	200	175	13
10	-8	-1	162	119	15
10	-8	0	155	153	17
10	-7	-6	138	130	18
10	-7	-5	144	146	17
10	-7	-4	165	171	15
10	-6	-9	148	160	20
10	-6	-6	160	161	17
10	-6	-5	215	223	12
10	-6	-4	353	337	9
10	-6	-3	274	272	10
10	-6	-2	203	188	12
10	-6	-1	202	196	12
10	-6	0	256	244	10
10	-6	1	236	216	11
11	0	0	175	147	13
11	0	1	174	169	15
11	0	2	202	193	14
11	1	-9	203	199	13
11	1	-8	268	272	10
11	1	-7	200	224	13
11	1	-5	148	143	15
11	1	-4	135	168	16
11	1	-3	377	388	9
11	1	-1	251	239	9
11	1	0	223	208	11

h	k	l	Fo	Fc	σ
8	14	-4	163	163	16
8	14	-3	166	184	17
8	14	-2	206	198	13
8	14	-1	157	156	18
9	-13	-5	140	124	20
9	-11	-2	178	209	16
9	-11	-1	230	231	13
9	-11	0	128	150	21
9	-11	1	133	102	21
9	-9	-7	196	200	15
9	-9	-6	156	162	17
9	-9	-5	142	154	18
9	-9	-4	159	168	15
9	-9	-3	273	264	10
9	-9	-2	228	218	12
9	-9	-1	129	137	20
9	-9	1	183	171	14
9	-9	2	186	186	16
9	-9	3	156	153	18
9	-7	-9	173	165	18
9	-7	-8	186	182	16
9	-7	-7	184	189	15
9	-7	-6	207	206	12
9	-7	-5	223	227	11
9	-7	-4	270	261	9
9	-7	-3	331	336	8
9	-7	-2	280	263	9
9	-7	-1	201	213	12
9	-7	0	212	203	12
9	-7	1	250	264	11
9	-7	2	234	236	12
9	-6	-3	168	156	13
9	-6	-2	164	137	13
9	-6	-1	132	129	17
9	-6	0	152	136	15
9	-6	1	136	125	18
9	-6	2	125	118	20
9	-5	-9	211	183	14
9	-5	-8	194	188	14
9	-5	-7	211	214	12
9	-5	-6	226	247	11
9	-5	-5	312	310	8
9	-5	-4	304	300	8
9	-5	-3	329	332	8
9	-5	-2	229	215	10
9	-5	-1	291	278	9
9	-5	0	262	266	10
9	-5	1	322	333	9
9	-5	2	225	248	12
9	-5	4	181	167	16
9	-5	5	168	166	18
9	-4	-10	182	121	15
9	-4	-6	159	167	14
9	-4	-5	351	354	9
10	-6	2	140	139	19
10	-6	3	142	115	19
10	-5	-7	133	120	18
10	-4	-10	161	164	18
10	-4	-9	160	150	18
10	-4	-8	139	131	19
10	-4	-7	200	195	12
10	-4	-6	285	282	9
10	-4	-5	263	265	9
10	-4	-4	287	268	8
10	-4	-3	180	174	12
10	-4	-2	251	249	10
10	-4	-1	350	341	8
10	-4	0	333	335	9
10	-4	1	228	228	11
10	-4	2	147	130	17
10	-4	3	202	185	15
10	-4	4	163	199	19
10	-2	-10	143	167	21
10	-2	-9	177	146	15
10	-2	-8	219	213	12
10	-2	-7	306	319	9
10	-2	-6	385	404	9
10	-2	-5	327	330	8
10	-2	-4	311	298	8
10	-2	-3	324	319	8
10	-2	-2	429	418	10
10	-2	-1	367	347	8
10	-2	0	319	313	8
10	-2	1	237	246	11
10	-2	2	242	241	12
10	-2	3	278	272	12
10	-2	4	219	224	15
10	-1	-2	128	142	17
10	-1	-1	118	71	17
10	0	-10	148	130	18
10	0	-9	157	163	17
10	0	-8	274	274	10
10	0	-7	324	316	8
10	0	-6	335	329	8
10	0	-5	258	250	9
10	0	-4	348	339	8
10	0	-3	469	460	9
10	0	-2	491	488	13
10	0	-1	406	409	10
10	0	0	277	294	9
10	0	1	296	295	9
10	0	2	360	366	9
10	0	3	301	299	11
10	0	4	208	181	15
11	7	-2	334	323	9
11	7	-1	323	327	10
11	7	0	262	264	11
11	7	1	203	197	14
11	7	2	202	209	15
11	8	-7	127	102	18
11	8	-6	171	181	15
11	8	-1	168	178	16
11	9	-7	172	172	14
11	9	-6	187	202	13
11	9	-5	169	177	14
11	9	-4	156	174	16
11	9	-3	220	240	12
11	9	-2	245	245	11

h	k	l	Fo	Fc	σ
10	2	2	364	365	9
10	2	3	240	251	13
10	2	4	187	172	17
10	3	-9	166	166	16
10	3	-8	239	246	11
10	3	-7	186	166	12
10	3	-6	126	168	17
10	3	-5	123	146	18
10	3	-4	384	387	8
10	3	-3	387	383	8
10	3	-2	212	183	10
10	3	-1	133	154	16
10	3	0	271	265	9
10	3	1	262	270	10
10	3	2	223	215	13
10	4	-10	125	99	20
10	4	-8	216	206	11
10	4	-7	256	264	10
10	4	-6	200	201	12
10	4	-5	295	291	9
10	4	-4	279	264	9
10	4	-3	295	296	9
10	4	-2	236	234	10
10	4	-1	244	244	10
10	4	0	288	285	9
10	4	1	305	303	10
10	4	2	237	229	12
10	4	4	165	148	19
10	5	-10	144	148	18
10	5	-9	225	223	12
10	5	-8	226	210	11
10	5	-7	209	193	11
10	5	-6	242	250	10
10	5	-5	380	382	9
10	5	-4	381	383	9
10	5	-3	222	212	10
10	5	-2	265	281	9
10	5	-1	356	368	8
10	5	0	452	475	11
10	5	1	316	319	10
10	5	2	243	214	12
12	1	-9	139	162	19
12	1	-8	190	173	13
12	1	-7	156	176	16
12	1	-6	242	245	11
12	1	-5	254	239	10
12	1	-4	331	337	8
12	1	-3	280	264	9
12	1	-2	173	187	14
12	1	-1	198	196	12
12	1	0	248	241	11
12	1	1	249	259	12
12	1	2	169	155	16
12	2	-4	132	132	17
12	2	0	150	103	16
12	3	-9	152	144	16
12	3	-8	148	140	17
12	3	-7	184	181	13
12	3	-6	223	227	11
12	3	-5	252	252	10
12	3	-4	209	200	12
12	3	-3	199	192	12
12	3	-2	255	265	10
12	3	-1	290	289	10
12	3	0	299	297	10
12	3	1	207	208	14
12	4	-6	132	122	17
12	4	-5	208	192	12
12	4	-4	119	137	19
12	4	0	164	156	16
12	4	1	133	120	20
12	5	-7	130	144	18
12	5	-6	184	171	13
12	5	-5	211	197	12
12	5	-4	161	177	15
12	5	-3	181	185	13
12	5	-2	189	177	13
12	5	-1	218	208	12
12	5	0	216	207	13
12	5	1	134	137	20
12	6	-7	150	170	16
12	6	-6	219	222	11
12	6	-5	132	160	18
12	6	-3	143	144	17
12	6	-2	259	246	10
12	6	-1	205	189	13
12	6	0	159	157	17
12	7	-5	152	150	15
12	7	-4	175	165	14
12	7	-3	170	154	14
12	7	-2	159	116	15
12	7	-1	133	137	19
12	8	-7	209	208	12
12	8	-4	140	163	18
12	8	-3	277	279	10
12	8	-2	246	254	11
10	7	-5	407	413	10
10	7	-4	350	352	8
10	7	-3	218	220	11
10	7	-2	246	249	10
10	7	-1	361	361	8
10	7	0	420	415	9
10	7	1	253	255	12
10	7	2	234	197	13
10	7	3	200	224	16
10	8	-3	125	134	18
10	8	-1	123	91	20
10	9	-8	172	140	14
10	9	-7	242	242	11
10	9	-6	309	306	9
10	9	-5	275	300	10
10	9	-4	204	223	12
10	9	-3	261	264	10
10	9	-2	373	375	9
10	9	-1	407	389	10
10	9	0	283	283	11
10	9	2	259	250	13
10	11	-7	212	205	12
10	11	-6	184	197	14
10	11	-5	160	182	15
10	11	-4	201	204	13
10	11	-3	280	271	10
10	11	-2	335	332	10
10	11	-1	277	276	11
10	11	0	207	210	14
10	12	-3	134	96	18
10	13	-3	203	211	13
11	-10	-4	128	119	20
11	-10	-3	152	126	17
11	-8	-6	138	103	19
11	-8	-4	188	180	14
11	-8	-2	131	121	19
11	-8	0	170	156	16
11	-8	1	137	145	20
11	-6	-8	142	116	19
11	-6	-7	197	176	14
11	-6	-6	214	197	12
12	8	-1	137	160	19
12	9	-2	122	61	19
12	10	-4	177	215	14
12	10	-3	240	252	11
13	-7	-6	130	126	20
13	-5	-7	151	134	16
13	-5	-6	127	129	19
13	-5	-5	132	106	18
13	-5	-2	171	150	15
13	-3	-8	142	119	18
13	-3	-6	165	110	14
13	-3	-4	134	157	19
13	-3	-3	195	195	13
13	-3	-2	149	154	17
13	-3	-1	131	124	18
13	-3	0	132	115	19
13	-2	-8	146	102	17
13	-1	-8	130	99	19
13	-1	-7	143	109	16
13	-1	-5	142	134	16
13	-1	-4	174	185	14
13	-1	-3	169	158	14
13	-1	0	134	140	19
13	0	-8	126	77	18
13	0	-5	152	132	15
13	0	-4	177	156	13
13	0	-3	150	138	15
13	0	-1	146	123	16
13	0	0	153	165	17
13	1	-6	135	120	17
13	1	-3	118	131	19
13	1	-1	161	137	15
13	1	0	137	146	19
13	2	-6	191	173	13
13	2	-5	199	180	12
13	2	-4	160	150	14
13	2	-3	119	102	19
13	2	-2	155	148	15
13	2	-1	207	184	12
13	2	0	201	173	13
13	3	-1	123	111	20
13	4	-8	139	101	16
13	4	-7	160	184	15
13	4	-6	221	204	11
13	4	-5	220	213	11
13	4	-4	169	153	14
13	4	-3	178	164	13
13	4	-2	221	211	12
13	4	-1	234	221	12
13	4	0	165	178	16
13	5	-5	125	57	17
13	6	-7	189	178	12
13	6	-6	161	176	15
13	6	-5	143	141	16
13	6	-4	125	158	19
11	-4	-2	240	241	11
11	-4	-1	274	268	10
11	-4	0	204	185	13
11	-4	1	178	137	14
11	-4	2	166	146	17
11	-4	3	165	164	18
11	-3	-6	149	153	16
11	-3	-5	127	138	18
11	-3	-3	172	162	13
11	-3	-2	229	228	11
11	-3	-1	167	176	15
11	-2	-9	136	128	19
11	-2	-8	195	179	13
11	-2	-7	202	197	12
11	-2	-6	205	216	12
11	-2	-5	204	229	12
11	-2	-4	166	169	13
11	-2	-3	235	223	10
11	-2	-2	234	224	10
11	-2	-1	215	204	11
11	-2	0	182	179	13
11	-2	2	184	190	16
11	-1	-8	206	179	12
11	-1	-7	204	199	12
11	-1	-6	121	123	18
11	-1	-5	175	171	13
11	-1	-4	189	176	11
11	-1	-3	297	283	8
11	-1	-2	273	273	9
11	-1	-1	181	200	13
11	-1	0	149	149	16
11	-1	1	164	148	15
11	-1	2	205	211	15
11	-1	3	231	195	13
11	0	-9	158	130	16
11	0	-6	137	130	16
11	0	-5	159	193	12
11	0	-4	217	193	10
11	0	-3	195	200	12
11	0	-2	172	195	13
13	6	-3	247	222	10
13	6	-2	202	230	13
13	6	-1	196	193	13
13	8	-4	189	190	13
14	-3	-6	122	55	18
14	-2	-3	135	109	17
14	0	-6	159	151	15
14	0	-5	171	164	14
14	0	-2	158	140	15
14	2	-7	123	111	18
14	2	-6	155	144	15
14	2	-5	189	163	12
14	2	-4	150	130	15
14	2	-2	158	157	15
14	4	-6	156	139	14
14	4	-5	140	139	16
14	4	-4	155	145	14
14	4	-3	173	164	14
11	1	1	292	286	10
11	1	2	258	250	12
11	1	3	141	164	21
11	2	-7	118	87	19
11	2	-6	132	112	16
11	2	-5	139	122	15
11	2	2	128	82	21
11	3	-10	149	116	17
11	3	-9	234	208	11
11	3	-8	206	202	12
11	3	-7	198	211	12
11	3	-6	258	246	9
11	3	-5	357	358	9
11	3	-4	387	380	9
11	3	-3	307	306	9
11	3	-2	263	246	9
11	3	-1	322	312	8
11	3	0	375	364	8
11	3	1	369	367	9
11	3	2	213	222	14
11	3	3	141	151	21
11	4	-3	124	98	17
11	5	-9	203	192	13
11	5	-8	183	191	13
11	5	-7	150	175	16
11	5	-6	274	271	10
11	5	-5	363	357	8
11	5	-4	297	299	9
11	5	-3	245	254	10
11	5	-2	326	333	8
11	5	-1	368	376	9
11	5	0	335	318	9
11	5	1	297	289	10
11	5	2	166	181	18
11	7	-9	152	139	15
11	7	-8	150	141	16
11	7	-7	217	220	12
11	7	-6	276	270	10
11	7	-5	282	277	9
11	7	-4	228	232	11
11	7	-3	278	266	9
11	9	-1	231	211	12
11	9	0	175	143	15
11	10	-7	164	171	14
11	10	-6	142	119	16
11	10	-3	218	203	12
11	10	-2	167	203	16
11	10	-1	161	139	16
11	11	-4	162	171	15
11	11	-3	186	200	14
11	11	-2	199	200	14
12	-8	0	151	91	16
12	-7	0	148	95	17
12	-6	-2	174	120	14
12	-5	-7	162	150	16
12	-5	-6	170	159	15
12	-5	-5	135	125	18
12	-5	-2	172	164	15
12	-5	-1	165	162	16
12	-5	0	142	114	18
12	-3	-9	137	85	18
12	-3	-8	176	154	15
12	-3	-7	142	174	18
12	-3	-6	215	194	11
12	-3	-5	162	148	14
12	-3	-4	192	177	13
12	-3	-3	248	230	11
12	-3	-2	290	273	9
12	-3	-1	192	179	13
12	-3	0	149	129	17
12	-1	-9	162	156	16
12	-1	-8	194	184	13
12	-1	-7	184	168	13
12	-1	-6	184	166	12
12	-1	-5	186	181	12
12	-1	-4	252	239	10
12	-1	-3	283	279	9
12	-1	-2	239	234	10
12	-1	-1	174	169	14
12	-1	0	168	165	15
12	-1	1	215	212	14
12	-1	2	210	213	14

Table A3: *Observed And Calculated Structure Factors For The [(o-Tol)₃PAu(6-MP)].C₂H₅OH Complex.*

10|F|o vs 10|F|c

h	k	l	Fo	Fc	sigF
0	0	4	2676	2460	10
0	0	6	2661	2520	10
0	0	8	358	331	6
0	0	10	1786	1822	8
0	0	12	640	650	6
0	0	14	1078	1119	7
0	0	16	804	843	8
0	0	18	855	889	8
0	0	20	941	1019	9
0	0	24	975	1030	10
0	0	26	523	561	15
0	0	28	440	440	13
0	0	30	392	433	12
0	1	1	1403	1560	6
0	1	2	428	449	3
0	1	3	3333	3158	13
0	1	4	1681	1719	7
0	1	5	1645	1635	7
0	1	6	443	408	5
0	1	7	2019	2007	8
0	1	8	399	373	6
0	1	9	740	742	6
0	1	10	795	754	6
0	1	11	922	944	7
0	1	12	483	453	8
0	1	13	1395	1437	8
0	1	14	270	326	8
0	1	15	400	405	9
0	1	17	1320	1344	8
0	1	18	379	376	9
0	1	19	415	433	12
0	1	21	891	944	10
0	1	23	857	920	11
0	1	24	213	215	14
0	1	25	331	311	10
0	1	27	759	802	13
0	1	29	252	251	17
0	1	30	192	152	23
0	1	31	267	291	19
0	1	33	286	301	21
0	2	0	2494	2409	10
0	2	1	119	134	4
0	2	2	1835	1824	7
0	2	3	482	506	4
0	2	4	2742	2694	11
0	2	5	1267	1293	6
0	2	6	3105	3166	12
0	2	7	1124	1159	6
0	2	8	1373	1405	6
0	2	9	108	87	9
0	2	10	2003	1988	9
0	2	11	483	475	7
0	2	12	545	518	7
0	2	13	214	188	7
0	2	14	1232	1207	8
0	12	13	245	236	11
0	12	14	200	190	14
0	12	15	496	474	14
0	13	2	393	377	13
0	13	4	239	225	10
0	13	6	220	226	11
0	13	8	331	327	10
0	13	11	194	153	14
1	0	-33	394	318	19
1	0	-29	705	637	20
1	0	-27	544	552	16
1	0	-25	477	497	16
1	0	-23	926	958	15
1	0	-19	807	866	14
1	0	-17	827	776	13
1	0	-15	980	1012	13
1	0	-13	1734	1743	13
1	0	-11	582	548	15
1	0	-9	2994	3166	16
1	0	-5	1202	1738	9
1	0	-3	3383	3245	13
1	0	-1	266	207	4
1	0	1	3192	3283	12
1	0	3	820	747	4
1	0	5	1031	1015	5
1	0	7	1107	1125	6
1	0	9	225	172	7
1	0	11	683	750	6
1	0	13	268	261	9
1	0	15	1537	1565	8
1	0	17	538	587	9
1	0	19	819	810	9
1	0	21	1315	1369	9
1	0	25	736	703	12
1	0	27	512	497	17
1	0	29	323	322	14
1	0	31	252	214	20
1	1	-32	409	387	17
1	1	-30	506	437	15
1	1	-26	812	795	18
1	1	-24	514	497	15
1	1	-22	700	688	17
1	1	-20	952	932	15
1	1	-19	276	224	13
1	1	-18	362	351	12
1	1	-16	1276	1271	14
1	1	-15	248	212	12
1	1	-14	545	476	14
1	1	-12	2114	2156	14
1	1	-11	394	427	10
1	1	-10	1970	1930	11
1	1	-9	204	70	7
1	1	-8	1040	1103	9
1	1	-6	2669	2765	11
1	1	-5	249	238	6
1	5	9	624	615	7
1	5	10	508	508	7
1	5	11	172	163	9
1	5	12	1074	1061	7
0	2	15	408	384	10
0	2	16	902	909	8
0	2	17	367	368	9
0	2	18	606	616	10
0	2	20	1133	1135	10
0	2	22	212	203	14
0	2	24	758	761	13
0	2	26	256	267	15
0	2	28	283	306	16
0	2	30	459	439	14
0	3	1	1236	1283	5
0	3	2	271	282	5
0	3	3	1813	1881	7
0	3	4	242	232	6
0	3	5	285	269	6
0	3	6	705	683	5
0	3	7	2043	2021	8
0	3	9	952	989	6
0	3	9	1721	1716	8
0	3	10	864	862	6
0	3	11	1641	1680	8
0	3	12	725	698	7
0	3	13	1177	1169	7
0	3	14	387	340	10
0	3	15	370	344	10
0	3	16	296	276	10
0	3	17	1615	1570	9
0	3	18	570	588	11
0	3	19	521	521	12
0	3	21	745	722	12
0	3	22	389	435	13
0	3	23	518	515	15
0	3	27	567	547	19
0	3	31	341	355	18
0	4	0	1588	1655	7
0	4	1	112	124	6
0	4	2	492	517	5
0	4	3	207	215	5
0	4	4	1465	1503	6
0	4	5	513	541	5
0	4	6	1228	1240	6
0	4	7	623	613	5
0	4	8	765	755	6
0	4	9	1004	954	6
0	4	10	1844	1770	8
0	4	11	632	608	7
0	4	12	356	364	10
0	4	13	648	642	7
0	4	14	1780	1755	9
0	4	15	848	871	8
0	4	16	731	703	8
0	4	17	455	445	11
0	4	18	654	677	10
0	4	19	431	401	13
0	4	20	526	522	12
1	1	-4	196	165	6
1	1	-3	163	186	4
1	1	-2	3269	2913	12
1	1	-1	180	222	5
1	1	0	2126	2004	8
1	1	1	1179	1136	5
1	1	2	801	765	4
1	1	3	1003	960	5
1	1	4	2190	2181	9
1	1	5	1625	1557	7
1	1	6	1448	1442	7
1	1	7	874	892	5
1	1	8	2292	2313	9
1	1	9	651	636	6
1	1	10	806	781	6
1	1	11	625	621	7
1	1	12	1636	1700	9
1	1	13	147	146	10
1	1	14	1678	1681	9
1	1	15	501	485	9
1	1	16	404	405	11
1	1	17	222	218	9
1	1	18	1576	1604	9
1	1	20	368	422	10
1	1	22	768	789	11
1	1	24	760	756	12
1	1	26	262	264	14
1	1	28	478	464	14
1	1	32	298	271	20
1	2	-33	393	400	19
1	2	-29	507	505	14
1	2	-27	407	369	13
1	2	-26	355	365	14
1	2	-25	368	368	13
1	2	-24	284	304	16
1	2	-23	877	893	16
1	2	-21	200	156	18
1	2	-20	521	510	13
1	2	-19	1434	1409	13
1	2	-18	483	463	12
1	2	-17	855	825	13
1	2	-15	1247	1190	11
1	2	-14	644	616	11
1	2	-13	1242	1112	10
1	2	-12	623	530	9
1	2	-11	193	151	9
1	2	-10	312	275	8
1	2	-9	2775	2615	12
1	2	-8	290	283	8
1	2	-7	1129	1142	6
1	2	-6	480	463	5
1	2	-5	2741	2623	11
1	2	-4	2208	2104	9
1	2	-3	1484	1428	6
1	2	-2	521	526	4
1	6	14	465	461	10
1	6	15	388	387	11
1	6	16	511	486	10
1	6	17	445	428	12
0	4	21	266	245	11
0	4	24	613	601	14
0	4	25	308	269	13
0	4	28	342	353	15
0	4	29	212	166	25
0	4	30	279	259	21
0	5	1	548	604	5
0	5	2	502	558	5
0	5	3	986	1019	6
0	5	4	348	317	6
0	5	5	350	325	7
0	5	6	698	665	6
0	5	7	1747	1721	8
0	5	8	1139	1085	6
0	5	9	387	365	9
0	5	10	360	329	9
0	5	11	1348	1310	7
0	5	12	897	886	7
0	5	13	1448	1389	8
0	5	14	604	594	8
0	5	15	162	168	12
0	5	16	862	825	8
0	5	17	899	853	9
0	5	18	250	211	10
0	5	19	329	331	9
0	5	21	512	496	13
0	5	22	461	417	11
0	5	23	328	317	11
0	5	24	196	181	18
0	5	25	228	194	17
0	5	26	276	263	15
0	5	27	314	302	15
0	6	0	1118	1156	6
0	6	1	1017	1050	6
0	6	2	285	299	9
0	6	3	182	192	6
0	6	4	1261	1279	7
0	6	5	1054	1047	6
0	6	6	993	979	6
0	6	7	614	568	6
0	6	8	826	822	6
0	6	9	476	479	8
0	6	10	1272	1242	7
0	6	11	809	816	7
0	6	12	285	286	7
0	6	13	541	529	9
0	6	14	779	753	8
0	6	15	687	637	9
0	6	16	655	633	9
0	6	17	139	117	16
0	6	18	340	333	11
0	6	19	757	723	10
0	6	20	724	681	11
0	6	21	331	339	10
0	6	23	292	256	12
1	2	-1	156	163	5
1	2	0	1331	1309	6
1	2	1	1630	1653	7
1	2	2	478	486	4
1	2	3	652	671	4
1	2	4	942	975	5
1	2	5	1682	1724	7
1	2	6	355	400	5
1	2	7	2337	2342	9
1	2	8	143	159	7
1	2	9	1161	1140	6
1	2	10	288	293	9
1	2	11	1615	1590	8
1	2	12	499	472	8
1	2	13	113	131	14
1	2	14	277	296	8
1	2	15	1442	1474	8
1	2	16	569	549	10
1	2	17	810	833	9
1	2	18	152	144	15
1	2	19	640	660	11
1	2	20	279	271	10
1	2	21	851	863	11
1	2	22	272	294	11
1	2	25	657	654	14
1	2	27	261	271	16
1	2	29	263	251	19
1	2	31	371	378	16
1	3	-30	343	337	17
1	3	-27	233	207	20
1	3	-26	600	562	18
1	3	-24	203	163	19
1	3	-23	250	211	16
1	3	-22	651	657	16
1	3	-20	987	984	13
1	3	-18	611	607	13
1	3	-17	707	681	12
1	3	-16	1514	1423	11
1	3	-15	139	78	15
1	3	-14	382	413	9
1	3	-13	355	298	9
1	3	-12	1862	1682	9
1	3	-10	1369	1250	8
1	3	-9	719	669	6
1	3	-8	635	618	6
1	3	-7	1113	1079	6
1	3	-6	1942	1902	8
1	3	-5	241	197	7
1	3	-4	215	189	5
1	3	-3	1053	1044	5
1	3	-2	1508	1503	6
1	3	-1	1492	1487	6
1	3	0	451	466	6
1	3	1	1543	1545	6
1	3	2	1386	1446	6
1	7	22	452	458	12
1	7	23	547	513	15
1	7	24	323	344	12
1	7	25	241	239	17
0	6	24	271	291	14
0	6	25	490	467	13
0	6	28	228	234	22
0	6	29	200	221	27
0	7	1	617	662	6
0	7	2	1195	1206	7
0	7	3	826	841	6
0	7	4	872	875	6
0	7	5	171	163	8
0	7	6	500	501	7
0	7	7	864	874	7
0	7	8	1001	994	7
0	7	11	584	545	8
0	7	12	625	577	8
0	7	13	607	573	9
0	7	14	315	297	10
0	7	15	324	293	10
0	7	16	330	330	10
0	7	17	466	443	12
0	7	18	482	473	13
0	7	20	265	227	11
0	7	21	392	376	12
0	7	22	516	510	15
0	7	23	434	422	13
0	7	25	284	249	14
0	7	26	265	243	16
0	7	27	287	292	17
0	7	28	343	326	15
0	8	0	856	879	7
0	8	1	1015	1011	7
0	8	2	130	112	10
0	8	3	266	280	8
0	8	4	919	931	7
0	8	5	1049	1043	7
0	8	6	447	453	8
0	8	9	727	702	7
0	8	10	637	642	8
0	8	11	574	548	9
0	8	13	187	190	11
0	8	14	485	469	11
0	8	15	692	676	9
0	8	16	170	173	14
0	8	18	266	265	10
0	8	19	438	412	15
0	8	20	313	310	10
0	8	21	431	406	12
0	8	23	236	162	15
0	8	24	391	391	12
0	8	25	450	456	15
0	9	1	395	407	9
0	9	2	1073	1094	7
0	9	3	531	545	8
0	9	4	434	431	9
0	9	6	509	496	9
0	9	7	358	335	11
1	3	3	721	736	5
1	3	4	1802	1803	7
1	3	5	786	801	5
1	3	6	167	164	5
1	3	7	298	322	7
1	3	8	2335	2354	10
1	3	9	795	810	6
1	3	10	1002	1029	6
1	3	12	1939	1948	9
1	3	13	584	573	8
1	3	14	1113	1121	8
1	3	15	639	615	9
1	3	16	375	371	13
1	3	18	1136	1148	9
1	3	19	313	304	10
1	3	21	135	143	21
1	3	22	726	727	12
1	3	23	254	230	13
1	3	24	423	423	13
1	3	26	257	223	16
1	3	28	494	475	15
1	3	29	220	209	23
1	4	-29	327	351	15
1	4	-27	306	295	14
1	4	-25	371	389	11
1	4	-24	397	406	12
1	4	-23	697	690	14
1	4	-22	155	160	21
1	4	-20	569	538	14
1	4	-19	1058	1003	11
1	4	-18	536	477	12
1	4	-17	737	743	11
1	4	-16	278	265	9
1	4	-15	1032	992	9
1	4	-14	551	484	10
1	4	-13	1734	1627	9
1	4	-12	418	407	9
1	4	-11	810	737	7
1	4	-10	842	810	7
1	4	-9	1395	1316	7
1	4	-8	586	526	6
1	4	-7	600	562	6
1	4	-6	426	379	6
1	4	-5	1054	1046	6
1	4	-4	659	682	5
1	4	-3	1486	1468	7
1	4	-2	353	319	6
1	4	-1	1166	1174	6
1	4	0	1071	1086	5
1	4	1	2028	2043	6
1	4	2	722	752	5
1	4	3	688	675	5
1	4	4	935	935	5
1	4	5	1877	1887	8
1	4	6	1203	1202	6
1	9	-21	333	388	11
1	9	-20	306	350	9
1	9	-17	378	396	12
1	9	-16	241	268	8
0	9	8	727	715	8
0	9	11	282	286	8
0	9	12	663	633	9
0	9	13	181	190	12
0	9	14	259	233	9
0	9	15	163	184	15
0	9	16	373	383	11
0	9	17	398	392	10
0	9	18	493	500	14
0	9	21	418	397	12
0	9	22	431	417	13
0	10	0	163	169	10
0	10	1	559	546	8
0	10	2	152	140	11
0	10	3	298	304	9
0	10	4	350	347	11
0	10	5	767	731	8
0	10	6	354	352	12
0	10	7	159	118	11
0	10	8	138	134	14
0	10	9	625	609	9
0	10	10	199	178	10
0	10	11	484	485	11
0	10	12	115	13	18
0	10	13	181	172	13
0	10	14	239	240	10
0	10	15	577	552	11
0	10	17	149	134	18
0	10	18	326	311	9
0	10	19	403	407	12
0	10	20	230	186	14
0	10	21	393	347	13
0	11	1	198	182	9
0	11	2	500	498	9
0	11	3	199	187	9
0	11	4	345	328	9
0	11	6	491	469	10
0	11	7	161	167	13
0	11	8	538	539	10
0	11	10	120	59	18
0	11	11	172	159	13
0	11	12	572	550	11
0	11	13	142	114	17
0	11	14	308	296	10
0	11	15	175	147	15
0	11	16	310	319	10
0	11	18	435	421	12
0	11	19	182	144	18
0	12	1	326	318	9
0	12	3	201	212	10
0	12	5	390	380	13
0	12	8	129	113	17
0	12	9	522	489	11
0	12	10	186	148	13
0	12	11	407	386	10
1	4	7	1551	1553	7
1	4	8	469	445	6
1	4	9	692	711	6
1	4	10	894	884	6
1	4	11	1725	1745	8
1	4	12	911	915	7
1	4	13	243	249	8
1	4	14	343	338	11
1	4	15	1297	1276	8
1	4	16	556	550	9
1	4	17	510	533	11
1	4	19	348	367	11
1	4	20	389	388	11
1	4	21	602	603	12
1	4	22	157	143	19
1	4	25	596	573	16
1	4	26	300	301	15
1	4	29	296	321	19
1	4	30	248	231	23
1	5	-30	223	186	20
1	5	-26	341	371	12
1	5	-25	318	293	12
1	5	-23	231	250	14
1	5	-22	538	525	14
1	5	-21	538	507	14
1	5	-20	612	622	12
1	5	-19	168	143	15
1	5	-18	340	305	11
1	5	-17	638	611	10
1	5	-16	1489	1448	9
1	5	-15	561	550	10
1	5	-14	343	329	9
1	5	-13	775	731	8
1	5	-12	901	903	7
1	5	-11	745	704	7
1	5	-10	1327	1299	7
1	5	-9	557	549	7
1	5	-8	467	419	7
1	5	-7	1101	1040	6
1	5	-6	1108	1075	6
1	5	-5	552	549	6
1	5	-4	104	88	9
1	5	-3	361	344	6
1	5	-2	1140	1141	6
1	5	-1	1496	1535	7
1	5	0	503	536	5
1	5	1	379	364	6
1	5	2	1746	1751	8
1	5	3	1321	1301	6
1	5	4	1310	1340	7
1	5	5	1159	1162	6
1	5	6	808	785	6
1	5	7	606	626	6
1	5	8	1994	1950	9
1	10	1	319	319	8
1	10	2	470	450	9
1	10	3	426	410	10
1	10	4	257	243	8

1	5	13	1033	1034	7
1	5	14	1177	1163	8
1	5	15	307	312	10
1	5	16	159	158	13
1	5	17	452	417	11
1	5	18	794	786	9
1	5	20	202	212	13
1	5	22	551	532	14
1	5	23	418	406	13
1	5	24	236	229	15
1	5	25	226	204	17
1	5	26	302	305	15
1	5	28	392	400	14
1	5	29	263	239	21
1	6	-30	173	189	25
1	6	-28	270	263	15
1	6	-25	228	212	15
1	6	-24	365	376	11
1	6	-23	383	366	12
1	6	-22	318	308	11
1	6	-20	224	223	12
1	6	-19	676	693	10
1	6	-18	657	646	10
1	6	-17	318	286	11
1	6	-15	637	630	9
1	6	-14	631	604	8
1	6	-13	994	996	8
1	6	-11	165	144	9
1	6	-10	896	876	7
1	6	-9	1158	1162	7
1	6	-8	556	526	7
1	6	-7	542	515	7
1	6	-6	681	659	6
1	6	-5	1167	1125	7
1	6	-4	1023	1022	6
1	6	-3	1113	1125	6
1	6	-2	591	626	6
1	6	-1	660	667	6
1	6	0	819	825	6
1	6	1	1356	1367	7
1	6	2	1548	1521	7
1	6	4	336	307	8
1	6	5	1197	1243	7
1	6	6	1007	993	6
1	6	7	760	766	6
1	6	8	449	415	8
1	6	9	562	530	7
1	6	10	830	826	7
1	6	11	1029	1002	7
1	6	12	200	180	9
1	6	13	268	272	8
1	12	5	154	146	14
1	12	6	543	547	11
1	12	10	531	506	12
1	12	12	423	412	14
1	12	14	172	195	16
1	13	-11	358	401	12
1	13	-10	136	148	13
1	13	-7	304	327	8
1	13	-5	249	244	9
1	13	-3	231	230	10
1	13	-1	369	370	10
1	13	3	424	407	13
1	13	5	208	185	12
1	13	7	315	320	10
1	13	9	427	393	10
2	0	-32	570	503	17
2	0	-28	458	463	15
2	0	-26	440	471	15
2	0	-24	436	484	14
2	0	-22	571	653	18
2	0	-18	939	1104	22
2	0	-16	566	820	19
2	0	-14	1051	1678	23
2	0	-12	898	1784	23
2	0	-8	2874	3396	13
2	0	-6	760	803	6
2	0	-4	3504	3498	13
2	0	-2	3315	3333	13
2	0	0	284	289	5
2	0	2	2174	2141	9
2	0	4	1771	1788	7
2	0	6	1359	1377	6
2	0	8	1151	1134	6
2	0	10	745	770	6
2	0	12	1576	1543	8
2	0	14	309	297	8
2	0	16	1830	1800	9
2	0	18	833	812	9
2	0	20	864	834	10
2	0	22	1009	962	10
2	0	26	580	614	16
2	0	28	198	194	21
2	0	30	286	299	18
2	1	-31	474	430	16
2	1	-29	592	547	19
2	1	-25	576	627	18
2	1	-23	232	281	22
2	1	-22	231	320	22
2	1	-21	557	718	16
2	1	-19	666	755	20
2	1	-18	402	438	12
2	1	-17	554	711	16
2	1	-15	911	1183	17
2	1	-14	496	618	17
2	1	-11	2047	2411	12
2	5	-4	746	748	6
2	5	5	1936	1990	8
2	5	6	353	375	8
2	5	7	473	463	7
2	5	8	991	996	6
2	5	9	1337	1322	7
2	5	10	653	658	7
2	5	11	736	748	7
2	5	12	275	272	9
2	5	13	542	551	8
2	5	14	692	676	8
2	5	15	487	491	10
2	5	18	434	436	12
2	5	19	636	631	11
2	5	20	448	475	14
2	5	23	564	539	15
2	5	24	344	345	12
1	6	19	514	508	12
1	6	20	622	604	12
1	6	21	422	421	11
1	6	22	471	413	15
1	6	25	394	400	12
1	6	26	388	369	12
1	6	29	361	333	16
1	7	-27	321	360	12
1	7	-26	323	343	11
1	7	-25	327	379	10
1	7	-24	214	228	14
1	7	-22	327	360	10
1	7	-21	363	393	11
1	7	-20	371	414	10
1	7	-17	440	473	12
1	7	-16	539	549	10
1	7	-15	284	274	8
1	7	-14	520	514	9
1	7	-13	677	666	8
1	7	-12	426	448	10
1	7	-11	854	860	7
1	7	-10	494	470	8
1	7	-9	187	177	8
1	7	-8	420	417	8
1	7	-7	1182	1178	7
1	7	-6	1117	1118	7
1	7	-5	715	693	6
1	7	-3	717	719	6
1	7	-2	1309	1321	7
1	7	-1	1295	1295	7
1	7	0	354	356	8
1	7	1	311	307	9
1	7	2	947	928	6
1	7	3	868	880	6
1	7	4	900	894	6
1	7	5	820	810	7
1	7	6	293	311	8
1	7	7	622	623	7
1	7	8	755	743	7
1	7	9	720	717	7
1	7	10	234	225	7
1	7	11	260	259	8
1	7	12	532	512	9
1	7	13	472	444	10
1	7	14	739	723	8
1	7	15	307	276	10
1	7	16	473	461	11
1	7	17	433	379	12
1	7	18	606	643	11
1	7	19	525	505	12
1	7	20	157	171	18
2	1	-9	1089	1248	9
2	1	-8	369	380	8
2	1	-7	1524	1596	8
2	1	-6	933	916	6
2	1	-5	2776	2737	11
2	1	-4	188	160	6
2	1	-3	469	452	4
2	1	-2	320	309	5
2	1	-1	1828	1804	7
2	1	0	529	519	4
2	1	1	241	256	7
2	1	2	758	717	5
2	1	3	2439	2426	10
2	1	4	187	183	6
2	1	5	1867	1894	8
2	1	6	391	399	6
2	1	7	399	391	7
2	1	8	378	395	8
2	1	9	2099	2121	9
2	1	10	769	764	6
2	1	11	688	677	7
2	1	12	472	474	8
2	1	13	1635	1635	8
2	1	14	171	166	10
2	1	15	1511	1555	9
2	1	16	288	276	9
2	1	17	345	308	9
2	1	19	1234	1249	9
2	1	21	272	278	10
2	1	23	555	539	14
2	1	25	538	507	15
2	1	27	226	183	18
2	1	28	186	126	23
2	1	29	348	369	14
2	2	-32	349	340	21
2	2	-29	252	212	24
2	2	-28	550	527	18
2	2	-26	341	353	17
2	2	-25	191	209	26
2	2	-24	343	402	16
2	2	-22	921	928	17
2	2	-20	179	162	20
2	2	-19	403	505	13
2	2	-18	1070	1190	16
2	2	-17	512	535	12
2	2	-16	481	512	15
2	2	-15	402	456	12
2	2	-14	1116	1182	12
2	2	-13	605	628	11
2	2	-12	1603	1677	11
2	2	-11	354	374	11
2	2	-10	180	185	8
2	2	-9	579	528	7
2	2	-8	1987	2024	9
2	2	-6	775	722	5
2	6	10	380	386	10
2	6	11	871	888	7
2	6	12	770	747	8
2	6	13	395	413	10
2	6	14	167	151	11
2	6	15	334	328	9
2	6	16	761	764	9
2	6	17	724	721	10
2	6	18	388	397	10
2	6	19	214	226	12
2	6	20	462	434	14
2	6	21	476	490	11
2	6	22	389	400	13
2	6	23	426	425	13
2	6	24	161	185	20
2	6	26	399	405	12
2	6	27	304	252	16
1	7	26	185	174	23
1	7	27	224	197	21
1	7	28	304	270	17
1	8	-27	285	293	12
1	8	-24	333	414	11
1	8	-23	270	307	10
1	8	-22	165	182	15
1	8	-20	309	346	9
1	8	-19	179	170	12
1	8	-18	395	429	12
1	8	-15	233	253	9
1	8	-14	675	720	8
1	8	-13	439	438	10
1	8	-12	357	358	11
1	8	-11	143	145	12
1	8	-10	723	732	7
1	8	-9	722	735	7
1	8	-8	790	813	7
1	8	-7	347	366	10
1	8	-6	361	346	9
1	8	-5	699	691	7
1	8	-4	1372	1346	7
1	8	-3	792	800	7
1	8	-2	384	375	9
1	8	-1	179	195	8
1	8	0	847	846	7
1	8	1	996	1011	7
1	8	2	979	985	7
1	8	3	199	222	8
1	8	4	143	163	10
1	8	5	376	361	9
1	8	6	844	851	7
1	8	7	197	204	8
1	8	8	121	121	13
1	8	9	112	115	15
1	8	10	423	422	10
1	8	11	612	600	9
1	8	12	486	471	10
1	8	13	147	103	13
1	8	14	343	328	9
1	8	15	430	398	12
1	8	16	575	545	10
1	8	19	358	377	12
1	8	20	472	427	14
1	8	21	237	231	13
1	8	22	410	381	12
1	8	25	321	306	13
1	8	26	326	287	14
1	9	-25	233	262	13
1	9	-24	238	281	12
1	9	-23	226	256	12
2	2	-5	1089	588	5
2	2	-4	2150	2064	9
2	2	-3	356	341	5
2	2	-2	3123	3091	12
2	2	-1	425	425	4
2	2	0	934	951	5
2	2	1	665	684	4
2	2	2	2819	2836	11
2	2	3	143	131	5
2	2	4	530	529	5
2	2	5	108	86	8
2	2	6	2121	2130	9
2	2	7	586	570	6
2	2	8	1494	1500	7
2	2	9	561	576	7
2	2	10	721	705	7
2	2	12	1727	1766	9
2	2	13	119	121	14
2	2	15	156	150	12
2	2	16	1119	1159	9
2	2	17	204	208	11
2	2	18	323	328	9
2	2	20	706	726	11
2	2	21	307	318	10
2	2	22	748	761	12
2	2	24	201	203	17
2	2	25	279	262	13
2	2	26	559	565	17
2	2	28	251	271	18
2	2	30	373	382	15
2	3	-31	247	267	26
2	3	-29	338	349	17
2	3	-26	328	377	16
2	3	-25	860	873	17
2	3	-24	221	217	20
2	3	-22	239	221	17
2	3	-21	1040	1133	16
2	3	-20	446	447	13
2	3	-19	1012	978	13
2	3	-18	187	184	16
2	3	-17	498	475	14
2	3	-16	409	424	11
2	3	-15	1575	1518	11
2	3	-14	342	318	10
2	3	-13	179	142	10
2	3	-12	348	299	11
2	3	-11	1115	1084	8
2	3	-10	975	929	7
2	3	-9	1022	980	7
2	3	-8	177	154	6
2	3	-7	708	689	6
2	3	-6	852	796	5
2	3	-5	2286	2209	9
2	3	-4	293	318	7
2	3	-2	904	916	5
2	7	17	362	354	10
2	7	18	551	550	11
2	7	19	530	568	13
2	7	20	560	548	13
2	7	23	310	329	12
2	7	24	336	344	12
2	7	25	195	145	20
2	8	-27	256	273	15
2	8	-26	234	290	15
2	8	-23	292	331	11
2	8	-22	229	234	13
2	8	-20	140	127	18
2	8	-19	346	350	11
2	8	-18	315	299	9
2	8	-17	503	519	11
2	8	-16	223	218	10
2	8	-15	176	157	12
1	9	-15	331	342	9
1	9	-13	205	230	9
1	9	-12	190	178	9
1	9	-11	630	660	8
1	9	-10	232	239	7
1	9	-9	123	108	13
1	9	-8	265	278	8
1	9	-7	818	840	7
1	9	-6	506	531	8
1	9	-5	471	449	9
1	9	-4	128	140	12
1	9	-3	591	605	8
1	9	-2	493	495	8
1	9	-1	941	928	7
1	9	0	359	367	10
1	9	2	368	375	10
1	9	3	843	828	7
1	9	4	584	582	8
1	9	5	276	249	9
1	9	6	211	209	8
1	9	7	390	386	10
1	9	8	412	409	10
1	9	9	724	691	8
1	9	12	373	357	12
1	9	13	588	587	10
1	9	14	181	178	12
1	9	15	285	270	9
1	9	16	352	338	11
1	9	17	369	382	11
1	9	18	379	376	11
1	9	19	506	500	14
1	9	22	312	318	11
1	9	23	369	383	12
1	10	-23	188	234	13
1	10	-21	159	203	14
1	10	-20	328	395	10
1	10	-19	181	203	12
1	10	-18	301	374	9
1	10	-17	148	191	13
1	10	-16	164	156	11
1	10	-14	499	562	10
1	10	-13	179	178	10
1	10	-12	236	259	8
1	10	-10	458	518	9
1	10	-8	724	759	8
1	10	-5	266	283	8
1	10	-4	798	818	8
1	10	-3	372	381	11
1	10	-2	281	266	9
1	10	0	666	644	8
2	3	-1	2673	2655	10
2	3	0	428	394	5
2	3	1	1801	1822	7
2	3	3	1701	1766	7
2	3	4	998	1043	5
2	3	5	1934	1991	8
2	3	6	666	649	5
2	3	7	276	315	8
2	3	8	448	450	7
2	3	9	1926	1990	9
2	3	10	623	638	7
2	3	11	466	478	8
2	3	12	322	324	11
2	3	13	1208	1179	8
2	3	14	597	592	9
2	3	15	980	1002	8
2	3	16	209	208	10
2	3	17	283	287	8
2	3	18	236	239	11
2	3	19	749	782	10
2	3	20	449	481	10
2	3	21	256	281	11
2	3	22	139	114	22
2	3	23	515	526	15
2	3	25	516	498	12
2	3	27	206	223	21
2	3	29	425	390	13
2	4	-32	236	220	26
2	4	-28	452	429	14
2	4	-27	250	252	19
2	4	-26	329	342	14
2	4	-24	457	448	14
2	4	-23	577	557	15
2	4	-22	871	882	14
2	4	-19	576	582	14
2	4	-18	1150	1115	11
2	4	-17	542	519	13
2	4	-16	555	564	12
2	4	-15	192	158	11
2	4	-14	1006	973	9
2	4	-13	741	708	8
2	4	-12	1168	1103	8
2	4	-11	261	264	7
2	4	-10	277	248	8
2	4	-9	506	507	7
2	4	-7	1311	1259	7
2	4	-6	637	647	6
2	4	-5	329	316	7
2	4	-4	1138	1119	6
2	4	-2	1957	1942	8
2	4	-1	109	107	8
2	4	0	1061	1109	6
2	4	1	891	897	5
2	9	-16	481	497	11
2	9	-15	296	312	9
2	9	-14	368	363	12
2	9	-12	373	394	12
2	9	-11	386	409	11
2	9	-10	657	672	8
2	9	-9	355	378	11
2	9	-7	193	192	9
2	9	-6	984	1020	7
2	9	-5	548	549	8
2	9	-4	455	451	9
2	9	-2	707	710	8
2	9	0	791	784	7
2	9	1	276	268	9
2	9	2	151	147	11
2	9	3	103	69	16
1	10	5	272	247	8
1	10	6	846	814	8
1	10	7	150	157	13
1	10	8	191	173	10
1	10	9	253	257	8
1	10	10	562	548	10
1	10	11	191	191	11
1	10	12	523	507	10
1	10	13	148	185	16
1	10	15	260	265	10
1	10	16	526	524	12
1	10	18	144	109	19
1	10	19	226	220	13
1	10	20	329	325	10
1	10	21	167	128	19
1	11	-20	160	199	13
1	11	-17	386	457	12
1	11	-16	151	146	12
1	11	-15	256	299	8
1	11	-13	206	234	9
1	11	-11	444	500	10
1	11	-8	146	164	12
1	11	-7	434	447	10
1	11	-6	198	215	9
1	11	-5	345	332	8
1	11	-3	409	401	11
1	11	-2	151	149	12
1	11	-1	443	458	10
1	11	0	348	316	12
1	11	1	110	64	16
1	11	3	702	682	9
1	11	4	219	210	9
1	11	5	349	312	9
1	11	7	465	451	11
1	11	8	146	150	15
1	11	9	626	576	10
1	11	13	510	515	12
1	11	15	290	271	9
1	11	16	220	210	13
1	11	19	356	323	11
1	12	-14	431	512	10
1	12	-13	219	232	9
1	12	-12	198	255	9
1	12	-10	251	283	8
1	12	-9	107	62	16
1	12	-8	354	388	12
1	12	-4	317	314	10
1	12	0	441	441	11
1	12	2	357	343	9
1	12	4	333	324	10
2	4	2	2692	2715	11
2	4	3	1183	1170	6
2	4	4	668	663	5
2	4	5	422	428	6
2	4	6	1807	1849	6
2	4	7	717	746	6
2	4	8	1490	1510	7
2	4	9	245	246	8
2	4	10	1004	1009	7
2	4	11	858	835	7
2	4	12	951	989	7
2	4	13	658	664	8
2	4	16	688	677	9
2	4	17	439	452	12
2	4	18	329	322	9
2	4	20	505	478	13
2	4	21	176	161	17
2	4	22	625	630	13
2	4	23	206	225	16
2	4	24	208	190	17
2	4	26	616	617	17
2	4	27	274	257	17
2	4	30	286	276	20
2	5	-30	216	230	25
2	5	-29	266	277	19
2	5	-27	213	193	21
2	5	-25	620	630	17
2	5	-24	258	247	15
2	5	-23	200	170	17
2	5	-22	244	259	14
2	5	-21	677	672	13
2	5	-20	545	536	14
2	5	-19	866	866	11
2	5	-18	163	154	16
2	5	-17	431	483	14
2	5	-16	628	615	11
2	5	-15	1255	1196	9
2	5	-14	221	200	9
2	5	-13	358	331	8
2	5	-12	485	468	9
2	5	-11	1276	1227	8
2	5	-10	1083	1049	7
2	5	-9	765	730	7
2	5	-7	752	727	6
2	5	-6	617	597	6
2	5	-5	1117	1093	6
2	5	-4	623	613	6
2	5	-3	184	147	6
2	5	-2	217	225	7
2	5	-1	1584	1603	7
2	5	0	1073	1114	6
2	5	1	892	918	6
2	5	2	211	163	7
2	5	3	1405	1451	7
2	10	12	244	235	9
2	10	13	428	443	12
2	10	14	207	222	12
2	10	15	275	286	9
2	10	16	291	301	9
2	10	17	404	401	10
2	10	20	194	191	15
2	11	-20	337	396	9
2	11	-16	341	385	10
2	11	-15	119	156	17
2	11	-14	279	299	9
2	11	-12	137	162	14
2	11	-10	419	437	11
2	11	-9	163	152	11
2	11	-6	458	468	10
2	11	-5	195	187	10

```
2  5  25  227  249 18    2  7 -25  226  238 16    2  8 -14  375  372  9    2  9   4  676  674  8    2 11  -4  193  197 10
2  5  26  188  153 22    2  7 -24  246  259 14    2  8 -13  811  825  8    2  9   5  281  265  8    2 11  -3  174  155 11
2  5  27  295  272 16    2  7 -23  217  206 15    2  8 -12  626  659  9    2  9   6  410  419 10    2 11  -2  479  463 10
2  5  29  400  405 15    2  7 -21  245  259 12    2  8 -11  410  416 10    2  9   7  280  287  9    2 11  -1  110  103 17
2  6 -28  228  271 19    2  7 -20  260  253 10    2  8  -9  798  795  8    2  9   8  282  302  8    2 11   0  717  703  9
2  6 -27  334  332 13    2  7 -19  280  269 10    2  8  -8 1105 1121  7    2  9   9  424  430 11    2 11   1  149  140 13
2  6 -24  316  321 12    2  7 -17  220  226 10    2  8  -7  654  664  7    2  9  10  764  764  8    2 11   3  147  128 13
2  6 -23  276  278 13    2  7 -16  564  579 10    2  8  -6  683  679  7    2  9  13  531  517 10    2 11   4  787  787  8
2  6 -22  626  637 13    2  7 -15  659  655  9    2  8  -5  272  258  8    2  9  14  678  689 10    2 11   6  439  421 11
2  6 -21  149  149 19    2  7 -14  309  299 10    2  8  -4  489  493  8    2  9  15  288  288  9    2 11   7  188  173 11
2  6 -19  534  530 12    2  7 -13  244  254  8    2  8  -3  793  787  7    2  9  16  234  237 11    2 11   8  406  385 12
2  6 -18  865  897 10    2  7 -12  904  920  8    2  8  -2  438  444  9    2  9  17  287  293  9    2 11   9  226  194 10
2  6 -17  547  550 11    2  7 -11  786  809  8    2  8  -1   98   83 14    2  9  18  372  384 11    2 11  10  516  541 11
2  6 -16  910  905  9    2  7 -10 1012  993  7    2  8   0   93   97 15    2  9  19  269  288 11    2 11  11  133  114 17
2  6 -15  396  386 12    2  7  -9  695  680  7    2  8   1  698  698  7    2  9  20  340  354 10    2 11  13  225  231 11
2  6 -14  428  408 11    2  7  -7  924  918  7    2  8   2  469  464  8    2 10 -23  324  400 11    2 11  14  323  333 10
2  6 -13  896  867  8    2  7  -6 1239 1232  7    2  8   3  254  248  7    2 10 -22  155  114 16    2 11  16  159  151 17
2  6 -12 1051 1057  8    2  7  -5  881  896  7    2  8   5  343  375 11    2 10 -19  272  300  9    2 11  18  256  233 11
2  6 -10  237  239  7    2  7  -4  778  796  7    2  8   6  292  290  9    2 10 -17  357  395 10    2 12 -16  137  154 15
2  6  -9  874  853  7    2  7  -3  139  144  9    2  8   7  631  621  8    2 10 -13  518  549 10    2 12 -13  314  360 10
2  6  -8 1242 1215  7    2  7  -2  337  357  9    2  8   8  329  314  8    2 10 -12  261  269  8    2 12 -11  164  186 12
2  6  -7  903  872  6    2  7  -1 1150 1133  7    2  8   9  171  188 10    2 10 -11  233  245  8    2 12  -9  207  220  9
2  6  -6  477  444  7    2  7   0  720  730  6    2  8  10  462  447  9    2 10 -10  114  114 15    2 12  -7  252  274  8
2  6  -5  426  411  8    2  7   1  340  349  9    2  8  11  703  709  8    2 10  -9  385  408 11    2 12  -5  182  160 11
2  6  -4 1127 1132  6    2  7   3  499  463  7    2  8  12  670  645  9    2 10  -8  363  383 11    2 12  -3  416  416 12
2  6  -3 1052 1062  6    2  7   4  646  657  7    2  8  13  483  499 11    2 10  -6  277  289  8    2 12   1  621  582 10
2  6  -2  790  799  6    2  7   5  633  619  7    2  8  14  175  176 12    2 10  -5  209  210  9    2 12   3  512  481 11
2  6  -1  534  533  6    2  7   6  314  293 10    2  8  15  444  436 11    2 10  -3  788  775  8    2 12   5  287  288 10
2  6   0  256  271  7    2  7   7  120  143 12    2  8  16  632  634 10    2 10  -2  324  306  9    2 12   7  622  593 10
2  6   1  492  493  7    2  7   8  736  722  7    2  8  17  700  705 10    2 10   1  529  516  9    2 12  11  296  323  9
2  6   2 1395 1411  7    2  7   9  803  794  7    2  8  18  224  222 12    2 10   2  254  236  7    2 12  13  257  250 10
2  6   3  987 1009  6    2  7  10  447  434  9    2  8  20  323  356 10    2 10   3  419  419 10    2 13 -10  238  270  9
2  6   4  257  250  7    2  7  11  372  356 11    2  8  21  447  444 11    2 10   5  293  289  9    2 13  -6  330  327 10
2  6   5  465  450  7    2  7  12  256  249  9    2  8  22  211  237 16    2 10   6  290  263  8    2 13  -4  254  257  9
2  6   6 1151 1177  7    2  7  13  466  450 10    2  8  23  291  285 12    2 10   7  717  701  8    2 13  -3  138   82 16
2  6   7  700  689  7    2  7  14  835  863  9    2  9 -22  145  163 19    2 10  10  381  383 12    2 13   0  442  402 12
2  6   8  680  675  7    2  7  15  562  553 10    2  9 -20  327  325  9    2 10  11  549  555 10    2 13   3  128  137 19
2  6   9  154  146 10    2  7  16  338  330 10    2  9 -19  144  134 17    3  3  22  184  241 17    3  4  27  479  488 15
2 13   4  468  460 12    3  1   3  734  727  6    3  2  10  251  251  7    3  3  24  604  587 14    3  4  28  226  236 22
2 13   6  232  209 11    3  1   4 1520 1547  7    3  2  11  929  924  7    3  3  25  261  244 15    3  5 -30  296  296 21
2 13   8  282  270  9    3  1   5  297  337  8    3  2  12  396  395 10    3  3  26  369  378 12    3  5 -29  375  345 16
3  0 -31  552  500 17    3  1   6 1827 1868  8    3  2  13 1370 1400  8    3  3  28  229  213 21    3  5 -28  382  364 15
3  0 -27  416  537 21    3  1   7  673  662  6    3  2  15  128  129 16    3  3  30  329  309 18    3  5 -25  314  306 16
3  0 -23  413  545 20    3  1   8  518  509  7    3  2  16  288  310  9    3  4 -31  375  390 19    3  5 -24  714  691 16
3  0 -21  598  818 18    3  1   9  292  297  7    3  2  17 1082 1123  9    3  4 -28  271  281 22    3  5 -23  172  204 23
3  0 -17  880 1527 29    3  1  10 2559 2540 11    3  2  18  190  211 13    3  4 -27  631  596 15    3  5 -22  337  358 12
3  0 -15  468  668 14    3  1  11  507  516  8    3  2  19  481  485 13    3  4 -26  256  282 20    3  5 -21  352  384 11
3  0 -13 1585 1930 14    3  1  12  688  719  8    3  2  21  611  636 12    3  4 -25  398  410 13    3  5 -20  624  605 14
3  0 -11 1598 1867 11    3  1  14 1148 1161  8    3  2  22  160  122 19    3  4 -23  384  384 12    3  5 -19  637  640 13
3  0  -9  866  869  7    3  1  16 1429 1464  9    3  2  23  591  603 14    3  4 -22  482  486 14    3  5 -18  929  926 11
3  0  -7 2544 2558 10    3  1  17  442  440 12    3  2  27  480  494 15    3  4 -21  967 1003 15    3  5 -15  678  612 10
3  0  -5  522  556  7    3  1  18  292  260  9    3  3 -31  254  196 28    3  4 -20  322  333 11    3  5 -14  797  778  9
3  0  -3 1658 1748  7    3  1  20  929  945 10    3  3 -30  358  301 20    3  4 -18  353  335 11    3  5 -13  384  343 12
3  0  -1  985  989  5    3  1  22  159  190 19    3  3 -28  438  414 15    3  4 -17  875  867 11    3  5 -12  118   85 15
3  0   1 1120 1114  6    3  1  23  249  260 13    3  3 -24  722  796 21    3  4 -16  410  374 10    3  5 -11  296  246  9
3  0   3 2383 2429 10    3  1  24  489  494 12    3  3 -23  213  197 21    3  4 -15  455  421 13    3  5 -10 1008  958  7
3  0   5  496  493  6    3  1  25  232  202 16    3  3 -20  703  734 16    3  4 -13  825  790  9    3  5  -9  682  667  7
3  0   7 2025 1996  9    3  1  26  293  284 14    3  3 -19  372  396 12    3  4 -12  603  589  9    3  5  -8  655  643  7
3  0   9  628  630  7    3  1  28  278  254 17    3  3 -18  703  715 14    3  4 -11 1172 1110  6    3  5  -7  154  139  9
3  0  11 1420 1411  8    3  1  30  349  344 16    3  3 -16  489  510 15    3  4 -10  249  218  7    3  5  -6  881  849  6
3  0  13 2064 2054 10    3  2 -31  452  439 18    3  3 -15  429  403 14    3  4  -9  550  517  7    3  5  -5 1023 1002  6
3  0  15  376  365 12    3  2 -28  260  263 26    3  3 -14 1436 1385 10    3  4  -8  245  189  6    3  5  -4 1145 1154  6
3  0  17 1475 1470  9    3  2 -27  590  595 19    3  3 -12  329  323  9    3  4  -7 1718 1614  8    3  5  -3 1180 1173  6
3  0  19  875  892  9    3  2 -25  410  487 16    3  3 -11  589  544  8    3  4  -6  749  752  6    3  5  -2  366  338  7
3  0  21  592  556 12    3  2 -23  628  682 16    3  3 -10 1067 1005  7    3  4  -5  749  755  6    3  5  -1 1024 1012  6
3  0  23  769  793 12    3  2 -22  427  461 13    3  3  -9  838  784  7    3  4  -4  550  543  6    3  5   0 1620 1672  7
3  0  27  389  371 12    3  2 -21  697  859 23    3  3  -8  908  887  7    3  4  -3 1773 1791  8    3  5   1 1051 1079  6
3  0  31  270  234 22    3  2 -20  477  590 14    3  3  -7  483  455  7    3  4  -2  985  991  6    3  5   2  774  779  6
3  1 -30  268  309 30    3  2 -17 1118 1295 16    3  3  -6 1171 1110  6    3  4  -1 1770 1783  8    3  5   3  176  177  7
3  1 -28  427  427 19    3  2 -16  500  523 16    3  3  -5  927  887  6    3  4   1  176  177  7    3  5   4 1063 1070  6
3  1 -24  454  603 18    3  2 -15  625  653 13    3  3  -4 2374 2366 10    3  4   2 1170 1164  6    3  5   5  661  686  6
3  1 -22  187  163 26    3  2 -14  442  452 14    3  3  -3  317  300  7    3  4   3 1586 1639  7    3  5   6 1373 1417  7
3  1 -20  653  892 19    3  2 -13 1085 1135 11    3  3  -2  396  430  6    3  4   4  872  878  6    3  5   7  279  264  7
3  1 -18  543  680 16    3  2 -12  209  169  9    3  3  -1  368  363  6    3  4   5  384  358  7    3  5   9  782  779  7
3  1 -17  234  310 16    3  2 -11 1567 1571 10    3  3   0 2433 2473 10    3  4   6  588  592  6    3  5  10 1186 1206  7
3  1 -16  827  975 17    3  2  -9  674  647  7    3  3   1 1063 1074  6    3  4   7 1031 1050  7    3  5  11  697  668  8
3  1 -15  219  302 15    3  2  -8  612  588  7    3  3   2 1067 1090  6    3  4   8  811  823  7    3  5  12  221  207  8
3  1 -14 1653 2000 15    3  2  -7 2295 2230 10    3  3   3  528  500  6    3  4   9  822  827  7    3  5  14  649  658  9
3  1 -12  175  194 12    3  2  -6  720  670  6    3  3   4 1879 1878  8    3  4  10  473  466  8    3  5  15  367  353  9
3  1 -11  589  582 10    3  2  -5  201  215  7    3  3   5  626  628  6    3  4  11  589  552  8    3  5  16  508  525 11
3  1 -10 2532 2586 12    3  2  -4  396  374  6    3  3   6 1419 1388  7    3  4  12  337  324  8    3  5  17  322  320  9
3  1  -9  150  129  9    3  2  -3 1621 1597  7    3  3   7  598  587  6    3  4  14  175  171 11    3  5  18  339  352  9
3  1  -8 1607 1628  8    3  2  -2  233  222  6    3  3   8  677  676  7    3  4  15  266  256  8    3  5  19  138  150 20
3  1  -7  475  442  7    3  2  -1 2161 2164  9    3  3   9  138  140 10    3  4  16  293  291  9    3  5  20  637  624 12
3  1  -6 1810 1784  8    3  2   0  138  129  6    3  3  10 1327 1326  8    3  4  17  743  751 10    3  5  21  412  412 12
3  1  -5  254  245  8    3  2   1 1481 1519  7    3  3  11  307  320  8    3  4  18  320  315 10    3  5  24  543  538 17
3  1  -4 2631 2611 10    3  2   2  481  511  6    3  3  12  620  647  8    3  4  19  315  301 10    3  5  25  275  284 15
3  1  -3  142  120  6    3  2   3 1865 1852  8    3  3  14 1119 1146  8    3  4  21  481  485 15    3  5  26  290  310 16
3  1  -2  456  478  5    3  2   4  632  618  6    3  3  15  246  239  9    3  4  22  266  243 12    3  5  28  236  245 22
3  1  -1  704  714  5    3  2   6  790  749  6    3  3  16  721  739  9    3  4  23  631  611 14    3  6 -27  353  328 14
3  1   0 1659 1725  7    3  2   7 1751 1802  8    3  3  18  480  491 12    3  4  26  192  202 22    3  6 -26  213  218 22
3  1   1  130   96  7    3  2   8  942  935  7    3  3  19  341  347 10    3  9  18  126  125 21    3 11  14  135  155 18
3  1   2 1188 1191  6    3  2   9  898  909  7    3  3  20  887  948 11    3  9  19  280  312 11    3 11  15  299  294  9
3  6 -25  408  385 11    3  7 -19  438  410 15    3  8  -5  320  332 11    3  9  20  214  204 14    3 12 -12  272  303  9
3  6 -24  269  273 15    3  7 -18  584  607 12    3  8  -4  135  132 11    3  9  21  282  287 12    3 12  -8  327  355 10
3  6 -23  299  294 13    3  7 -17  278  278  9    3  8  -3  443  452  9    3 10 -22  269  273 11    3 12  -6  322  319 10
3  6 -22  457  462 12    3  7 -16  205  181 12    3  8  -2  768  778  7    3 10 -18  263  286 10    3 12  -4  267  251  9
3  6 -21  654  635 13    3  7 -15  922  893  9    3  8  -1  376  402 10    3 10 -17  179  181 13    3 12  -2  569  553 10
3  6 -18  696  663 11    3  7 -14  685  679  9    3  8   0  118   70 12    3 10 -16  408  420 12    3 12   0  124  109 17
3  6 -17  809  803 10    3  7 -13  378  378  9    3  8   1  222  218  7    3 10 -12  592  620  9    3 12   2  480  482 11
3  6 -16  515  500 12    3  7 -12  129  160 15    3  8   2  849  834  7    3 10 -11  429  450 11    3 12   3  175  163 13
3  6 -15  649  623 10    3  7 -11  705  694  8    3  8   3  364  336 10    3 10 -10  160  163 12    3 12   4  434  431 12
3  6 -14  464  455 12    3  7 -10  879  883  8    3  8   4  606  600  8    3 10  -7  288  287  8    3 12   8  377  374 10
3  6 -13  592  565  9    3  7  -9 1203 1180  8    3  8   5  209  216  8    3 10  -6  508  527  9    3 12  12  258  267 10
3  6 -12  764  714  8    3  7  -8  518  534  8    3  8   6  390  397 10    3 10  -5  250  253  8    3 13  -5  367  379 11
3  6 -11  689  650  8    3  7  -7  201  185  8    3  8   7  694  698  8    3 10  -4  305  313  9    3 13  -3  245  220 10
3  6 -10  519  516  9    3  7  -6  381  391  9    3  8   8  786  781  8    3 10  -2  718  702  8    3 13  -1  308  282 10
3  6  -9  257  258  8    3  7  -5  840  827  8    3  8   9  422  421 10    3 10   0  190  176 10    3 13   1  372  362 11
3  6  -8  580  556  8    3  7  -4  769  770  7    3  8  10  210  208  9    3 10   2  515  524  9    3 13   5  376  352 10
3  6  -7  934  917  7    3  7  -3  564  584  7    3  8  12  805  806  8    3 10   3  262  257  8    3 13   7  177  174 14
3  6  -6  972  945  7    3  7  -1  349  360  9    3  8  14  562  568 10    3 10   4  563  562  9    4  0 -26  409  499 24
3  6  -5  141  137  9    3  7   0  889  886  7    3  8  16  239  238 10    3 10   6  300  313 10    4  0 -22  721  877 22
3  6  -4  316  298  9    3  7   1  753  753  7    3  8  17  401  415 10    3 10   7  390  410 12    4  0 -20  936 1094 26
3  6  -3 1109 1095  7    3  7   2  443  439  8    3  8  18  556  565 13    3 10   8  646  644  9    4  0 -18  338  355 15
3  6  -2 1013  995  6    3  7   3  207  196  7    3  8  21  154  185 21    3 10  11  287  292  9    4  0 -16 1784 1979 15
3  6  -1  681  672  6    3  7   4  395  407  9    3  8  22  291  283 12    3 10  12  523  534 11    4  0 -14  594  657 13
3  6   0  253  280  7    3  7   5 1010 1011  7    3  9 -25  266  255 13    3 10  13  206  197 11    4  0 -12 1247 1343  9
3  6   1  299  306  9    3  7   6  859  843  7    3  9 -21  223  264 13                              4  0 -10 1459 1489  8
3  6   2 1019 1018  7    3  7   7  201  186  8    3  9 -19  424  411 14                              4  0  -8  164  167  8
3  6   3 1162 1202  7    3  7   9  696  693  8    3  9 -18  209  243 12                              4  0  -6 1966 2008  9
3  6   4  622  632  7    3  7  10  727  749  8    3  9 -15  734  739  9
3  6   5  307  330 10    3  7  11  666  675  8
3  6   6  663  660  7    3  7  12  257  258  8
```

```
3  6   7  840  846  7    3  7  14  670  705  9    3  9 -14  438  450 11    3 10  14  307  319 10    4  0  -4  683  675  6
3  6   8  891  879  7    3  7  15  797  790  9    3  9 -13  349  352  9    3 10  16  207  227 13    4  0  -2  767  784  5
3  6   9  629  646  8    3  7  16  398  407 10    3  9 -11  539  554  9    3 10  17  156  150 17    4  0   0 2059 2115  9
3  6  11  388  388 10    3  7  17  432  419 13    3  9 -10  350  322 12    3 10  18  339  332 10    4  0   2  892  965  6
3  6  12  602  609  9    3  7  18  237  213 11    3  9  -9  644  680  8    3 11 -19  249  290 11    4  0   4 2370 2367 10
3  6  13  552  558  9    3  7  19  277  266 10    3  9  -8  527  544  9    3 11 -13  277  278  9    4  0   6  703  727  7
3  6  14  474  465 10    3  7  20  394  387 12    3  9  -7  147  156 12    3 11 -11  265  292  8    4  0   8 2481 2372 11
3  6  15  223  213 10    3  7  21  377  420 11    3  9  -5  872  890  8    3 11 -10  139  153 14    4  0  10 1728 1657  9
3  6  16  201  162 11    3  7  24  241  245 16    3  9  -4  387  386 10    3 11  -9  473  495 10    4  0  12 1030 1060  8
3  6  17  707  708 10    3  7  25  208  231 20    3  9  -3  410  409 10    3 11  -8  225  232  9    4  0  14 1201 1198  9
3  6  18  678  698 11    3  8 -22  457  478 11    3  9  -1  547  536  8    3 11  -7  205  208 10    4  0  18  709  705 10
3  6  20  196  180 15    3  8 -21  265  282 12    3  9   0  503  511  9    3 11  -5  655  662  9    4  0  20  374  373 12
3  6  21  449  487 11    3  8 -20  210  194 14    3  9   1  789  789  8    3 11  -4  224  213 10    4  0  22  327  310 10
3  6  22  297  295 12    3  8 -18  581  565 12    3  9   2  177  159 10    3 11  -3  346  314  9    4  0  24  483  469 13
3  6  23  378  369 12    3  8 -17  534  518 11    3  9   5  669  674  8    3 11  -1  439  436 11    4  0  28  489  439 13
3  6  24  202  205 19    3  8 -16  470  470 12    3  9   6  461  476 10    3 11   0  252  227  8    4  1 -29  367  406 25
3  6  25  198  181 20    3  8 -15  220  217 10    3  9   7  467  471 10    3 11   1  700  684  9    4  1 -27  367  380 23
3  6  27  278  315 18    3  8 -14  210  184 10    3  9   8  258  257  8    3 11   4  230  228 10    4  1 -25  336  415 23
3  7 -28  246  222 19    3  8 -13  497  469 10    3  9   9  445  461 11    3 11   5  597  583 10    4  1 -23  877  990 25
3  7 -25  237  265 16    3  8 -12  913  905  8    3  9  10  420  402 11    3 11   7  327  322 10    4  1 -19 1359 1479 19
3  7 -24  234  251 16    3  8 -11  593  608  9    3  9  11  643  621  9    3 11   8  200  192 11    4  1 -17  982 1052 17
3  7 -23  201  182 17    3  8 -10  169  145 11    3  9  14  329  341 11    3 11   9  323  319  9    4  1 -15 1003 1068 15
3  7 -22  281  263 12    3  8  -8  741  769  8    3  9  15  563  581 11    3 11  10  157  145 14    4  1 -14  149  151 16
3  7 -21  498  459 14    3  8  -7  632  655  8    3  9  16  156  172 16    3 11  11  326  312 11    4  1 -13 1858 1888 11
3  7 -20  474  517 15    3  8  -6  635  639  8    4  3  13  388  404 12    4  4  23  360  375 12    4  1 -12  203  216 10
4  1 -10  313  273  9    4  2   2  794  747  6    4  3  14  404  394 12    4  4  24  546  557 16    4  6 -26  446  416 14
4  1  -9 1804 1741  9    4  2   3  229  229  7    4  3  15  797  805  9    4  5 -29  365  351 18    4  6 -25  182  213 25
4  1  -8  382  375  8    4  2   4 2279 2200 10    4  3  16  590  607 11    4  5 -28  299  265 20    4  6 -24  377  345 12
4  1  -7 1454 1409  7    4  2   5  718  730  7    4  3  17  836  847 10    4  5 -27  504  469 15    4  6 -23  280  281 15
4  1  -6  517  510  7    4  2   6  219  171  7    4  3  19  296  293 10    4  5 -25  221  164 21    4  6 -21  530  508 16
4  1  -5  512  542  6    4  2   7  182  156  8    4  3  20  330  329 11    4  5 -24  325  287 14    4  6 -20  633  563 14
4  1  -4  140  119  7    4  2   8 1759 1768  9    4  3  21  679  670 12    4  5 -23  648  586 17    4  6 -18  153  171 18
4  1  -3 1376 1422  7    4  2   9  183  178  9    4  3  22  277  306 12    4  5 -21  267  218 14    4  6 -17  670  636 11
4  1  -2  458  451  6    4  2  10  927  938  8    4  3  25  410  399 12    4  5 -20  212  206 17    4  6 -16  507  481 12
4  1  -1  743  766  6    4  2  11  199  173  9    4  3  26  192  176 22    4  5 -19  532  492 15    4  6 -15  681  655 10
4  1   0  309  299  8    4  2  12  565  551  9    4  3  27  300  246 15    4  5 -18  317  293 10    4  6 -12  644  628  9
4  1   1 2001 2043  9    4  2  13  412  425 11    4  4 -30  479  398 16    4  5 -17  314  296 10    4  6 -11  870  840  8
4  1   2  473  475  7    4  2  14 1069 1070  8    4  4 -26  604  500 15    4  5 -15  326  311  9    4  6 -10  648  638  8
4  1   3 1217 1173  7    4  2  17  470  477 12    4  4 -25  269  239 19    4  5 -14  703  687 10    4  6  -9  387  397 10
4  1   4  328  289  8    4  2  18  877  866 10    4  4 -24  358  363 15    4  5 -13  945  899  9    4  6  -8  433  435  9
4  1   5 1661 1643  8    4  2  19  237  252 12    4  4 -22  504  467 14    4  5 -12  449  409 10    4  6  -7  525  528  8
4  1   6  179  136  8    4  2  20  421  418 11    4  4 -21  232  226 17    4  5 -11  156  157 12    4  6  -6 1028 1034  7
4  1   7 1964 1969  9    4  2  22  610  629 14    4  4 -20  506  500 13    4  5 -10  447  408 10    4  6  -5  691  697  7
4  1   8  212  200  7    4  2  23  244  276 15    4  4 -19  264  240 13    4  5  -9 1439 1372  8    4  6  -4  103   57 13
4  1   9  795  777  7    4  2  24  461  492 13    4  4 -17  242  202 12    4  5  -8  747  725  7    4  6  -3  618  609  7
4  1  10  316  299  8    4  2  25  300  281 13    4  4 -16  696  676 12    4  5  -7  802  779  7    4  6  -2 1076 1065  7
4  1  11 1920 1900  9    4  2  28  474  468 16    4  4 -15  410  388 10    4  5  -6  296  267  7    4  6  -1  754  730  7
4  1  12  217  211  9    4  3 -29  428  393 19    4  4 -14  457  400 12    4  5  -5 1278 1258  7    4  6   0 1043 1032  7
4  1  13  443  460 10    4  3 -28  265  250 26    4  4 -13  351  359  9    4  5  -4 1190 1186  7    4  6   1  159  154  9
4  1  14  294  264  9    4  3 -27  487  492 15    4  4 -12  951  903  9    4  5  -3 1569 1607  8    4  6   2  294  289  7
4  1  15  820  839  9    4  3 -25  318  281 18    4  4 -11  623  580  9    4  5  -2  413  403  8    4  6   3  666  668  7
4  1  17  717  692 10    4  3 -23  751  781 20    4  4 -10 1335 1248  8    4  5  -1  269  259  7    4  6   4 1020 1014  7
4  1  21  568  533 13    4  3 -22  330  331 15    4  4  -8  736  718  7    4  5   0 1043 1045  7    4  6   5  442  446  9
4  1  25  479  462 13    4  3 -19  825  814 15    4  4  -7 1145 1111  7    4  5   1 1240 1239  7    4  6   6  213  217  8
4  1  26  199  186 21    4  3 -17  795  774 13    4  4  -6 2089 2042  9    4  5   2  544  549  7    4  6   7  450  465  9
4  1  27  228  201 20    4  3 -15  584  586 13    4  4  -5  667  658  6    4  5   3  691  683  7    4  6   8  882  876  7
4  1  29  272  266 20    4  3 -14  432  393 13    4  4  -4  509  500  6    4  5   4  300  309 10    4  6   9  797  802  8
4  2 -30  477  377 19    4  3 -13 1266 1223 10    4  4  -3  363  368  8    4  5   5  699  697  7    4  6  10  409  415 11
4  2 -26  556  551 17    4  3 -11  179  172 10    4  4  -2 1547 1531  7    4  5   6  728  738  7    4  6  11  255  243  8
4  2 -24  358  363 18    4  3 -10  933  878  8    4  4  -1  935  930  6    4  5   7  897  896  7    4  6  12  713  716  9
4  2 -22  444  509 14    4  3  -9 1952 1867  9    4  4   0 1364 1357  7    4  5   8  324  311 11    4  6  13  582  578 10
4  2 -20  880  878 18    4  3  -8  718  671  7    4  4   1  158  172  8    4  5   9  173  155 10    4  6  14  739  729  9
4  2 -18  402  433 12    4  3  -7 1191 1162  7    4  4   2 1003 1030  6    4  5  10  374  355 10    4  6  15  497  500 12
4  2 -16 1495 1500 14    4  3  -6  297  304  9    4  4   3  852  874  6    4  5  11  793  793  8    4  6  16  171  165 14
4  2 -14  773  757 11    4  3  -5 1536 1490  7    4  4   4 1278 1245  7    4  5  12  460  470 11    4  6  18  601  611 12
4  2 -13  255  246  9    4  3  -4  779  742  6    4  4   7  231  218  8    4  5  14  159  134 14    4  6  19  455  434 15
4  2 -12 1112 1092  9    4  3  -3 2094 2060  9    4  4   8  964  935  7    4  5  15  781  777  9    4  6  20  165  184 19
4  2 -11  480  515 10    4  3  -2  598  595  6    4  4   9  573  558  8    4  5  16  701  692 10    4  6  22  412  421 13
4  2 -10 1364 1342  8    4  3  -1  130   98  8    4  4  10  543  523  9    4  5  17  458  462 13    4  6  23  228  259 17
4  2  -9  692  687  7    4  3   0  124  115  9    4  4  12  597  602  9    4  5  18  311  324  9    4  6  24  317  328 13
4  2  -8  441  439  8    4  3   1 2208 2168  9    4  4  13  311  273 10    4  5  19  432  449 11    4  7 -27  235  215 20
4  2  -7  668  626  6    4  3   2  649  682  6    4  4  14 1026 1016  9    4  5  20  312  314 10    4  7 -24  396  395 13
4  2  -6 1924 1876  8    4  3   3  636  595  6    4  4  15  345  331 10    4  5  21  592  614 14    4  7 -23  374  348 13
4  2  -5  208  174  6    4  3   5 1404 1355  7    4  4  16  289  281  9    4  5  22  327  318 11    4  7 -22  258  247 14
4  2  -4  796  789  6    4  3   6  506  493  8    4  4  17  272  258 10    4  5  25  360  381 12    4  7 -19  482  484 14
4  2  -3  825  779  6    4  3   7  877  868  7    4  4  18 1022 1072 10    4  5  26  255  279 18    4  7 -18  506  533 12
4  2  -2 2242 2264  9    4  3   9  167  162 10    4  4  19  401  401 11    4  5  27  256  226 18    4  7 -17  484  475 13
4  2  -1  828  811  6    4  3  10  225  225  8    4  4  20  319  326 10    4  6 -27  225  239 23    4  7 -16  169  179 15
4  2   0 1557 1518  7    4  3  11 1148 1161  8    4  4  22  460  506 12    4 12  -1  505  510 11    5  1   1  254  159  7
4  2   1  554  533  6    4  3  12  202  181  9    4 10 -17  343  359 11    4 12   3  371  388 10    5  1   2 1612 1684  8
4  7 -15  488  461 11    4  8  -2  334  345 11    4 10 -16  207  221 11    4 12   5  287  281  9    5  1   3  454  462  8
4  7 -14  775  766  9    4  8  -1  703  707  8    4 10 -15  358  371 10    4 12   9  259  269 10    5  1   4  603  598  7
4  7 -13  849  862  9    4  8   0  332  316 10    4 10 -14  282  309  8    4 13  -4  425  397 14    5  1   5  225  191  7
4  7 -12  475  468 11    4  8   2  419  409  9    4 10 -13  180  206 12    4 13  -2  165  173 15    5  1   6 1630 1609  8
4  7 -10  412  422 10    4  8   3  924  904  7    4 10 -11  537  510  9    4 13   0  298  270  9    5  1   8 1469 1451  8
4  7  -9  655  635  8    4  8   4  676  676  8    4 10 -10  375  381 12    4 13   2  320  318 10    5  1   9  275  302  8
4  7  -8  982 1023  7    4  8   5  659  640  8    4 10  -8  108  109 17    5  0 -25  680  711 21    5  1  10  359  352  8
4  7  -7  271  279  9    4  8   7  415  402 10    4 10  -7  552  587  9    5  0 -23  233  273 29    5  1  11  282  303  9
4  7  -6  148  125 10    4  8   8  693  688  8    4 10  -6  278  266  8    5  0 -21  816  940 25    5  1  12 1186 1191  8
4  7  -5  442  453  9    4  8   9  882  898  8    4 10  -5  469  483 10    5  0 -19  930 1049 17    5  1  14  275  293  8
4  7  -4  604  611  7    4  8  10  292  274  9    4 10  -3  278  284  8    5  0 -17  149  173 20    5  1  15  143  146 16
4  7  -3  788  764  7    4  8  11  168  146 12    4 10  -2  235  212  9    5  0 -15 1136 1190 11    5  1  16  819  814  9
4  7  -2  336  336 10    4  8  12  387  409  9    4 10  -1  589  572  9    5  0 -13  586  600 10    5  1  17  169  176 15
4  7  -1  144  119 10    4  8  13  570  556 10    4 10   2  245  228  8    5  0 -11 1053 1069  8    5  1  18  496  490 13
4  7   0  519  493  8    4  8  14  445  441 13    4 10   3  569  574  9    5  0  -9 1140 1133  7    5  1  20  388  370 12
4  7   1  786  791  7    4  8  15  387  396 10    4 10   4  233  232  9    5  0  -7 1116 1112  7    5  1  22  638  599 13
4  7   2  584  577  8    4  8  17  210  212 13    4 10   5  444  394 10    5  0  -5 1052 1099  7    5  1  26  520  528 14
4  7   3  380  396 10    4  8  18  252  268 12    4 10   7  397  389 12    5  0  -3  281  203  7    5  1  28  270  257 20
4  7   4  232  219  7    4  8  19  327  325 10    4 10   8  265  261  8    5  0  -1 2541 2589 10    5  2 -31  312  277 31
4  7   5  593  617  8    4  9 -24  240  280 16    4 10   9  568  571 10    5  0   1 1726 1760  8    5  2 -29  530  499 19
4  7   6  913  893  7    4  9 -22  218  242 15    4 10  12  195  184 12    5  0   3 1530 1568  8    5  2 -25  660  615 19
4  7   7  608  598  8    4  9 -20  284  314 11    4 10  13  449  484 13    5  0   5 1924 1966  9    5  2 -24  263  282 24
4  7   8  330  335  9    4  9 -19  278  297 10    4 10  14  154  156 16    5  0   9 1571 1546  8    5  2 -21  451  432 14
4  7   9  328  318  9    4  9 -18  579  606 12    4 10  15  256  254 10    5  0  11  934  907  8    5  2 -20  263  225 16
4  7  10  627  655  9    4  9 -17  426  432 10    4 10  18  161  161 18    5  0  13  773  754  9    5  2 -19  836  854 17
4  7  11  638  650  9    4  9 -14  673  698 10    4 10  19  343  341 11    5  0  15  821  816  9    5  2 -18  291  327 14
4  7  12  788  788  9    4  9 -13  440  471 12    4 11 -18  261  302 10    5  0  17  245  222 10    5  2 -15 1449 1435 11
4  7  15  552  549 11    4  9 -12  340  358  9    4 11 -14  312  365  9    5  0  19  715  721 12    5  2 -13  189  178 11
4  7  16  517  524 12    4  9 -11  202  201 10    4 11 -13  188  210 11    5  0  21  298  280 11    5  2 -12  367  316 12
4  7  17  245  244 11    4  9 -10  417  438 10    4 11 -12  222  244  9    5  0  23  481  441 12    5  2 -11 1460 1414  9
4  7  18  235  236 12    4  9  -9  317  323  9    4 11 -10  350  365  9    5  0  25  385  358 12    5  2 -10  154  139 11
4  7  19  316  310 10    4  9  -7  237  252  8    4 11  -9  131  144 15    5  1 -32  359  310 32    5  2  -9 1246 1205  7
4  7  20  231  214 13    4  9  -5  286  299  9    4 11  -8  522  544 10    5  1 -28  412  518 26    5  2  -8  321  339 10
4  7  21  281  305 12    4  9  -4  578  586  8    4 11  -7  202  194 10    5  1 -26  587  512 18    5  2  -7  714  669  7
4  7  22  215  204 16    4  9  -3  388  389 11    4 11  -6  113  104 17    5  1 -24  373  357 20    5  2  -6  196  198  7
4  7  24  165  140 24    4  9  -2  500  499  9    4 11  -4  659  664  9    5  1 -22  844  853 23    5  2  -5 1833 1783  8
4  7  25  243  231 18    4  9   1  369  347 11    4 11  -3  190  160 11    5  1 -20  201  234 22    5  2  -4  930  928  6
4  8 -25  277  293 15    4  9   2  751  747  8    4 11  -2  340  322 10    5  1 -19  422  430 14    5  2  -3  198  187  6
4  8 -24  219  225 17    4  9   5  510  511  9    4 11   0  379  396  9    5  1 -18  932  961 16    5  2  -2  161   93  8
4  8 -21  590  605 14    4  9   6  642  641  9    4 11   1  193  156 11    5  1 -16  983 1047 13
4  8 -20  408  402 12    4  9   7  419  409 11    4 11   2  515  522 11    5  1 -15  531  529 13
4  8 -19  224  210 13
4  8 -17  527  524 12
```

Structure factor table (columns: h k l F_o F_c σ)

h	k	l	Fo	Fc	σ
4	8	-16	443	438	13
4	8	-15	553	563	11
4	8	-14	236	218	10
4	8	-13	227	208	9
4	8	-12	482	502	10
4	8	-11	587	608	9
4	8	-10	500	509	9
4	8	-7	409	404	10
4	8	-6	350	362	11
4	8	-5	337	348	11
4	8	-4	248	249	8
4	8	-3	363	390	10
5	2	11	648	664	9
5	2	13	707	699	9
5	2	14	258	259	9
5	2	15	894	895	9
5	2	16	247	256	10
5	2	19	773	779	11
5	2	21	228	246	14
5	2	22	194	216	17
5	2	23	478	476	12
5	2	25	460	459	14
5	3	-28	357	376	22
5	3	-26	347	348	20
5	3	-24	218	222	25
5	3	-23	275	308	19
5	3	-22	551	525	15
5	3	-20	208	202	19
5	3	-19	430	420	14
5	3	-18	1017	1004	13
5	3	-17	462	457	12
5	3	-16	731	709	12
5	3	-15	429	435	11
5	3	-14	506	493	12
5	3	-13	821	779	10
5	3	-12	1510	1464	9
5	3	-10	156	146	11
5	3	-9	345	327	11
5	3	-8	1847	1803	9
5	3	-7	1079	1042	7
5	3	-6	611	609	7
5	3	-5	391	334	8
5	3	-4	1322	1281	7
5	3	-3	476	487	7
5	3	-2	1406	1418	7
5	3	-1	894	954	6
5	3	0	241	229	8
5	3	1	271	237	7
5	3	2	1681	1637	8
5	3	3	262	234	8
5	3	4	554	547	8
5	3	5	229	213	7
5	3	6	917	910	7
5	3	7	479	477	9
5	3	8	938	936	8
5	3	10	317	318	9
5	3	11	554	572	10
5	3	12	1228	1198	9
5	3	13	195	184	12
5	3	14	193	212	12
5	3	16	887	883	10
5	3	17	330	330	10
5	3	18	799	809	11
5	3	19	246	261	12
5	3	20	350	349	11
5	3	21	195	212	16
5	3	22	596	616	14
5	9	-23	347	358	11
5	9	-22	286	297	12
5	9	-21	189	218	16
5	9	-20	146	196	20
5	9	-19	311	305	9
5	9	-18	254	283	11
5	9	-17	488	503	12
5	9	-16	401	432	10
5	9	-13	435	481	12
5	9	-12	286	267	8
5	9	-11	296	303	8
5	9	-10	179	186	10
5	9	-9	334	348	8
5	9	-8	229	231	8
5	9	-7	458	457	10
5	9	-5	108	109	16
5	9	-4	237	231	8
5	9	-3	528	531	9
5	9	-2	229	208	8
5	9	-1	426	429	11
5	9	0	261	252	9
5	9	1	502	491	10
5	9	2	538	539	10
5	9	3	689	683	9
5	9	4	213	188	9
5	9	5	227	219	9
5	9	6	233	221	9
5	9	7	627	612	10
5	9	8	343	306	10
5	9	10	138	91	16
5	9	11	371	371	10
5	9	12	203	202	12
5	9	13	320	295	10
5	9	16	207	164	13
5	9	17	363	369	10
5	10	-20	319	350	9
5	10	-19	261	277	10
5	10	-17	140	141	17
5	10	-16	402	416	13
5	10	-15	218	234	10
5	10	-14	287	312	9
5	10	-13	240	283	9
5	10	-12	280	308	9
5	10	-10	515	556	10
5	10	-8	142	157	13
5	10	-6	441	466	10
5	10	-5	212	223	9
5	10	-4	434	463	11
5	10	-2	211	187	10
5	10	-1	274	242	8
5	10	0	665	637	9
5	10	3	201	213	10
5	10	4	501	490	11
5	10	5	299	260	9
5	10	6	276	295	8
6	5	-16	419	392	10
4	9	8	283	278	9
4	9	10	460	454	11
4	9	11	289	288	9
4	9	12	441	443	12
4	9	14	123	132	19
4	9	15	199	186	12
4	9	16	399	396	11
4	9	20	233	247	14
4	9	21	164	151	21
4	10	-21	289	304	10
4	10	-20	166	171	16
4	10	-19	152	161	17
5	3	23	340	329	11
5	3	26	327	324	14
5	4	-29	434	383	18
5	4	-26	241	242	24
5	4	-25	408	439	15
5	4	-24	222	208	22
5	4	-23	415	385	13
5	4	-21	530	499	13
5	4	-20	423	379	14
5	4	-19	573	558	16
5	4	-17	232	223	13
5	4	-16	580	573	13
5	4	-15	957	915	10
5	4	-14	357	338	11
5	4	-13	472	426	11
5	4	-12	247	220	9
5	4	-11	1382	1346	8
5	4	-10	905	867	8
5	4	-9	1468	1414	8
5	4	-7	704	715	7
5	4	-6	601	576	7
5	4	-5	1779	1744	8
5	4	-4	513	519	7
5	4	-3	358	385	9
5	4	-2	233	242	7
5	4	-1	1050	1045	7
5	4	0	733	736	7
5	4	1	585	582	7
5	4	3	495	478	8
5	4	4	827	793	7
5	4	5	1141	1105	8
5	4	6	564	558	8
5	4	7	235	205	8
5	4	8	202	192	9
5	4	9	924	931	8
5	4	10	486	464	10
5	4	11	505	484	11
5	4	13	630	637	10
5	4	14	522	519	11
5	4	15	1024	1058	9
5	4	16	392	417	11
5	4	17	191	176	14
5	4	19	704	716	12
5	4	20	379	383	13
5	4	21	249	266	13
5	4	23	289	290	13
5	4	24	210	225	18
5	4	25	294	311	15
5	5	-28	353	307	18
5	5	-26	425	403	14
5	5	-23	425	411	13
5	5	-22	617	609	17
5	5	-19	368	358	11
5	5	-18	522	498	14
5	5	-17	492	450	14
6	0	20	822	753	12
6	0	24	492	458	14
6	0	26	436	415	15
6	1	-31	398	353	30
6	1	-27	500	580	22
6	1	-25	659	587	18
6	1	-24	270	280	23
6	1	-23	426	440	15
6	1	-21	981	1010	18
6	1	-17	880	904	12
6	1	-15	453	424	13
6	1	-14	242	208	10
6	1	-13	548	549	10
6	1	-11	1280	1250	8
6	1	-10	378	372	11
6	1	-9	142	172	12
6	1	-7	1357	1343	8
6	1	-6	545	551	8
6	1	-5	788	789	7
6	1	-4	128	96	12
6	1	-3	1783	1817	8
6	1	-2	203	176	8
6	1	-1	1700	1731	8
6	1	0	275	271	8
6	1	1	621	637	7
6	1	2	347	340	10
6	1	3	1862	1861	9
6	1	5	431	396	9
6	1	6	355	344	11
6	1	7	1309	1281	8
6	1	9	981	983	8
6	1	10	159	139	12
6	1	11	375	357	9
6	1	13	1001	997	9
6	1	16	155	134	16
6	1	17	712	705	11
6	1	18	235	192	12
6	1	19	480	488	14
6	1	21	311	311	11
6	1	23	516	514	12
6	2	-28	502	432	18
6	2	-24	558	550	15
6	2	-21	216	167	20
6	2	-20	658	671	17
6	2	-19	375	394	11
6	2	-18	796	808	14
6	2	-17	135	99	22
6	2	-15	455	406	13
6	2	-14	1342	1363	10
6	2	-13	400	376	13
6	2	-12	203	194	10
6	2	-10	1283	1248	8
6	2	-9	340	310	11
6	6	2	547	513	9
4	11	5	139	140	15
4	11	6	465	423	11
4	11	8	207	201	11
4	11	10	263	271	9
4	11	11	134	149	17
4	11	12	239	225	10
4	12	-11	329	356	10
4	12	-7	436	456	12
4	12	-6	152	117	14
4	12	-5	362	358	9
4	12	-3	244	249	10
4	12	-2	146	93	15
5	5	-16	350	336	9
5	5	-15	178	128	14
5	5	-14	701	655	10
5	5	-13	802	789	9
5	5	-12	875	857	8
5	5	-11	447	423	10
5	5	-9	703	679	8
5	5	-8	1373	1363	8
5	5	-7	883	903	7
5	5	-6	1030	1042	7
5	5	-5	202	181	8
5	5	-4	973	950	7
5	5	-3	804	815	7
5	5	-2	1181	1167	7
5	5	-1	229	200	7
5	5	1	339	354	10
5	5	2	1022	996	7
5	5	3	614	632	8
5	5	4	360	346	12
5	5	5	119	73	13
5	5	6	714	709	8
5	5	7	641	625	8
5	5	8	898	845	8
5	5	9	254	259	8
5	5	10	469	453	11
5	5	11	181	185	12
5	5	12	1033	1009	9
5	5	13	605	606	10
5	5	14	151	152	16
5	5	16	709	704	11
5	5	17	406	398	11
5	5	18	464	464	14
5	5	20	239	266	13
5	5	21	240	235	14
5	5	22	446	458	12
5	5	23	211	191	17
5	5	26	230	245	20
5	6	-26	404	387	13
5	6	-25	398	388	13
5	6	-24	255	235	17
5	6	-23	222	193	19
5	6	-22	251	269	16
5	6	-21	280	281	13
5	6	-20	526	515	16
5	6	-19	491	466	15
5	6	-18	230	209	13
5	6	-17	420	410	11
5	6	-16	478	481	13
5	6	-15	773	753	10
5	6	-14	674	672	10
5	6	-13	135	126	15
5	6	-11	545	530	9
5	6	-10	615	604	9
5	6	-9	695	723	8
5	6	-8	205	196	8
6	2	-8	1132	1109	12
6	2	-7	419	438	9
6	2	-6	528	538	8
6	2	-5	281	293	8
6	2	-4	1585	1598	8
6	2	-3	755	761	7
6	2	-2	336	371	10
6	2	-1	272	255	8
6	2	0	1375	1407	8
6	2	1	278	280	8
6	2	2	1009	1009	7
6	2	4	577	537	8
6	2	5	342	341	11
6	2	6	1471	1409	8
6	2	8	130	117	14
6	2	10	1134	1093	8
6	2	11	120	114	17
6	2	12	551	524	10
6	2	14	708	723	10
6	2	15	234	214	11
6	2	16	717	733	11
6	2	17	222	214	12
6	2	20	611	622	13
6	2	21	205	188	16
6	2	22	261	266	14
6	3	-28	95	105	11
6	3	-27	360	360	20
6	3	-25	399	374	16
6	3	-23	274	263	19
6	3	-21	764	765	17
6	3	-18	167	111	19
6	3	-17	1001	980	12
6	3	-16	519	540	14
6	3	-15	790	773	11
6	3	-13	1011	994	9
6	3	-12	472	413	11
6	3	-11	1499	1455	9
6	3	-8	175	174	10
6	3	-7	1292	1259	8
6	3	-6	493	492	8
6	3	-5	442	417	8
6	3	-4	276	285	8
6	3	-3	767	780	7
6	3	-1	837	861	7
6	3	2	1292	1271	8
6	3	4	134	146	11
6	3	5	458	465	9
6	3	6	235	224	8
6	3	7	931	906	8
6	3	8	416	420	11
6	3	11	606	576	10
6	8	-8	360	382	11
5	1	-14	482	468	12
5	1	-12	1328	1319	9
5	1	-11	318	319	9
5	1	-9	163	154	9
5	1	-8	1242	1252	7
5	1	-7	396	384	8
5	1	-6	953	950	7
5	1	-4	1055	1089	6
5	1	-3	367	352	8
5	1	-2	1751	1763	8
5	1	-1	672	655	7
5	1	0	296	299	9
5	7	-27	258	267	16
5	7	-26	258	269	18
5	7	-23	441	421	14
5	7	-22	526	532	12
5	7	-21	218	211	15
5	7	-19	322	309	10
5	7	-18	453	426	10
5	7	-17	649	613	11
5	7	-16	385	390	10
5	7	-14	323	293	8
5	7	-13	543	528	10
5	7	-12	700	722	9
5	7	-11	440	447	10
5	7	-10	155	171	11
5	7	-9	309	325	9
5	7	-8	289	277	9
5	7	-7	557	582	8
5	7	-6	452	453	9
5	7	-5	134	115	11
5	7	-4	256	253	7
5	7	-3	710	723	7
5	7	-2	671	667	7
5	7	-1	253	259	8
5	7	0	115	116	14
5	7	1	717	686	8
5	7	2	863	829	7
6	10	5	480	477	12
5	2	-1	1906	1937	9
5	2	0	444	465	7
5	2	1	1210	1234	7
5	2	2	515	528	7
5	2	3	891	903	7
5	2	4	555	521	8
5	2	5	1556	1483	8
5	2	6	377	350	10
5	2	7	126	85	13
5	2	8	470	467	10
5	2	9	1405	1375	8
5	2	10	153	174	13
5	7	3	525	517	9
5	7	4	314	329	9
5	7	5	128	121	14
5	7	6	807	773	8
5	7	7	837	852	8
5	7	8	485	465	10
5	7	9	535	502	10
5	7	10	363	377	9
5	7	11	474	474	11
5	7	12	581	577	10
5	7	13	501	476	11
5	7	16	323	332	11
5	7	17	254	264	11
5	7	18	196	192	15
5	7	21	228	230	15
5	7	22	258	248	15
5	7	23	159	152	24
5	8	-25	301	249	14
5	8	-24	310	285	13
5	8	-21	250	245	13
5	8	-20	488	499	14
5	8	-19	380	390	12
5	8	-16	344	334	11
5	8	-15	429	431	12
5	8	-14	461	446	11
5	8	-13	235	228	9
5	8	-12	218	225	9
5	8	-11	365	387	8
5	8	-10	477	501	9
5	8	-9	291	310	9
5	8	-7	217	227	8
5	8	-6	483	497	9
5	8	-5	536	533	8
5	8	-4	483	502	9
5	8	-3	194	180	9
5	8	-2	386	400	10
5	8	-1	376	375	11
5	8	0	800	809	8
5	8	1	397	387	11
5	8	2	231	229	8
5	8	3	537	532	9
5	8	4	859	839	8
5	8	5	735	731	9
5	8	6	596	599	9
5	8	8	399	388	12
5	8	9	518	507	10
5	8	10	593	588	10
5	8	11	258	232	9
5	8	12	148	144	15
5	8	13	202	193	12
5	8	14	318	323	10
5	8	15	231	221	11
5	8	18	231	228	13
5	8	19	180	188	17
5	8	20	229	207	15
7	1	16	157	165	17
5	6	-7	401	422	10
5	6	-6	629	645	7
5	6	-5	1160	1197	7
5	6	-4	232	231	8
5	6	-3	461	468	8
5	6	-2	755	769	7
5	6	-1	1044	1065	7
5	6	0	692	690	7
5	6	1	833	826	7
5	6	2	103	116	15
5	6	3	460	404	9
5	6	4	846	835	8
5	6	5	779	761	8
5	6	6	649	658	8
5	6	8	126	90	15
5	6	9	839	836	8
5	6	10	920	909	9
5	6	11	251	233	9
5	6	13	688	682	10
5	6	14	513	537	12
5	6	15	423	419	14
5	6	16	325	343	10
5	6	18	195	196	15
5	6	19	469	468	15
5	6	20	256	251	13
5	6	21	249	230	14
5	6	23	262	229	15
5	6	24	261	246	16
5	6	25	209	206	21
6	3	12	432	449	13
6	3	13	983	978	9
6	3	14	425	424	13
6	3	15	162	147	15
6	3	17	592	591	12
6	3	18	184	183	15
6	3	19	376	378	13
6	3	20	258	263	12
6	3	21	278	290	12
6	3	23	356	354	11
6	4	-24	386	374	14
6	4	-20	546	583	18
6	4	-19	341	334	11
6	4	-18	794	747	12
6	4	-17	135	117	21
6	4	-16	316	312	24
6	4	-15	460	440	13
6	4	-14	1186	1144	9
6	4	-13	458	460	12
6	4	-12	400	384	12
6	4	-11	477	488	11
6	4	-10	1188	1164	8
6	4	-9	785	774	8
6	4	-8	1004	995	8
6	4	-6	538	528	8
6	4	-5	433	433	9
6	4	-4	915	922	7
6	4	-3	343	337	10
6	4	-2	246	240	7
6	4	-1	128	104	11
6	4	0	706	738	7
6	4	1	442	445	9
6	4	2	701	704	8
6	4	4	533	497	9
6	4	5	489	509	10
6	4	6	1266	1226	8
6	4	7	301	310	10
6	4	8	157	165	13
6	4	9	237	249	9
6	4	10	1158	1182	9
6	4	11	565	578	10
6	4	12	543	555	11
6	4	14	543	548	11
6	4	15	241	244	11
6	4	16	761	786	11
6	4	17	196	173	14
6	4	19	237	217	13
6	4	20	444	480	12
6	4	21	216	240	16
6	5	-25	293	285	17
6	5	-22	377	358	12
6	5	-20	454	433	13
6	5	-19	223	203	15
6	5	-18	227	224	14
6	5	-17	841	816	11

h	k	l	Fo	Fc	σ
6	5	-15	602	602	11
6	5	-13	669	615	9
6	5	-12	627	647	9
6	5	-11	1013	1015	8
6	5	-10	273	273	8
6	5	-8	800	798	8
6	5	-7	1092	1091	7
6	5	-6	427	431	9
6	5	-5	802	804	7
6	5	-4	411	421	9
6	5	-3	446	447	8
6	5	-2	584	608	8
6	5	-1	749	758	7
6	5	0	448	421	9
6	5	1	180	153	9
6	5	2	384	381	10
6	5	3	786	756	9
6	5	4	756	738	8
6	5	5	144	131	13
6	5	6	160	149	12
6	5	7	855	831	8
6	5	8	445	439	11
6	5	9	560	547	10
6	5	11	429	410	12
6	5	12	418	424	13
6	5	13	834	811	10
6	5	14	478	512	13
6	5	16	218	199	12
6	5	17	481	494	14
6	5	18	411	419	11
6	5	19	289	285	11
6	6	-24	340	318	13
6	6	-23	315	297	13
6	6	-20	177	157	18
6	6	-19	506	490	15
6	6	-18	425	418	11
6	6	-17	240	262	12
6	6	-16	222	204	11
6	6	-15	294	291	9
6	6	-14	726	736	9
6	6	-13	349	378	10
6	6	-12	272	288	8
6	6	-11	292	299	8
6	6	-10	663	659	8
6	6	-9	419	442	10
6	6	-8	655	687	8
6	6	-7	157	155	11
6	6	-5	821	833	7
6	6	-4	1000	1021	7
6	6	-3	255	262	8
6	6	-2	322	321	8
6	6	-1	647	665	8
6	6	0	871	850	7
6	6	1	836	832	8
7	3	-8	172	175	10
7	3	-7	281	259	9
7	3	-6	968	991	8
7	3	-5	377	393	10
7	3	-4	365	355	10
7	3	-3	157	164	10
7	3	-2	935	953	7
7	3	-1	239	254	7
7	3	0	850	893	7
7	3	1	185	205	9
7	3	3	318	307	9
7	3	4	1304	1286	8
7	3	5	180	199	11
7	3	6	434	428	11
7	3	7	215	222	10
7	3	8	1072	1044	9
7	3	9	599	574	10
7	3	10	783	783	9
7	3	11	226	254	10
7	3	12	406	403	13
7	3	13	233	243	11
7	3	14	829	833	10
7	3	15	252	246	11
7	3	18	474	478	15
7	3	19	172	205	18
7	3	20	333	318	10
7	4	-24	230	199	21
7	4	-23	423	415	14
7	4	-21	206	206	19
7	4	-20	319	330	12
7	4	-19	740	730	13
7	4	-18	357	378	11
7	4	-17	692	689	12
7	4	-15	332	314	9
7	4	-14	357	349	11
7	4	-13	938	943	9
7	4	-12	462	472	11
7	4	-11	429	451	11
7	4	-10	320	321	10
7	4	-9	858	860	8
7	4	-8	335	326	8
7	4	-7	454	498	10
7	4	-6	149	147	11
7	4	-5	347	374	11
7	4	-4	450	440	9
7	4	-3	777	792	8
7	4	0	143	125	11
7	4	1	882	921	8
7	4	2	429	442	10
7	4	3	540	538	9
7	4	4	184	152	10
7	4	5	774	768	9
7	4	6	617	598	10
7	4	7	1099	1085	9
7	4	8	252	264	9
8	2	-10	348	345	10
8	2	-8	1066	1069	8
8	2	-7	134	101	15
8	2	-6	939	922	8
8	2	-5	272	282	9
8	2	-4	219	203	9
8	2	-3	340	346	8
8	2	-2	948	979	8
8	2	1	505	518	9
8	2	2	749	775	8
8	2	3	261	285	9
8	2	4	534	553	9
8	2	6	572	538	10
8	2	7	192	166	11
6	6	3	152	145	12
6	6	4	467	462	10
6	6	5	666	651	9
6	6	6	594	555	9
6	6	7	597	583	9
6	6	10	629	650	10
6	6	11	609	593	10
6	6	12	277	260	9
6	6	14	434	424	10
6	6	15	357	326	11
6	6	16	350	343	10
6	6	19	220	227	15
6	7	-22	333	330	11
6	7	-21	410	396	12
6	7	-20	229	214	14
6	7	-18	185	169	14
6	7	-17	348	348	9
6	7	-16	399	410	10
6	7	-15	477	499	12
6	7	-12	484	493	10
6	7	-11	463	454	10
6	7	-8	495	533	9
6	7	-7	620	630	8
6	7	-6	610	658	8
6	7	-5	353	370	10
6	7	-4	165	170	10
6	7	-3	412	441	10
6	7	-2	908	951	8
6	7	-1	691	679	8
6	7	0	207	200	9
6	7	1	363	352	11
6	7	2	636	644	9
6	7	3	843	802	8
6	7	4	538	544	10
6	7	7	533	530	10
6	7	8	672	658	10
6	7	9	329	309	10
6	7	10	269	280	9
6	7	11	267	246	9
6	7	12	417	366	13
6	7	13	339	320	11
6	7	14	278	294	10
6	7	17	354	346	11
6	7	18	287	308	12
6	8	-20	153	115	19
6	8	-19	377	405	12
6	8	-18	237	241	11
6	8	-15	223	242	10
6	8	-14	219	214	10
6	8	-13	260	296	8
6	8	-12	160	156	12
6	8	-11	182	202	11
6	8	-10	323	330	9
6	8	-9	478	513	10
7	4	9	173	149	13
7	4	10	360	364	10
7	4	11	896	903	10
7	4	12	559	569	11
7	4	13	373	356	10
7	4	15	367	360	11
7	4	16	253	255	11
7	4	17	384	385	12
7	4	19	150	133	20
7	5	-22	254	201	15
7	5	-21	406	410	12
7	5	-20	458	428	12
7	5	-19	183	174	17
7	5	-17	452	464	11
7	5	-16	732	723	11
7	5	-15	311	293	10
7	5	-14	450	480	13
7	5	-13	201	196	11
7	5	-12	475	482	11
7	5	-11	589	621	9
7	5	-10	762	764	8
7	5	-9	302	306	9
7	5	-7	467	478	9
7	5	-6	722	739	8
7	5	-5	219	224	8
7	5	-4	228	227	8
7	5	-3	232	232	8
7	5	-2	540	538	8
7	5	-1	415	427	10
7	5	0	561	551	8
7	5	1	408	420	10
7	5	2	447	449	10
7	5	3	311	283	10
7	5	4	916	906	9
7	5	5	457	452	11
7	5	7	200	211	11
7	5	8	866	849	9
7	5	9	509	520	11
7	5	10	700	685	10
7	5	12	261	261	10
7	5	13	328	328	10
7	5	14	620	591	11
7	5	16	159	150	18
7	5	17	236	251	13
7	5	18	303	326	11
7	5	19	303	312	11
7	6	-22	327	330	12
7	6	-19	396	398	12
7	6	-18	441	448	15
7	6	-17	536	552	12
7	6	-14	565	602	11
7	6	-13	707	730	9
7	6	-12	169	174	12
7	6	-11	221	214	9
7	6	-10	404	404	11
8	4	-21	211	188	17
8	4	-20	179	182	20
8	4	-19	296	267	12
8	4	-18	658	708	14
8	4	-17	280	268	11
8	4	-16	626	610	12
8	4	-14	177	187	14
8	4	-13	343	351	11
8	4	-12	626	642	10
8	4	-11	225	236	10
8	4	-10	213	200	10
8	4	-8	572	585	9
8	4	-7	389	394	11
8	4	-6	420	435	11
6	8	-6	252	255	7
6	8	-5	853	894	8
6	8	-4	574	575	9
6	8	-3	495	526	9
6	8	-1	478	473	10
6	8	0	562	534	9
6	8	1	860	830	8
6	8	2	558	522	9
6	8	4	335	301	9
6	8	5	675	665	9
6	8	6	370	339	9
6	8	7	463	432	11
6	8	9	242	227	10
6	8	10	270	254	9
6	8	11	354	345	11
6	8	12	170	156	14
6	8	14	150	137	18
6	8	15	327	312	11
6	9	-17	167	175	14
6	9	-16	294	317	8
6	9	-15	210	233	11
6	9	-12	361	384	9
6	9	-10	347	365	8
6	9	-8	352	376	12
6	9	-7	337	368	8
6	9	-6	465	496	10
6	9	-5	122	135	15
6	9	-4	213	204	9
6	9	-3	374	372	11
6	9	-2	609	615	9
6	9	-1	412	394	11
6	9	0	238	255	9
6	9	1	189	204	11
6	9	2	472	462	11
6	9	3	407	378	12
6	9	4	573	537	10
6	9	5	208	201	11
6	9	6	252	249	9
6	9	7	194	169	12
6	9	8	490	459	12
6	9	9	195	183	12
6	9	12	321	304	10
6	10	-13	301	337	9
6	10	-11	207	228	10
6	10	-9	466	516	11
6	10	-7	156	166	12
6	10	-6	175	165	10
6	10	-5	390	397	11
6	10	-4	302	301	8
6	10	-3	335	340	9
6	10	-1	336	313	10
6	10	0	438	389	12
6	10	1	489	461	11
6	10	2	246	208	9
7	6	-9	622	625	9
7	6	-8	425	437	10
7	6	-7	697	714	8
7	6	-5	231	217	8
7	6	-4	557	615	9
7	6	-3	695	713	8
7	6	-2	457	481	10
7	6	-1	166	174	11
7	6	0	168	164	11
7	6	1	621	627	9
7	6	2	918	913	8
7	6	3	335	296	10
7	6	4	241	252	9
7	6	5	510	496	11
7	6	6	499	497	11
7	6	7	481	445	11
7	6	8	349	331	10
7	6	9	143	160	16
7	6	10	244	246	10
7	6	11	547	542	12
7	6	12	347	344	11
7	6	13	201	173	13
7	6	15	359	377	10
7	6	17	380	391	10
7	7	-20	265	254	12
7	7	-19	264	280	11
7	7	-17	193	229	13
7	7	-16	242	253	10
7	7	-15	394	423	13
7	7	-14	275	284	8
7	7	-13	251	267	9
7	7	-12	130	131	15
7	7	-11	524	563	10
7	7	-10	620	644	9
7	7	-7	517	525	9
7	7	-6	510	511	9
7	7	-5	667	698	8
7	7	-2	500	517	9
7	7	-1	693	724	8
7	7	0	482	469	10
7	7	1	319	305	10
7	7	2	353	351	10
7	7	3	389	355	12
7	7	4	491	484	11
7	7	5	482	453	11
7	7	6	146	136	15
7	7	9	396	382	13
7	7	10	321	307	10
7	7	13	298	280	10
7	7	14	364	338	12
7	7	15	226	229	13
8	5	-18	366	409	11
8	5	-17	202	232	12
8	5	-9	243	230	10
8	5	9	569	573	12
8	5	10	418	419	10
8	5	11	420	418	10
8	5	14	295	304	10
8	5	15	384	375	12
8	5	16	209	267	15
8	6	-20	236	243	14
8	6	-19	164	128	18
8	6	-18	341	343	10
8	6	-17	274	294	10
8	6	-16	439	476	14
8	6	-14	149	155	16
8	6	-13	419	448	13
6	10	6	201	167	12
6	10	7	304	294	10
6	11	-2	387	366	10
7	0	-27	285	422	27
7	0	-23	797	858	19
7	0	-21	368	386	12
7	0	-19	578	590	15
7	0	-17	882	867	11
7	0	-15	183	178	14
7	0	-13	1093	1052	9
7	0	-11	291	321	9
7	0	-9	1214	1170	8
7	0	-7	973	996	8
7	0	-5	1164	1181	8
7	0	-3	2143	2154	10
7	0	1	1510	1572	8
7	0	3	1004	992	7
7	0	5	682	714	8
7	0	7	866	850	8
7	0	9	145	121	14
7	0	11	563	550	10
7	0	13	588	538	11
7	0	15	715	666	11
7	0	17	687	654	12
7	0	19	199	196	17
7	0	21	692	617	15
7	1	-26	520	533	17
7	1	-24	326	402	18
7	1	-20	773	772	15
7	1	-16	649	620	12
7	1	-15	194	145	13
7	1	-14	403	393	10
7	1	-12	721	718	9
7	1	-11	332	303	10
7	1	-10	1077	1073	8
7	1	-9	365	354	12
7	1	-8	473	444	10
7	1	-7	112	95	16
7	1	-6	1658	1681	9
7	1	-5	366	340	11
7	1	-4	815	840	7
7	1	-2	1178	1181	7
7	1	0	1263	1300	8
7	1	1	283	289	9
7	1	2	466	479	9
7	1	4	1298	1334	8
7	1	6	370	384	11
7	1	7	302	287	10
7	1	8	582	571	9
7	1	10	706	720	10
7	1	11	163	138	13
7	1	12	382	361	10
7	1	14	765	741	10
7	1	15	328	334	10
7	8	-14	318	357	9
7	8	-13	292	297	9
7	8	-12	370	392	9
7	8	-10	278	287	8
7	8	-9	437	460	10
7	8	-8	600	650	9
7	8	-7	476	521	10
7	8	-5	227	209	8
7	8	-4	544	566	9
7	8	-3	457	448	10
7	8	-2	538	552	9
7	8	-1	136	111	14
7	8	0	269	269	9
7	8	1	299	276	9
7	8	3	572	564	10
7	8	5	269	265	9
7	8	6	350	331	11
7	8	7	257	229	10
7	8	8	239	229	11
7	8	10	188	169	14
7	8	11	299	285	9
7	8	12	280	276	10
7	9	-12	143	144	14
7	9	-11	435	479	11
7	9	-10	169	160	11
7	9	-9	226	250	9
7	9	-7	405	439	11
7	9	-6	299	286	9
7	9	-5	542	576	9
7	9	-4	153	179	13
7	9	-3	196	211	10
7	9	-2	280	271	9
7	9	-1	528	562	10
7	9	0	416	397	13
7	9	1	239	219	10
7	9	3	448	415	12
7	9	4	170	159	14
7	9	8	263	235	10
7	9	9	411	409	13
7	10	-8	366	405	12
7	10	-7	136	136	13
7	10	-6	121	96	15
7	10	-4	387	414	12
7	10	-3	302	287	10
7	10	-2	286	308	9
7	10	0	285	280	9
7	10	1	213	204	12
7	10	2	373	355	10
7	10	3	206	188	12
8	0	-22	587	581	19
8	0	-18	473	457	12
8	0	-16	925	880	11
8	0	-14	372	359	12
8	7	3	189	183	12
8	7	4	253	246	10
8	7	5	394	391	10
8	7	6	290	276	9
8	7	7	194	209	13
8	7	9	286	267	10
8	7	10	360	360	12
8	7	11	293	278	10
8	8	-13	369	376	12
8	8	-11	303	325	10
8	8	-9	335	376	9
8	8	-8	376	379	12
7	1	18	694	668	12
7	1	20	404	392	13
7	1	22	317	291	12
7	2	-23	701	665	18
7	2	-21	282	307	15
7	2	-20	196	223	19
7	2	-19	412	417	12
7	2	-18	373	334	11
7	2	-17	701	701	13
7	2	-15	577	555	12
7	2	-13	1238	1229	10
7	2	-12	494	488	11
7	2	-11	302	275	8
7	2	-10	221	211	9
7	2	-9	1081	1088	8
7	2	-8	331	313	9
7	2	-7	993	980	8
7	2	-6	159	191	11
7	2	-5	748	746	8
7	2	-3	1272	1309	8
7	2	-2	214	214	8
7	2	-1	220	221	8
7	2	0	554	568	8
7	2	1	1383	1404	8
7	2	2	157	149	11
7	2	3	656	702	8
7	2	4	374	397	11
7	2	5	558	524	9
7	2	6	142	138	14
7	2	7	1099	1093	8
7	2	8	234	235	9
7	2	11	1010	1011	9
7	2	12	301	286	9
7	2	13	316	319	9
7	2	14	184	178	13
7	2	15	546	560	12
7	2	17	530	520	13
7	2	18	197	195	15
7	2	19	142	129	21
7	2	21	483	503	12
7	3	-26	386	421	18
7	3	-24	379	363	15
7	3	-23	270	310	18
7	3	-22	476	434	15
7	3	-21	364	340	12
7	3	-20	751	718	15
7	3	-17	222	230	14
7	3	-16	840	808	11
7	3	-15	562	542	12
7	3	-14	669	648	11
7	3	-12	726	693	9
7	3	-11	291	279	9
7	3	-10	733	738	9
7	3	-9	446	456	10
8	0	-12	1257	1217	9
8	0	-10	160	139	14
8	0	-8	1185	1162	9
8	0	-6	846	842	8
8	0	-4	503	511	9
8	0	-2	746	737	8
8	0	0	111	108	15
8	0	2	707	733	8
8	0	4	607	618	9
8	0	6	476	484	10
8	0	8	519	503	11
8	0	10	202	184	11
8	0	12	792	763	10
8	0	14	367	358	12
8	0	16	738	699	12
8	0	18	570	522	15
8	1	-25	386	394	16
8	1	-23	403	382	13
8	1	-19	606	580	16
8	1	-17	168	206	19
8	1	-15	904	872	11
8	1	-14	331	320	10
8	1	-13	545	543	12
8	1	-12	186	171	14
8	1	-11	1019	992	9
8	1	-10	259	241	10
8	1	-9	1209	1196	9
8	1	-7	399	407	12
8	1	-5	1410	1422	9
8	1	-3	506	534	9
8	1	-2	203	228	9
8	1	-1	672	689	8
8	1	0	196	178	9
8	1	1	927	966	8
8	1	3	180	179	10
8	1	4	197	209	9
8	1	5	741	758	8
8	1	7	187	179	11
8	1	9	832	821	9
8	1	11	644	624	10
8	1	12	305	300	10
8	1	13	475	447	13
8	1	15	708	691	11
8	1	19	549	525	15
8	2	-23	263	247	18
8	2	-22	565	583	14
8	2	-21	269	288	15
8	2	-20	204	195	18
8	2	-18	694	669	14
8	2	-17	388	360	12
8	2	-16	591	584	13
8	2	-15	244	215	12
8	2	-14	483	455	13
8	2	-12	936	906	9
8	2	-11	326	325	9
8	2	-10	221	211	9
9	1	-23	201	210	24
9	1	-22	244	206	18
9	1	-20	384	366	12
9	1	-18	616	573	15
9	1	-16	210	144	15
9	1	-14	940	857	11
9	1	-13	230	228	13
9	1	-12	363	323	11
9	1	-10	836	795	9
9	1	-9	317	282	10
9	1	-8	975	932	9
9	1	-7	246	226	9
9	1	-6	148	167	14
9	1	-4	857	862	8

h	k	l	Fo	Fc	σ
8	2	8	875	860	9
8	2	9	444	450	12
8	2	10	234	253	10
8	2	12	799	786	10
8	2	13	215	194	12
8	2	14	227	219	12
8	2	16	465	467	15
8	2	18	465	440	11
8	3	-23	451	424	13
8	3	-21	459	458	14
8	3	-20	289	307	14
8	3	-19	586	563	15
8	3	-18	209	221	16
8	3	-16	204	155	14
8	3	-15	794	774	11
8	3	-14	244	230	11
8	3	-13	478	459	12
8	3	-11	463	472	11
8	3	-10	158	141	13
8	3	-9	561	552	10
8	3	-6	376	414	12
8	3	-5	991	1018	8
8	3	-4	304	300	9
8	3	-3	399	384	10
8	3	-2	529	547	9
8	3	-1	870	887	8
8	3	0	556	573	9
8	3	1	883	923	8
8	3	3	379	361	11
8	3	4	189	192	11
8	3	5	1190	1183	9
8	3	6	541	508	10
8	3	7	176	160	13
8	3	9	703	700	10
8	3	10	333	353	11
8	3	11	481	475	12
8	3	12	266	275	10
8	3	13	305	303	9
8	3	15	475	481	14
8	4	-23	289	271	15
8	4	-22	635	621	17
9	3	-19	234	234	16
9	3	-18	512	487	16
9	3	-17	281	258	12
9	3	-14	409	388	11
9	3	-13	219	239	13
9	3	-12	268	256	10
9	3	-10	564	548	11
9	3	-9	214	198	11
9	3	-8	714	703	9
9	3	-6	175	187	12
9	3	-5	323	318	10
9	3	-4	1042	1057	8
9	3	-3	277	295	9
9	3	-2	300	288	8
9	3	0	867	909	8
9	3	1	220	236	9
9	3	2	742	767	9
9	3	3	250	267	8
9	3	4	323	336	9
9	3	6	742	747	10
9	3	7	341	348	11
9	3	8	153	145	15
9	3	10	391	397	10
9	3	12	358	345	12
9	3	14	210	196	13
9	4	-21	492	493	13
9	4	-19	182	201	19
9	4	-18	199	167	16
9	4	-17	344	356	11
9	4	-16	232	240	13
9	4	-15	458	482	14
9	4	-12	306	292	9
9	4	-11	564	558	11
9	4	-10	224	225	10
9	4	-7	656	638	9
9	4	-6	386	418	13
9	4	-5	388	364	12
9	4	-3	443	451	11
9	4	-2	351	357	9
9	4	-1	888	915	8
9	4	0	280	293	9
9	4	2	218	219	9
9	4	3	860	894	9
9	4	4	315	313	9
9	4	5	326	307	11
9	4	7	381	378	10
9	4	8	291	286	9
9	4	9	370	355	11
9	4	10	169	153	15
9	4	13	357	347	12
9	5	-19	258	250	12
9	5	-18	390	387	12
9	5	-15	250	264	11
9	5	-14	491	514	13
9	5	-13	270	270	10
11	1	4	463	459	11
11	1	6	296	296	9
11	1	7	134	106	17
11	1	8	556	533	12
11	2	-15	480	425	12
11	2	-13	429	398	12
11	2	-11	251	250	13
11	2	-9	515	497	13
11	2	-8	127	132	21
11	2	-5	615	585	10
11	2	-4	299	313	10
11	2	-3	293	311	8
11	2	-2	162	163	14
11	2	-1	384	384	12
11	2	0	150	137	14
11	2	1	530	521	10
11	2	2	180	190	12
11	2	5	561	601	11
11	2	7	223	229	10
11	3	-13	262	242	13
11	3	-12	636	595	13
11	3	-10	267	233	11
11	3	-9	194	155	14
11	3	-8	531	513	13
11	3	-7	240	247	11
11	3	-6	486	471	12
11	3	-4	225	222	10
8	4	-4	296	305	10
8	4	-3	564	578	9
8	4	-2	974	1013	8
8	4	-1	146	144	12
8	4	0	196	211	10
8	4	1	268	273	9
8	4	2	1146	1181	8
8	4	3	532	552	10
8	4	4	434	458	12
8	4	6	602	615	10
8	4	7	502	488	12
8	4	8	782	753	10
8	4	9	397	399	10
8	4	12	555	503	11
8	4	13	181	189	15
8	4	14	224	224	12
8	4	16	233	230	13
8	4	17	226	209	13
8	5	-21	312	305	12
8	5	-20	266	290	14
8	5	-19	643	648	13
8	5	-16	343	323	10
8	5	-15	646	660	11
8	5	-14	163	152	15
8	5	-13	375	343	10
8	5	-11	381	400	9
8	5	-10	423	442	12
8	5	-9	509	540	10
8	5	-8	186	153	10
8	5	-6	390	432	12
8	5	-5	606	625	9
8	5	-4	402	410	11
8	5	-3	292	293	8
8	5	-1	757	777	8
8	5	0	719	747	8
8	5	1	632	646	9
8	5	2	189	198	10
8	5	3	384	422	9
8	5	4	464	437	11
8	5	5	856	845	9
8	5	6	302	320	10
9	5	-12	249	250	10
9	5	-10	358	363	10
9	5	-9	468	487	11
9	5	-8	359	375	10
9	5	-7	219	244	10
9	5	-6	204	221	10
9	5	-5	190	206	11
9	5	-4	654	671	9
9	5	-3	417	419	11
9	5	-2	224	228	9
9	5	0	562	572	10
9	5	1	413	431	12
9	5	2	549	580	10
9	5	4	201	181	12
9	5	5	396	412	10
9	5	6	645	612	11
9	5	8	167	175	15
9	5	10	364	320	11
9	5	11	183	172	15
9	5	12	256	260	11
9	6	-17	274	282	11
9	6	-16	304	319	9
9	6	-15	353	370	10
9	6	-13	215	213	11
9	6	-12	414	442	13
9	6	-11	399	425	13
9	6	-10	293	293	9
9	6	-7	431	420	11
9	6	-6	490	496	10
9	6	-5	288	280	9
9	6	-4	160	171	13
9	6	-3	323	332	10
9	6	-2	380	403	12
9	6	-1	418	436	11
9	6	0	224	247	9
9	6	2	215	209	10
9	6	3	414	427	13
9	6	5	327	307	10
9	6	7	241	246	11
9	6	8	324	307	10
9	6	9	438	411	15
9	7	-14	388	409	10
9	7	-13	281	298	9
9	7	-12	212	239	11
9	7	-10	278	273	8
9	7	-9	455	495	11
9	7	-8	301	322	9
9	7	-7	255	282	9
9	7	-6	168	185	12
9	7	-5	277	300	8
9	7	-4	323	347	10
9	7	-3	343	390	9
9	7	1	256	277	9
11	3	-2	547	554	11
11	3	-1	234	253	10
11	3	0	135	142	15
11	3	2	356	364	9
11	3	3	197	203	11
11	3	4	267	271	8
11	4	-11	327	299	11
11	4	-10	355	351	10
11	4	-9	585	579	12
11	4	-6	215	195	12
11	4	-5	602	602	11
11	4	-4	223	244	11
11	4	-3	280	267	9
11	4	-1	326	343	11
11	4	0	204	226	11
11	4	1	350	371	9
11	5	-8	484	439	12
11	5	-7	275	289	10
11	5	-6	474	470	12
11	5	-4	153	129	15
11	5	-3	265	266	9
11	5	-2	423	430	12
11	5	0	130	115	16
12	0	-8	382	369	10
12	0	-4	617	601	12
12	0	-2	232	201	12
12	1	-7	481	459	14
8	6	-12	606	608	10
8	6	-11	174	176	12
8	6	-10	125	133	16
8	6	-9	321	326	10
8	6	-8	327	326	9
8	6	-7	482	478	10
8	6	-6	406	425	11
8	6	-5	157	133	12
8	6	-4	479	499	10
8	6	-3	565	570	9
8	6	-2	559	580	9
8	6	-1	404	402	11
8	6	0	164	162	12
8	6	1	224	225	9
8	6	2	550	581	10
8	6	3	574	562	10
8	6	4	413	362	13
8	6	6	367	335	10
8	6	7	429	428	14
8	6	8	515	488	12
8	6	11	179	172	15
8	6	12	363	357	12
8	6	13	181	181	15
8	6	14	181	183	16
8	7	-16	324	335	9
8	7	-15	328	331	9
8	7	-14	313	339	9
8	7	-13	193	214	12
8	7	-12	220	240	10
8	7	-11	288	307	9
8	7	-10	529	570	10
8	7	-9	636	667	9
8	7	-8	203	218	10
8	7	-7	187	186	10
8	7	-6	396	425	11
8	7	-5	500	525	10
8	7	-4	466	507	10
8	7	-1	455	484	11
8	7	0	401	443	12
8	7	1	421	393	12
8	7	2	210	200	11
9	7	2	247	258	9
9	7	5	296	279	9
9	7	6	393	362	11
9	7	7	224	217	12
9	8	-10	248	278	9
9	8	-8	180	201	11
9	8	-7	256	264	8
9	8	-6	280	321	9
9	8	-5	226	265	9
9	8	-2	314	320	10
9	8	-1	188	189	11
9	8	0	180	193	12
9	8	3	271	245	10
10	0	-20	635	604	18
10	0	-16	801	756	13
10	0	-14	616	564	13
10	0	-12	423	398	11
10	0	-10	867	811	10
10	0	-6	461	416	12
10	0	-4	284	286	9
10	0	-2	240	269	9
10	0	0	728	738	9
10	0	4	771	777	9
10	0	6	353	366	10
10	0	8	576	587	12
10	0	10	588	546	12
10	0	12	184	175	17
10	1	-19	464	439	12
10	1	-17	735	661	14
10	1	-13	926	833	11
10	1	-11	335	283	10
10	1	-9	521	518	12
10	1	-7	654	650	10
10	1	-5	136	98	15
10	1	-3	672	682	9
10	1	-1	350	372	9
10	1	0	159	131	19
10	1	1	478	498	11
10	1	3	535	548	10
10	1	5	337	385	10
10	1	6	139	131	15
10	1	7	762	779	10
10	1	8	139	91	18
10	1	11	601	564	12
10	1	13	358	331	10
10	2	-20	565	530	13
10	2	-18	214	186	18
10	2	-16	572	535	15
10	2	-14	477	402	16
10	2	-13	143	123	21
10	2	-12	402	388	11
10	2	-11	146	131	19
10	2	-10	796	752	10
10	2	-8	159	174	15
10	2	-7	215	229	11
12	1	-6	178	157	16
12	1	-5	432	434	10
12	1	-3	237	231	11
12	1	-1	592	555	11
8	8	-7	532	563	10
8	8	-6	286	279	8
8	8	-4	270	296	8
8	8	-3	381	430	12
8	8	-2	393	383	12
8	8	-1	300	302	8
8	8	1	222	225	10
8	8	2	196	186	12
8	8	3	379	343	10
8	8	6	187	206	14
8	8	7	288	269	10
8	8	8	255	229	11
8	8	9	223	190	12
8	9	-10	429	495	11
8	9	-9	281	290	8
8	9	-8	154	167	12
8	9	-6	332	371	9
8	9	-5	302	311	8
8	9	-4	336	363	9
8	9	-3	195	185	10
8	9	-1	197	183	11
8	9	0	357	349	10
8	9	1	197	160	12
8	9	2	138	139	18
8	9	4	276	258	10
9	0	-21	430	383	13
9	0	-17	712	665	14
9	0	-15	738	713	12
9	0	-13	403	385	11
9	0	-11	1101	1041	10
9	0	-7	965	978	9
9	0	-5	408	390	12
9	0	-3	572	558	9
9	0	-1	933	952	8
9	0	3	745	755	9
9	0	5	472	471	10
9	0	7	780	771	10
9	0	9	798	772	10
9	0	13	821	776	11
9	0	15	322	322	11
10	2	-6	547	553	11
10	2	-5	230	225	10
10	2	-4	516	488	10
10	2	-2	460	455	11
10	2	0	547	573	10
10	2	1	240	280	9
10	2	2	153	164	13
10	2	4	603	639	9
10	2	5	282	292	9
10	2	6	253	256	9
10	2	10	486	468	13
10	3	-19	285	293	14
10	3	-17	441	407	13
10	3	-13	542	518	13
10	3	-11	322	292	10
10	3	-10	212	181	13
10	3	-9	584	580	11
10	3	-8	180	186	14
10	3	-7	698	680	10
10	3	-5	305	295	9
10	3	-4	299	320	9
10	3	-3	838	866	9
10	3	-2	360	375	9
10	3	-1	239	219	9
10	3	1	572	617	10
10	3	2	240	231	9
10	3	3	450	465	11
10	3	4	207	202	10
10	3	5	177	190	12
10	3	7	346	355	9
10	3	11	374	359	11
10	4	-16	252	239	13
10	4	-15	211	187	14
10	4	-14	310	303	10
10	4	-12	216	212	13
10	4	-11	201	209	13
10	4	-10	559	566	12
10	4	-9	184	203	14
10	4	-7	219	183	11
10	4	-6	776	746	10
10	4	-5	295	303	8
10	4	-4	334	335	10
10	4	-3	127	101	16
10	4	-2	421	448	12
10	4	-1	314	346	10
10	4	0	574	582	10
10	4	1	147	114	13
10	4	3	297	316	9
10	4	4	405	431	12
10	4	5	201	214	11
10	4	6	176	187	14
10	4	8	224	222	12
10	4	10	158	152	16
10	4	10	287	266	10
9	1	-2	159	164	12
9	1	0	633	649	8
9	1	2	648	673	9
9	1	3	162	187	12
9	1	4	321	324	9
9	1	6	713	725	9
9	1	7	135	141	17
9	1	8	183	158	13
9	1	10	801	782	10
9	1	12	467	477	14
9	1	14	349	314	10
9	1	15	141	98	21
9	1	16	574	546	14
9	2	-21	458	470	15
9	2	-17	669	614	14
9	2	-16	212	192	15
9	2	-15	578	530	13
9	2	-13	356	304	12
9	2	-12	237	218	11
9	2	-11	757	738	10
9	2	-9	335	291	10
9	2	-8	326	303	10
9	2	-7	839	829	9
9	2	-5	706	724	9
9	2	-4	366	359	9
9	2	-3	593	610	9
9	2	-2	150	164	13
9	2	-1	816	838	8
9	2	0	266	290	9
9	2	1	245	270	8
9	2	3	784	816	8
9	2	4	339	367	9
9	2	5	401	395	11
9	2	6	241	238	9
9	2	7	590	606	10
9	2	9	760	729	10
9	2	10	234	211	11
9	2	13	601	610	12
9	2	15	155	179	19
9	3	-22	318	309	14
9	3	-20	311	323	13
10	5	-14	194	163	14
10	5	-13	385	376	11
10	5	-12	253	264	11
10	5	-11	215	194	12
10	5	-9	432	429	13
10	5	-8	374	407	10
10	5	-7	415	447	13
10	5	-5	162	180	13
10	5	-4	351	367	10
10	5	-3	602	610	10
10	5	-2	242	261	9
10	5	0	209	220	10
10	5	1	365	384	9
10	5	2	302	305	9
10	5	3	335	359	10
10	5	5	273	264	10
10	5	7	386	388	11
10	6	-12	123	109	20
10	6	-11	298	301	10
10	6	-10	239	235	10
10	6	-9	261	259	9
10	6	-7	150	148	15
10	6	-6	411	433	13
10	6	-5	333	348	10
10	6	-4	244	257	9
10	6	-2	212	224	10
10	6	-1	332	355	10
10	6	0	403	420	13
10	6	4	374	357	11
10	6	5	286	296	10
10	7	-7	248	253	9
10	7	-4	227	232	9
10	7	-2	230	248	9
11	0	-15	506	453	12
11	0	-13	438	418	12
11	0	-9	554	508	13
11	0	-5	489	472	12
11	0	-3	415	416	14
11	0	1	623	596	10
11	0	5	700	730	11
11	0	7	340	345	10
11	1	-16	472	434	13
11	1	-12	494	485	15
11	1	-10	263	245	11
11	1	-8	323	287	10
11	1	-7	176	155	14
11	1	-6	403	396	10
11	1	-5	183	173	13
11	1	-4	243	249	10
11	1	-2	601	602	10
11	1	2	621	631	10

Table A4: *Observed And Calculated Structure Factors For The [Cycl₃PAu(6p2-TU)] Complex.*

10|F|o vs 10|F|c

h	k	l	Fo	Fc	sigF
0	0	2	3218	3272	8
0	0	4	3475	3505	9
0	0	6	2181	2248	10
0	0	8	870	832	13
0	0	10	286	297	15
0	0	12	136	40	35*
0	0	14	414	446	15
0	0	16	465	462	14
0	0	18	481	491	16
0	0	20	466	451	16
0	0	22	277	328	27
0	1	1	136	729	6
0	1	2	1009	991	7
0	1	3	494	491	10
0	1	4	2361	2307	9
0	1	5	642	596	12
0	1	6	2242	2251	10
0	1	7	977	934	12
0	1	8	1436	1456	12
0	1	9	215	215	19
0	1	10	1296	1311	14
0	1	11	199	126	23
0	1	12	1022	989	16
0	1	13	93	192	74*
0	1	14	736	721	14
0	1	15	113	218	77*
0	1	16	481	470	14
0	1	17	0	158	77*
0	1	18	199	207	33
0	1	19	0	82	79*
0	1	20	199	61	33
0	1	21	132	12	81*
0	1	22	87	12	82*
0	2	0	3450	3449	8
0	2	1	381	368	9
0	2	2	2255	2229	8
0	2	3	168	134	14
0	2	4	2870	2925	9
0	2	5	277	293	11
0	2	6	1549	1498	10
0	2	7	404	364	9
0	2	8	720	683	14
0	2	9	0	89	62*
0	2	10	93	68	44*
0	2	11	0	83	67*
0	2	12	284	262	18
0	2	13	64	24	73*
0	2	14	515	510	12
0	2	15	0	54	76*
0	2	16	454	467	14
0	2	17	182	154	32*
0	2	18	443	452	15
0	2	19	132	128	48*
0	2	20	311	368	23
0	2	21	0	98	80*
0	2	22	236	235	28
0	3	1	1415	1401	7
0	3	2	652	643	10
0	3	3	1118	1097	9
0	3	4	606	576	12
0	3	5	820	822	11
0	3	6	1353	1344	11
0	3	7	1225	1233	11
0	3	8	1690	1654	12
0	3	9	960	1036	14
0	3	10	1277	1248	14
0	3	11	1002	1023	16
0	3	12	970	991	16
0	3	13	682	682	14
0	3	14	662	626	15
0	3	15	509	499	13
0	3	16	225	234	25
0	3	17	342	325	18
0	3	18	15	118	78*
0	3	19	0	151	79*
0	3	20	0	9	79*
0	3	21	138	33	80*
0	4	0	1147	1211	8
0	4	1	1727	1698	8
0	4	2	1624	1597	9
0	4	3	1333	1356	9
0	4	4	1275	1238	10
0	4	5	1518	1498	10
0	4	6	1068	1028	11
0	4	7	923	883	13
0	4	8	667	677	15
0	4	9	246	242	17
0	4	10	125	42	65*
0	4	11	61	118	69*
0	4	12	207	227	24
0	4	13	180	159	30
0	4	14	494	511	13
0	4	15	394	377	15
0	4	16	325	329	18
0	4	17	211	237	28
0	4	18	117	273	80*
0	4	19	0	166	78*
0	4	20	0	205	80*
0	4	21	0	138	79*
0	5	1	98	121	26*
0	5	2	92	79	51*
0	5	3	866	861	11
0	5	4	796	800	12
0	5	5	1017	1004	11
0	5	6	847	874	12
0	5	7	1660	1658	12
0	5	8	655	667	11
0	5	9	1653	1635	13
0	5	10	1006	992	15
0	5	11	1525	1485	14
0	5	12	561	589	13
0	5	13	1013	1010	17
0	5	14	375	358	15
0	5	15	568	560	14
0	5	16	189	231	29
0	5	17	322	333	20
0	5	18	114	104	65*
0	5	19	86	137	78*
0	5	20	0	3	77*
0	5	21	146	21	76*
0	6	0	1219	1230	10
0	6	1	1990	2045	10
0	6	2	234	235	12
0	6	3	2034	2030	10
0	6	4	628	599	13
0	6	5	1468	1451	11
0	6	6	0	44	58*
0	6	7	989	979	13
0	6	8	165	152	24
0	6	9	560	525	14
0	6	10	82	106	67*
0	6	11	0	47	70*
0	6	12	35	145	71*
0	6	13	261	321	22
0	6	14	102	117	61*
0	6	15	366	407	17
0	6	16	0	61	74*
0	6	17	271	336	22
0	6	18	0	44	77*
0	6	19	235	249	26
0	6	20	106	39	63*
0	6	21	26	204	80*
0	7	1	1001	958	11
0	7	2	805	778	12
0	7	3	687	740	13
0	7	4	553	573	11
0	7	5	1288	1301	12
0	7	6	356	378	12
0	7	7	1651	1633	13
0	7	8	94	85	48*
0	7	9	1371	1357	14
0	7	10	102	191	52*
0	7	11	1119	1116	16
0	7	12	124	72	71*
0	7	13	914	862	17
0	7	14	0	67	72*
0	7	15	520	481	12
0	7	16	138	128	40*
0	7	17	346	325	18
0	7	18	0	109	77*
0	7	19	145	129	76*
0	7	20	179	25	32*
0	8	0	434	418	10
0	8	2	696	686	14
0	8	3	1958	1986	11
0	8	4	377	379	11
0	8	5	1142	1176	13
0	8	6	687	702	15
0	8	7	520	516	11
0	8	8	287	310	17
0	8	9	254	221	19
0	8	10	282	287	18
0	8	11	132	86	71*
0	8	12	139	109	36*
0	8	13	228	263	24
0	8	14	97	93	55*
0	8	15	280	274	20
0	8	16	128	139	75*
0	8	17	289	362	22
0	8	18	91	126	77*
0	8	19	318	371	21
0	8	20	115	90	75*
0	9	1	682	613	15
0	9	2	197	217	19
0	9	3	636	656	16
0	9	4	487	472	11
0	9	5	1297	1310	13
0	9	6	339	362	14
0	9	7	966	1002	15
0	9	8	218	229	22
0	9	9	819	853	17
0	9	10	331	315	15
0	9	11	603	623	15
0	9	12	323	332	17
0	9	13	582	584	13
0	9	14	217	228	26
0	9	15	388	396	16
0	9	16	238	162	23
0	9	17	234	211	24
0	9	18	0	90	75*
0	9	19	110	81	58*
0	9	20	143	80	74*
0	10	0	1545	1554	13
0	10	1	2139	2159	12
0	10	2	1336	1347	13
0	10	3	1387	1398	13
0	10	4	1014	967	14
0	10	5	1025	1056	15
0	10	6	498	493	11
0	10	7	732	724	18
0	10	8	242	224	21
0	10	9	183	174	28
0	10	10	261	232	20
0	10	11	0	64	69*
0	10	12	0	96	73*
0	10	13	196	260	28
0	10	14	83	28	72*
0	10	15	327	338	17
0	10	16	133	145	76*
0	10	17	152	297	78*
0	10	18	83	208	65*
0	10	19	224	324	28
0	11	1	62	87	57*
0	11	2	439	452	12
0	11	3		331	16
0	11	4	792	772	16
0	11	5	494	508	11
0	11	6	824	820	18
0	11	7	593	638	15
0	11	8	853	813	18
0	11	9	582	636	13
0	11	10	564	575	13
0	11	11	447	508	13
0	11	12	486	473	13
0	11	13	391	393	15
0	11	14	414	414	15
0	11	15	152	174	37*
0	11	16	318	290	19
0	11	17	145	46	38*
0	11	18	185	231	32*
0	11	19	59	20	75*
0	12	0	1106	1114	15
0	12	1	793	784	17
0	12	2	1195	1147	15
0	12	3	660	690	14
0	12	4	879	835	16
0	12	5	763	730	18
0	12	6	651	651	14
0	12	7	577	592	13
0	12	8	204	140	26
0	12	9	91	75	72*
0	12	10	111	79	71*
0	12	11	127	145	72*
0	12	12	22	95	72*
0	12	13	116	238	73*
0	12	14	171	169	32*
0	12	15	288	270	20
0	12	16	277	230	21
0	12	17	194	224	30
0	12	18	174	211	33*
0	13	1	111	30	71*
0	13	2	398	393	15
0	13	3	0	54	72*
0	13	4	619	652	15
0	13	5	179	131	30*
0	13	6	799	778	19
0	13	7	344	390	17
0	13	8	927	955	19
0	13	9	226	244	24
0	13	10	836	894	19
0	13	11	167	185	33*
0	13	12	683	710	15
0	13	13	10	147	64*
0	13	14	478	494	14
0	13	15	0	12	74*
0	13	16	274	251	21
0	13	17	43	55	76*
0	14	0	908	862	18
0	14	1	322	333	18
0	14	2	952	920	18
0	14	3	142	135	75*
0	14	4	733	702	15
0	14	5	172	154	32*
0	14	6	801	742	20
0	14	7	53	79	76*
0	14	8	315	328	20
0	14	9	0	27	76*
0	14	10	102	82	77*
0	14	11	189	110	29
0	14	12	0	131	75*
0	14	13	0	127	76*
0	14	14	66	263	78*
0	14	15	0	82	75*
0	14	16	215	255	28
0	15	1	176	113	31*
0	15	2	355	352	18
0	15	3	126	133	74*
0	15	4	396	366	15
0	15	5	76	86	53*
0	15	6	750	746	16
0	15	7	65	46	76*
0	15	8	793	822	15
0	15	9	138	83	79*
0	15	10	760	730	16
0	15	11	169	131	36*
0	15	12	609	621	14
0	15	13	167	87	34*
0	15	14	322	395	20
0	15	15	164	75	35*
0	16	0	790	738	15
0	16	1	297	247	21
0	16	2	678	637	16
0	16	3	222	266	28
0	16	4	550	542	13
0	16	5	347	315	19
0	16	6	345	334	19
0	16	7	345	377	19
0	16	8	155	116	78*
0	16	9	108	182	67*
0	16	10	147	9	42*
0	16	11	101	74	77*
0	16	12	22	83	78*
0	16	13	95	26	74*
0	16	14	103	166	53*
0	17	1	104	31	79*
0	17	2	287	334	24
0	17	3	46	49	79*
0	17	4	500	438	15
0	17	5	156	107	81*
0	17	6	548	566	15
0	17	7	105	228	83*
0	17	8	474	493	16
0	17	9	244	200	28
0	17	10	381	387	19
0	17	11	245	220	28
0	17	12	272	351	25
0	17	13	118	149	79*
0	18	0	562	553	14
0	18	1	712	659	17
0	18	2	481	467	16
0	18	3	581	491	15
0	18	4	330	338	22
0	18	5	455	418	17
0	18	6	133	166	70*
0	18	7	112	256	86*
0	18	8	46	40	58*
0	18	9	0	127	84*
0	18	10	0	32	82*
0	18	11	177	59	37*
0	18	12	62	71	57*
0	19	1	0	116	85*
0	19	2	0	93	83*
0	19	3	245	254	31
0	19	4	191	220	39*
0	19	5	346	313	22
0	19	6	266	222	27
0	19	7	292	316	26
0	19	8	283	240	25
0	19	9	131	208	85*
0	19	10	109	144	70*
0	20	0	263	205	29
0	20	1	586	618	15
0	20	2	260	242	30
0	20	3	501	525	18
0	20	4	181	172	43*
0	20	5	367	344	21
0	20	6	127	125	66*
0	20	7	142	222	87*
0	20	8	0	56	86*
0	21	1	89		
0	21	2	0	17	90*
0	21	3	99	172	89*
0	21	4	0	27	88*
0	21	5	304	240	25
1	0	-22	311	294	29
1	0	-20	324	296	26
1	0	-18	149	119	79*
1	0	-16	71	27	58*
1	0	-12	708	734	16
1	0	-10	2300	2317	11
1	0	-8	2162	2128	9
1	0	-6	2828	2807	8
1	0	-2	4346	4266	8
1	0	2	1621	1622	5
1	0	4	576	587	9
1	0	6	665	665	10
1	0	8	332	312	10
1	0	10	212	267	18
1	0	12	702	704	17
1	0	14	848	899	18
1	0	16	759	759	14
1	0	18	675	626	16
1	0	20	468	430	16
1	1	-22	205	141	42*
1	1	-21	216	90	37*
1	1	-20	344	222	23
1	1	-19	160	106	84*
1	1	-18	427	367	18
1	1	-17	172	177	39*
1	1	-16	647	609	14
1	1	-15	113	131	77*
1	1	-14	817	775	19
1	1	-13	163	146	32*
1	1	-12	879	875	17
1	1	-11	205	157	22
1	1	-10	1131	1099	13
1	1	-9	962	843	13
1	1	-8	766	791	13
1	1	-7	468	506	10
1	1	-6	759	778	10
1	1	-5	314	273	8
1	1	-4	343	369	8
1	1	-3	431	436	7
1	1	-2	348	355	6
1	1	-1	671	665	4
1	1	0	1846	1768	5
1	1	1	606	583	5
1	1	2	954	928	6
1	1	3	149	154	10
1	1	4	1346	1356	7
1	1	5	874	870	9
1	1	6	1815	1827	9
1	1	7	413	383	9
1	1	8	742	813	13
1	1	9	326	254	11
1	1	10	1116	1142	13
1	1	11	166	159	25
1	1	12	701	731	17
1	1	13	303	310	17
1	1	14	379	382	15
1	1	15	167	156	31*
1	1	16	161	100	34*
1	1	17	98	74	53*
1	1	18	0	109	77*
1	1	20	157	179	80*
1	1	21	0	79	81*
1	2	-22	281	224	30
1	2	-21	218	44	35
1	2	-20	323	314	25
1	2	-19	160	18	85*
1	2	-18	237	239	30
1	2	-17	0	34	80*
1	2	-16	181	186	34*
1	2	-15	221	155	27
1	2	-14	0	56	75*
1	2	-13	126	73	72*
1	2	-12	533	502	13
1	2	-11	230	145	19
1	2	-10	900	838	14
1	2	-9	141	119	24*
1	2	-8	1659	1653	10
1	2	-7	457	464	10
1	2	-6	2136	2200	7
1	2	-5	1292	1320	7
1	2	-4	2036	2085	6
1	2	-3	1677	1694	6
1	2	-2	1634	1627	5
1	2	-1	402	404	6
1	2	0	2072	2048	6
1	2	1	387	379	7
1	2	2	1422	1383	6
1	2	3	405	377	8
1	2	4	1262	1283	7
1	2	5	190	221	13
1	2	6	562	535	12
1	2	7	828	831	12
1	2	8	752	694	13
1	2	9	0	83	59*
1	2	10	622	616	12
1	2	11	316	298	14
1	2	12	839	836	17
1	2	13	284	267	18
1	2	14	791	787	18
1	2	15	299	341	19
1	2	16	640	638	16
1	2	17	193	245	32
1	2	18	510	492	14
1	2	19	221	194	28
1	2	20	342	345	20
1	2	21	53	70	81*
1	3	-22	118	61	88*
1	3	-21	170	166	88*
1	3	-20	0	148	85*
1	3	-19	340	307	22
1	3	-18	332	297	21
1	3	-17	460	446	15
1	3	-16	531	539	13
1	3	-15	575	543	14
1	3	-14	819	849	19
1	3	-13	665	682	14
1	3	-12	727	725	18
1	3	-11	786	792	16
1	3	-10	945	986	13
1	3	-9	962	931	12
1	3	-8	447	456	11
1	3	-7	453	463	9
1	3	-6	283	289	8
1	3	-5	256	304	7
1	3	-4	120	76	11
1	3	-3	82	37	17*
1	3	-2	539	559	7
1	3	-1	1383	1393	6
1	3	0	613	607	7
1	3	1	2860	2835	7
1	3	2	611	579	9
1	3	3	2008	1952	8
1	3	4	1895	1822	8
1	3	5	1558	1509	9
1	3	6	1784	1784	10
1	3	7	1565	1529	11
1	3	8	1441	1428	11
1	3	9	1259	1242	13
1	3	10	1030	1032	14
1	3	11	918	891	15
1	3	12	486	475	12
1	3	13	629	596	15
1	3	14	131	55	71*
1	3	15	251	224	21
1	3	16	0	74	75*
1	3	17	67	117	76*
1	3	18	125	123	64*
1	3	19	0	49	81*
1	3	20	131	91	81*
1	3	21	136	126	81*
1	4	-21	194	103	37*
1	4	-20	165	222	45*
1	4	-19	0	75	83*
1	4	-18	200	149	33
1	4	-17	0	138	81*
1	4	-16	122	194	77*
1	4	-15	0	12	77*
1	4	-14	0	33	73*
1	4	-13	412	406	14
1	4	-12	424	398	12
1	4	-11	510	508	12
1	4	-10	731	749	14
1	4	-9	1050	1073	12
1	4	-8	927	926	10
1	4	-7	1235	1256	9
1	4	-6	1100	1134	8
1	4	-5	1156	1209	7
1	4	-4	1174	1210	7
1	4	-3	1411	1411	7
1	4	-2	1059	1053	7
1	4	-1	1566	1580	7
1	4	0	1611	1616	7
1	4	1	1314	1300	7
1	4	2	722	688	9
1	4	3	1130	1088	9
1	4	4	757	725	11
1	5	13	437	453	13
1	5	14	218	178	24
1	5	15	122	225	75*
1	5	16	0	50	76*
1	7	-18	0	134	80*
1	7	-17	494	481	14
1	7	-16	97	108	73*
1	7	-15	607	681	13
1	8	-4	527	509	11
1	8	-3	1946	1973	10
1	8	-2	620	590	14
1	8	-1	2013	1979	11
1	9	10	440	423	13
1	9	11	628	595	15
1	9	12	251	254	21
1	9	13	492	483	13

```
1   4   5   746  746 11     1   5  17   167   27 34*    1   7 -14   133   41 69*    1   8   0   740  719 13     1   9  14   151  207 77*
1   4   6   161  127 18     1   5  18     0   58 76*    1   7 -13   943  931 16     1   8   1  1085 1123 11     1   9  15   163  140 35*
1   4   7   482  498 12     1   5  19    71   77 78*    1   7 -12   196  222 23     1   8   2  1096 1040 11     1   9  16     0   89 77*
1   4   8   370  377 11     1   5  20   149   87 78*    1   7 -11   930  882 14     1   8   3  1022 1034 12     1   9  17   130   58 76*
1   4   9   370  341 12     1   5  21     0   99 79*    1   7 -10   338  368 11     1   8   4   608  637 11     1   9  18    92   52 77*
1   4  10   705  714 16     1   6 -21   114  182 82*    1   7  -9  1006 1080 10     1   8   5    65  161 50*    1   9  19     0  130 79*
1   4  11   517  495 12     1   6 -20    56   19 81*    1   7  -8   335  360  9     1   8   6   199  238 19     1  10 -19   180  194 32*
1   4  12   774  795 18     1   6 -19   214  183 30     1   7  -7   653  658 13     1   8   7   228  219 18     1  10 -18    33   30 77*
1   4  13   686  679 14     1   6 -18   111   21 78*    1   7  -6   376  386  9     1   8   8   281  271 16     1  10 -17   220  160 27
1   4  14   481  490 13     1   6 -17   124  147 48*    1   7  -5   203  203 14     1   8   9   314  305 16     1  10 -16    42   64 78*
1   4  15   423  416 14     1   6 -16     0   27 63*    1   7  -4   430  425 11     1   8  10     0   57 71*    1  10 -15     0   64 76*
1   4  16   379  380 16     1   6 -15   144   70 37*    1   7  -3     0  103 51*    1   8  11   764  711 19     1  10 -14     0   47 52*
1   4  17   375  384 17     1   6 -14    69   93 50*    1   7  -2   428  384 10     1   8  12     0  152 73*    1  10 -13   109  135 63*
1   4  18   276  244 22     1   6 -13   432  398 13     1   7  -1  1202 1185 10     1   8  13   549  564 14     1  10 -12   259  275 16
1   4  19   124  176 51*    1   6 -12   247  190 18     1   7   0   551  550 13     1   8  14     0   58 75*    1  10 -11   236  275 19
1   4  20   162  162 37*    1   6 -11   817  773 14     1   7   1  1213 1202 10     1   8  15   631  650 13     1  10 -10   229  243 20
1   4  21   175  136 35*    1   6 -10   185  146 19     1   7   2   524  514 10     1   8  16   206  129 28     1  10  -9   874  885 16
1   5 -21   117  140 71*    1   6  -9  1079 1080 11     1   7   3  1548 1613 10     1   8  17   553  541 13     1  10  -8   684  675 17
1   5 -20     0  107 84*    1   6  -8   132  130 18     1   7   4   412  382 10     1   8  18   202  124 29     1  10  -7  1078 1079 14
1   5 -19   420  386 17     1   6  -7  1491 1532  9     1   7   5  1847 1847 11     1   8  19   369  391 18     1  10  -6   980  984 14
1   5 -18   233  266 29     1   6  -6   497  468 12     1   7   6   210  157 17     1   8  20     0   77 78*    1  10  -5  1324 1329 13
1   5 -17   554  539 14     1   6  -5  1735 1752  9     1   7   7  1472 1533 13     1   9 -20     0  102 77*    1  10  -4  1003  992 14
1   5 -16   265  325 23     1   6  -4   268  302  9     1   7   8     0   32 65*    1   9 -19   187  215 32*    1  10  -3  1746 1790 12
1   5 -15   876  923 19     1   6  -3  1344 1370  9     1   7   9  1482 1490 14     1   9 -18    84  113 64*    1  10  -2  1305 1312 13
1   5 -14   501  524 12     1   6  -2   651  621 10     1   7  10   381  367 14     1   9 -17   274  340 22     1  10  -1  1885 1892 12
1   5 -13  1083 1063 15     1   6  -1  1685 1688  9     1   7  11   842  822 18     1   9 -16   116  118 74*    1  10   0   999  968 13
1   5 -12   624  646 14     1   6   0   300  265  9     1   7  12     0   42 70*    1   9 -15   430  379 14     1  10   1  1175 1195 13
1   5 -11  1211 1258 13     1   6   1  1285 1280  9     1   7  13   492  421 12     1   9 -14    56  153 62*    1  10   2   450  460 10
1   5 -10   506  572 12     1   6   2    89   46 49*    1   7  14   163  155 33*    1   9 -13   709  718 13     1  10   3   779  770 16
1   5  -9   878  890 12     1   6   3  1019 1043 10     1   7  15   232  271 25     1   9 -12   262  273 15     1  10   4    99  181 65*
1   5  -8   535  540 13     1   6   4   161  100 18     1   7  16     0   27 75*    1   9 -11   467  471 10     1  10   5   284  276 16
1   5  -7   470  479  8     1   6   5   557  555 10     1   7  17    67   16 74*    1   9 -10    39   70 47*    1  10   6   193  193 23
1   5  -6   139  139 14     1   6   6   497  468 12     1   7  18    93   25 65*    1   9  -9   757  795 15     1  10   7   110   24 57*
1   5  -5   161  179 12     1   6   7    84  148 62*    1   7  19     0  130 79*    1   9  -8   192  156 21     1  10   8   138  122 71*
1   5  -4    82   65 23*    1   6   8     0   33 62*    1   7  20   161  100 37*    1   9  -7   849  833 14     1  10   9    80   96 72*
1   5  -3   325  347  8     1   6   9   661  635 12     1   8 -20   151   69 40*    1   9  -6     0   76 63*    1  10  10   211  221 24
1   5  -2   282  263  8     1   6  10   131  115 67*    1   8 -19   187  215 32*    1   9  -5   208  214 18     1  10  11   512  541 12
1   5  -1   273  266  8     1   6  11   784  782 17     1   8 -18     0   40 76*    1   9  -4   169  123 20     1  10  12   117  106 72*
1   5   0   510  562 11     1   6  12    86   59 70*    1   8 -17     0  101 76*    1   9  -3   280  260 13     1  10  13   488  491 13
1   5   1   982  987  8     1   6  13   865  869 18     1   8 -16     0   57 74*    1   9  -2   399  396 10     1  10  14   292  317 21
1   5   2  1039 1027  9     1   6  14   138  215 74*    1   8 -15     0    5 72*    1   9  -1   894  930 13     1  10  15   488  501 14
1   5   3  1746 1782  9     1   6  15   594  546 13     1   8 -14   156  115 31*    1   9   0   546  486 11     1  10  16   303  309 21
1   5   4  1352 1312 10     1   6  16   182  162 31*    1   8 -13   220  155 23     1   9   1  1238 1243 12     1  10  17   384  404 18
1   5   5  2248 2242 10     1   6  17   441  452 15     1   8 -12   121  148 66*    1   9   2   708  717 14     1  10  18   295  275 21
1   5   6   980 1005 12     1   6  18     0   54 77*    1   8 -11   431  459 10     1   9   3  1364 1417 12     1  10  19   274  287 23
1   5   7  2030 2038 11     1   6  19   266  266 24     1   8 -10   363  400 10     1   9   4   631  626 15     1  11 -19     0   89 79*
1   5   8   904  913 14     1   6  20    46   21 77*    1   8  -9   847  817 13     1   9   5  1251 1269 13     1  11 -18   228  250 28
1   5   9  1558 1573 13     1   6  21   168  192 38*    1   8  -8   523  502 12     1   9   6   330  307 13     1  11 -17   149  185 83*
1   5  10   679  693 12     1   7 -21     0  135 82*    1   8  -7  1517 1503 11     1   9   7   971 1017 16     1  11 -16   365  299 18
1   5  11  1112 1107 15     1   7 -20     0   39 81*    1   8  -6   347  304 10     1   9   8   240  289 20     1  11 -15   267  313 20
1   5  12   289  331 18     1   7 -19   357  335 19     1   8  -5  1902 1905 11     1   9   9   622  659 14     1  11 -14   338  343 14
1  11 -13   349  417 14     1  12   5   421  458 13     1  14 -10   608  562 14     1  15  12   418  417 16     1  17   9   250  242 28
1  11 -12   446  445 12     1  12   6   136   26 71*    1  14  -9     0   36 76*    1  15  13     0   38 77*    1  17  10   429  392 17
1  11 -11   398  418 14     1  12   7     0   76 72*    1  14  -8   691  688 15     1  15  14   186  178 33*    1  17  11     0  149 85*
1  11 -10   494  466 12     1  12   8   131  183 74*    1  14  -7     0  111 73*    1  15  15     0   59 78*    1  17  12    31  199 83*
1  11  -9   374  401 14     1  12   9   326  345 18     1  14  -6   725  755 14     1  16 -14     0   47 84*    1  17  13    41  142 80*
1  11  -8   587  620 12     1  12  10   290  320 20     1  14  -5   131   58 71*    1  16 -13   112  107 83*    1  18 -12    96   59 82*
1  11  -7   133  153 37*    1  12  11   323  359 19     1  14  -4   739  713 14     1  16 -12   217  206 32     1  18 -11   155  197 45*
1  11  -6   315  345 16     1  12  12   402  385 16     1  14  -3   115  164 73*    1  16 -11   214  231 32     1  18 -10   151   90 44*
1  11  -5    81   70 67*    1  12  13   385  392 16     1  14  -2   775  806 19     1  16 -10   242  277 28     1  18  -9   287  276 24
1  11  -4    87   10 65*    1  12  14   386  397 17     1  14  -1     0   63 73*    1  16  -9   269  302 25     1  18  -8   225  256 31
1  11  -3   106  101 40*    1  12  15   247  236 24     1  14   0   728  722 14     1  16  -8   451  443 16     1  18  -7   456  446 16
1  11  -2   433  437 11     1  12  16   320  352 20     1  14   1   154   70 34*    1  16  -7   315  305 21     1  18  -6   359  394 20
1  11  -1   320  321 14     1  12  17   182  179 33*    1  14   2   627  628 15     1  16  -6   690  698 16     1  18  -5   515  474 15
1  11   0   628  597 13     1  12  18   198  272 32     1  14   3     0   30 75*    1  16  -5   248  257 25     1  18  -4   469  481 16
1  11   1   604  613 13     1  13 -17   125   39 38*    1  14   4   583  541 13     1  16  -4   661  663 14     1  18  -3   632  598 15
1  11   2   714  729 17     1  13 -16   363  418 15     1  14   5     0   95 76*    1  16  -3   211  219 28     1  18  -2   448  457 17
1  11   3   576  588 14     1  13 -15    50  151 57*    1  14   6    79   15 74*    1  16  -2   764  773 15     1  18  -1   599  576 14
1  11   4   799  792 17     1  13 -14   582  578 13     1  14   7   137   70 40*    1  16  -1   362  340 17     1  18   0   360  348 20
1  11   5   821  817 17     1  13 -13     0  162 79*    1  14   8   219  241 27     1  16   0   573  576 13     1  18   1   456  418 17
1  11   6   838  846 17     1  13 -12   613  606 14     1  14   9     0   98 78*    1  16   1   265  286 24     1  18   2    95  179 84*
1  11   7   790  807 18     1  13 -11   100  194 78*    1  14  10   319  363 21     1  16   2   286  304 22     1  18   3   376  352 19
1  11   8   530  485 13     1  13 -10   600  610 14     1  14  11   171  142 34*    1  16   3   302  319 21     1  18   4   147   27 45*
1  11   9   347  368 16     1  13  -9   203  155 27     1  14  12   445  475 15     1  16   4   248  207 25     1  18   5   110  153 85*
1  11  10   706  675 14     1  13  -8   405  420 15     1  14  13    78  105 76*    1  16   5   268  245 24     1  18   6     0   89 84*
1  11  11   354  386 17     1  13  -7   111   71 72*    1  14  14   350  389 19     1  16   6   116   90 79*    1  18   7     0   56 84*
1  11  12   367  375 16     1  13  -6   104   66 61*    1  14  15     0   76 78*    1  16   7     0   78 81*    1  18   8   183  148 39*
1  11  13   139   72 39*    1  13  -5   120   58 71*    1  14  16   278  281 22     1  16   8   198  218 32     1  18   9     0   19 86*
1  11  14   334  345 19     1  13  -4   127   84 71*    1  15 -16   384  387 19     1  16   9   154   84 77*    1  18  10     0  137 87*
1  11  15     0   43 78*    1  13  -3     0   62 70*    1  15 -15   185   73 37*    1  16  10   240  259 28     1  18  11    68  132 84*
1  11  16   135  173 78*    1  13  -2   282  263 18     1  15 -14   471  498 17     1  16  11     0  119 83*    1  18  12   153  226 84*
1  11  17     0   74 77*    1  13  -1   120  111 71*    1  15 -13     0   23 84*    1  16  12   249  305 28     1  19 -10     0  183 85*
1  11  18    82   19 77*    1  13   0   742  755 13     1  15 -12   542  562 15     1  16  13   168  144 38*    1  19  -9    88  203 83*
1  12 -18   136   89 83*    1  13   1   132  109 71*    1  15 -11   129   32 79*    1  16  14   328  324 19     1  19  -8     0  157 86*
1  12 -17   202  196 32     1  13   2  1001 1055 17     1  15 -10   523  566 14     1  17 -13     0  138 85*    1  19  -7   157  155 84*
1  12 -16   134   18 68*    1  13   3   166  108 30*    1  15  -9   130   33 45*    1  17 -12   280  295 26     1  19  -6   155  150 84*
1  12 -15   102  122 68*    1  13   4   927  917 18     1  15  -8   411  425 16     1  17 -11     0   90 82*    1  19  -5     0   63 83*
1  12 -14   147   88 35*    1  13   5   278  280 20     1  15  -7   127  115 76*    1  17 -10   359  392 20     1  19  -4   132   10 82*
1  12 -13     0   46 75*    1  13   6  1267 1253 16     1  15  -6     0  113 74*    1  17  -9     0   84 79*    1  19  -3   144   98 65*
1  12 -12   328  258 17     1  13   7   186  189 31     1  15  -5     0  186 74*    1  17  -8   382  394 18     1  19  -2   102   79 84*
1  12 -11   105  174 73*    1  13   8  1062 1042 17     1  15  -4    67   47 72*    1  17  -7     0   17 67*    1  19  -1   297  306 24
1  12 -10   466  444 13     1  13   9     0  110 75*    1  15  -3     0   48 74*    1  17  -6   216  236 30     1  19   0   143  161 85*
1  12  -9   472  476 13     1  13  10   738  750 15     1  15  -2   322  287 18     1  17  -5     0   94 81*    1  19   1   378  387 21
1  12  -8   666  678 14     1  13  11     0   19 76*    1  15  -1    77   35 73*    1  17  -4     0   62 81*    1  19   2   312  265 23
1  12  -7   574  613 13     1  13  12   538  545 13     1  15   0   578  602 14     1  17  -3     0   57 78*    1  19   3   430  385 19
1  12  -6   840  860 18     1  13  13     0   89 77*    1  15   1   152   91 35*    1  17  -2   306  279 21     1  19   4   282  232 26
1  12  -5   594  583 15     1  13  14   259  204 23     1  15   2   819  748 19     1  17  -1   191  154 32*    1  19   5   380  355 20
1  12  -4  1054 1120 16     1  13  15    75  139 65*    1  15   3     0   98 76*    1  17   0   573  572 13     1  19   6   227  253 33
1  12  -3   533  516 12     1  13  16   122  102 65*    1  15   4  1061 1057 18     1  17   1   194  181 33*    1  19   7   302  272 24
1  12  -2   932  919 15     1  13  17     0   89 75*    1  15   5   224  146 27     1  17   2   626  600 15     1  19   8     0  155 86*
1  12  -1   668  658 13     1  14 -16    75   83 77*    1  15   6  1032 1008 18     1  17   3   154  237 83*    1  19   9   203  254 38*
1  12   0   651  638 13     1  14 -15     0   99 82*    1  15   7   290  248 22     1  17   4   645  650 15     1  19  10     0  118 86*
1  12   1   645  645 13     1  14 -14     0  108 82*    1  15   8   863  893 21     1  17   5   398  348 18     1  20  -8     0  154 87*
1  12   2   601  604 14     1  14 -13   133   96 81*    1  15   9   199  135 31     1  17   6   562  536 14     1  20  -7   376  431 21
1  12   3   669  630 13     1  14 -12   320  277 21     1  15  10   686  644 17     1  17   7   381  327 18     1  20  -6    84  141 87*
1  12   4   347  306 15     1  14 -11    85   61 78*    1  15  11   188  107 33*    1  17   8   471  433 16     1  20  -5   514  533 16
1  20  -4   212  182 34     2   1 -11   322  380 14     2   2  -1  1448 1418  6     2   3  12   269  309 18     2   5 -20   124  164 83*
1  20  -3   511  568 17     2   1 -10   355  364 12     2   2   0  1248 1250  6     2   3  13   112   59 57*    2   5 -19   402  434 17
1  20  -2   104  170 87*    2   1  -9   327  330 11     2   2   1   406  385  9     2   3  14   141  163 34*    2   5 -18   252  258 26
1  20  -1   500  541 17     2   1  -8   273  284 11     2   2   2   718  716  7     2   3  15    83   23 71*    2   5 -17   565  606 13
1  20   0   156  207 88*    2   1  -7   101   44 24*    2   2   3   135  117 13     2   3  16   311  287 18     2   5 -16   341  374 18
1  20   1   402  424 21     2   1  -6   785  807  9     2   2   4   501  522 10     2   3  17    66  145 57*    2   5 -15   570  632 14
1  20   2    88  150 67*    2   1  -5   950  963  7     2   2   5   446  436  8     2   3  19   245  206 25     2   5 -14   314  381 18
1  20   3   103  211 91*    2   1  -4  4160 4064  8     2   2   6  1425 1307 29     2   3  20   127  207 80*    2   5 -13   638  677 14
1  20   4     0   76 88*    2   1  -3  1221 1237  6     2   2   7   121  163 22*    2   3  21     0  178 81*    2   5 -12   385  383 13
1  20   5   184  147 42*    2   1  -2  4160 4064  8     2   2   8  1277 1294 11     2   4 -21   105   12 84*    2   5 -11   413  427 11
1  20   6     0   18 89*    2   1  -1   258  254  6     2   2   9   401  373  9     2   4 -20     0   82 83*    2   5 -10   323  312 12
1  20   7     0    3 90*    2   1   0  1221 1219  6     2   2  10  1377 1388 12     2   4 -19     0   47 81*    2   5  -9   138   48 23
1  20   8    90   74 66*    2   1   1   286  283  6     2   2  11   477  459 12     2   4 -18     0  110 78*    2   5  -8   118   25 22*
1  21  -5     0   32 86*    2   1   2  3309 3333  7     2   2  12  1154 1147 14     2   4 -17     0  110 78*    2   5  -7   358  342  9
1  21  -4     0    8 84*    2   1   3   272  308  7     2   2  13   525  545 12     2   4 -16   215  175 27     2   5  -6   452  441  9
1  21  -3     0   99 88*    2   1   4  2292 2299  8     2   2  14   739  776 18                                  2   5  -5   672  636  9
1  21  -2     0   10 87*                                2   2  15   313  283 17                                  2   5  -4   202  225 10
```

```
 1 21 -1  153  173 88*    2  1  5  101   61 19*    2  2 16  619  615 13    2  4 -15  382  344 15    2  5 -3 1214 1238  8
 1 21  0  105   29 85*    2  1  6 1338 1368  9    2  2 17  205  225 28    2  4 -14  324  343 17    2  5 -2  911  952  8
 1 21  1  276  271 29     2  1  7  553  568 12    2  2 18  391  364 16    2  4 -13  707  681 13    2  5 -1 2197 2204  8
 1 21  2    0   26 88*    2  1  8  708  729 12    2  2 19  108   65 54*   2  4 -12  697  718 17    2  5  0 1210 1222  8
 1 21  3  305  350 27     2  1  9  169  210 19    2  2 20    0  187 79*   2  4 -11  842  842 14    2  5  1 2929 2951  8
 1 21  4    0   47 87*    2  1 10  691  689 15    2  2 21    0   35 66*   2  4 -10  687  675 15    2  5  2 1553 1523  8
 2  0 -22    0  112 91*   2  1 11  294  312 14    2  3 -21  219  203 34    2  4  -9 1081 1066 11    2  5  3 3091 3130  9
 2  0 -20  101   45 87*   2  1 12   69   30 66*   2  3 -20  231  217 31    2  4  -8  845  891 11    2  5  4 1408 1430  9
 2  0 -18    0  115 71*   2  1 13   94  154 51*   2  3 -19  354  333 20    2  4  -7  982 1021 10    2  5  5 2612 2571 10
 2  0 -16  249  213 26    2  1 14  220  226 22    2  3 -18  331  345 21    2  4  -6  929  939  9    2  5  6  974  970 12
 2  0 -14  494  476 14    2  1 15    0   48 69*   2  3 -17  396  413 17    2  4  -5 1120 1176  8    2  5  7 1371 1363 11
 2  0 -12  817  839 17    2  1 16  376  376 15    2  3 -16  456  489 14    2  4  -4  801  850  8    2  5  8  444  456  9
 2  0 -10 1631 1584 12    2  1 17    0  107 73*   2  3 -15  492  492 13    2  4  -3  917  926  7    2  5  9  959  985 14
 2  0  -8 2233 2197 10    2  1 18  364  392 18    2  3 -14  394  423 15    2  4  -2  979  948  7    2  5 10  467  473 11
 2  0  -6 2077 2093  8    2  1 19  128  104 77*   2  3 -13  531  555 13    2  4  -1  759  778  8    2  5 11  313  351 15
 2  0  -4 2407 2436  7    2  1 20  320  304 20    2  3 -12  245  263 19    2  4   0  525  581  9    2  5 12   73    2 68*
 2  0  -2 2023 2045  6    2  1 21    0   96 78*   2  3 -11  660  679 12    2  4   1  400  395  8    2  5 13  144   44 33*
 2  0   0  957  978  6    2  2 -22    0  122 88*   2  3 -10  179  108 20    2  4   2    0   20 43*   2  5 14   43   28 59*
 2  0   2 1263 1245  6    2  2 -21    0    7 85*   2  3  -9  282  292 12    2  4   3  175  194 12    2  5 15   67   31 71*
 2  0   4  952  937  7    2  2 -20  103   91 84*   2  3  -8  192  113 14    2  4   4  527  494 12    2  5 16    0  116 76*
 2  0   6  587  611 10    2  2 -19  163   51 83*   2  3  -7  353  376  8    2  4   5 1237 1179 10    2  5 17  198  174 29
 2  0   8 1506 1517 10    2  2 -18    0   37 83*   2  3  -6  525  502 10    2  4   6  991  977 11    2  5 18  145  159 77*
 2  0  10 1367 1387 12    2  2 -17  122   54 50*   2  3  -5  453  474 10    2  4   7  984  954 12    2  5 19  245  217 26
 2  0  12 1423 1449 13    2  2 -16  265  252 24    2  3  -4  742  752  8    2  4   8 1084 1050 12    2  5 20  125  130 65*
 2  0  14 1128 1121 15    2  2 -15  133  118 74*   2  3  -3 1583 1618  7    2  4   9 1011 1025 13    2  6 -21    0   55 80*
 2  0  16  743  738 14    2  2 -14  526  514 12    2  3  -2 1145 1169  7    2  4  10 1117 1136 13    2  6 -20  129   34 78*
 2  0  18  452  427 14    2  2 -13  220  214 23    2  3  -1 1916 1956  7    2  4  11  705  716 17    2  6 -19  134   22 78*
 2  0  20  217  214 29    2  2 -12  872  879 15    2  3   0 1882 1856  7    2  4  12  640  629 14    2  6 -18    0    9 77*
 2  1 -22    0  188 90*   2  2 -11  348  320 13    2  3   1 2018 2012  7    2  4  13  603  635 14    2  6 -17  147  136 77*
 2  1 -21    0   72 90*   2  2 -10 1251 1283 12    2  3   2 1565 1578  7    2  4  14  423  400 13    2  6 -16   28   54 75*
 2  1 -20  292  239 26    2  2  -9  788  791 13    2  3   3 1519 1532  8    2  4  15  474  495 13    2  6 -15  450  422 14
 2  1 -19    0  109 85*   2  2  -8 1737 1760 10    2  3   4 1728 1739  8    2  4  16  319  311 18    2  6 -14    0   51 71*
 2  1 -18  263  286 27    2  2  -7  862  911 10    2  3   5 1422 1419  9    2  4  17  244  248 23    2  6 -13  820  812 17
 2  1 -17  153  106 41*   2  2  -6 1874 1899  8    2  3   6 1598 1634 10    2  4  18  215  171 27    2  6 -12   95  178 70*
 2  1 -16  416  420 16    2  2  -5  849  889  8    2  3   7 1144 1141 11    2  4  19  214  146 28    2  6 -11  921  845 14
 2  1 -15  105  178 78*   2  2  -4 2059 2101  7    2  3   8  618  609 14    2  4  20  137  111 78*   2  6 -10  108  114 61*
 2  1 -14  444  423 14    2  2  -3 1254 1232  6    2  3   9 1025 1011 13    2  4  21   17   79 79*   2  6  -9 1245 1272 11
 2  1 -13  186  202 28    2  2  -2 1836 1807  6    2  3  10  184  190 21    2  5 -21  208  241 33    2  6  -8  410  427  9
 2  6  -7 1279 1298 10    2  7  7 1420 1404 13    2  9 -19  230  199 28    2 10  -3 1096 1084 13    2 11 14   63    5 65*
 2  6  -6  405  423 10    2  7  8  369  361 12    2  9 -18    0   65 80*   2 10  -2  543  552 12    2 11 15  197  197 31
 2  6  -5 1187 1204  9    2  7  9  718  674 17    2  9 -17  296  274 23    2 10  -1  669  662 15    2 11 16  190  127 32*
 2  6  -4  433  390  9    2  7 10  398  372 13    2  9 -16   72   59 79*   2 10   0  209  212 18    2 11 17  126  212 52*
 2  6  -3 1612 1617  8    2  7 11  244  135 21    2  9 -15  414  403 16    2 10   1  208  177 18    2 11 18   70  156 80*
 2  6  -2  176  184 13    2  7 12    0  125 71*   2  9 -14    0  166 76*   2 10   2  112  140 34*   2 12 -18    0   37 88*
 2  6  -1  845  883  9    2  7 13  100   27 69*   2  9 -13  335  378 16    2 10   3  298  262 14    2 12 -17    0    3 81*
 2  6   0  185  147 12    2  7 14   89   37 60*   2  9 -12    0   80 66*   2 10   4  104   74 53*   2 12 -16    0  167 76*
 2  6   1    0   62 49*   2  7 15    0  210 76*   2  9 -11  386  386 12    2 10   5  396  410 12    2 12 -15  171  156 31*
 2  6   2  381  388  9    2  7 16  147   41 37*   2  9 -10   99   26 62*   2 10   6  165  162 27    2 12 -14  297  283 19
 2  6   3  279  269 10    2  7 17  265  291 23    2  9  -9  214  192 19    2 10   7  547  581 12    2 12 -13  254  241 21
 2  6   4  322  387 10    2  7 18  119   74 78*   2  9  -8  162  161 24    2 10   8  305  316 17    2 12 -12  430  440 14
 2  6   5 1247 1225 11    2  7 19  202  277 32    2  9  -7  321  313 13    2 10   9  606  683 13    2 12 -11  344  337 16
 2  6   6  151  174 22    2  7 20   74   73 77*   2  9  -6  370  351 11    2 10  10  474  477 13    2 12 -10  649  616 14
 2  6   7 1349 1369 12    2  8 -20   78   30 59*   2  9  -5  817  806  9    2 10  11  810  814 19    2 12  -9  561  558 13
 2  6   8  372  355 12    2  8 -19   74    3 77*   2  9  -4  384  427 10    2 10  12  575  530 14    2 12  -8  760  757 19
 2  6   9 1236 1250 14    2  8 -18   83   36 79*   2  9  -3 1378 1376 11    2 10  13  631  656 13    2 12  -7  449  428 13
 2  6  10  136   89 32*   2  8 -17  191  102 32*   2  9  -2  524  492 11    2 10  14  464  428 15    2 12  -6  959  920 15
 2  6  11 1163 1191 15    2  8 -16    0  121 65*   2  9  -1 1742 1713 11    2 10  15  499  469 14    2 12  -5  486  504 12
 2  6  12  167  178 30*   2  8 -15  272  258 23    2  9   0  626  626 14    2 10  16  359  355 19    2 12  -4  879  826 16
 2  6  13  737  711 18    2  8 -14  215  187 26    2  9   1 1405 1357 11    2 10  17  131  296 82*   2 12  -3  665  676 13
 2  6  14  254  290 22    2  8 -13  554  532 13    2  9   2  412  439 10    2 10  18  243  192 26    2 12  -2  573  580 14
 2  6  15  570  547 14    2  8 -12  329  305 15    2  9   3 1178 1245 12    2 11 -19    0  123 87*   2 12  -1  573  625 14
 2  6  16    0  123 75*   2  8 -11  866  820 14    2  9   4  377  428 11    2 11 -18  122  187 88*   2 12   0  254  254 19
 2  6  17  356  342 18    2  8 -10  396  383 10    2  9   5 1091 1105 13    2 11 -17  245  206 28    2 12   1  282  227 17
 2  6  18   99   61 58*   2  8  -9 1286 1316 11    2  9   6  303  260 14    2 11 -16  141  191 81*   2 12   2   75   45 68*
 2  6  19  236  221 26    2  8  -8  281  314 13    2  9   7  624  643 13    2 11 -15    0  198 76*   2 12   3  134  174 35*
 2  6  20    0   24 78*   2  8  -7 1737 1722 11    2  9   8  359  350 14    2 11 -14  256  253 20    2 12   4  172  181 30*
 2  7 -20    0   42 80*   2  8  -6  354  324 10    2  9   9  427  488 13    2 11 -13  186  221 26    2 12   5  384  418 15
 2  7 -19  281  347 23    2  8  -5 1533 1537 11    2  9  10  183  169 28    2 11 -12  241  231 20    2 12   6  661  648 14
 2  7 -18  147   81 76*   2  8  -4  296  327 11    2  9  11  252  254 22    2 11 -11    0  112 69*   2 12   7  676  666 14
 2  7 -17  413  435 16    2  8  -3 1621 1582 10    2  9  12  132  165 74*   2 11 -10  228  222 22    2 12   8  590  600 13
 2  7 -16   63   90 76*   2  8  -2  618  625 13    2  9  13  118   29 45*   2 11  -9  192  168 26    2 12   9  478  519 14
 2  7 -15  511  512 13    2  8  -1  381  388  9    2  9  14   36   33 76*   2 11  -8    0   17 68*   2 12  10  689  649 15
 2  7 -14    0   92 72*   2  8   0  797  789 12    2  9  15  259  244 23    2 11  -7  169  145 27    2 12  11  505  502 13
 2  7 -13  514  516 12    2  8   1  467  453 11    2  9  16  128   55 78*   2 11  -6  387  371 13    2 12  12  628  616 14
 2  7 -12  430  414 12    2  8   2  571  560 14    2  9  17  386  375 17    2 11  -5  379  379 13    2 12  13  235  268 26
 2  7 -11  358  361 13    2  8   3  519  465 11    2  9  18   69   61 78*   2 11  -4  782  766 16    2 12  14  450  428 15
 2  7 -10  341  322 11    2  8   4  103  145 57*   2  9  19  269  259 23    2 11  -3  688  692 12    2 12  15    0  161 78*
 2  7  -9  262  232 13    2  8   5  674  691 15    2 10 -18  115   85 84*   2 11  -2  958  993 15    2 12  16  320  371 21
 2  7  -8  323  316 10    2  8   6   63  112 63*   2 10 -17  110   57 58*   2 11  -1  784  757 15    2 12  17  171  157 37*
 2  7  -7  300  275 10    2  8   7  864  860 15    2 10 -16   69  129 79*   2 11   0  993 1005 14    2 13 -17  144   61 39*
 2  7  -6  139  152 21    2  8   8  151  151 29*   2 10 -15  247  210 25    2 11   1  738  783 16    2 13 -16  329  365 18
 2  7  -5  999  979 11    2  8   9  889  951 17    2 10 -14  249  252 21    2 11   2  888  936 15    2 13 -15    0   58 78*
 2  7  -4    0   69 51*   2  8  10  206  182 24    2 10 -13  378  379 13    2 11   3  985  989 15    2 13 -14  373  379 17
 2  7  -3 1497 1497  9    2  8  11 1026 1056 17    2 10 -12  356  355 13    2 11   4  813  844 16    2 13 -13  127   31 75*
 2  7  -2  928  921 10    2  8  12    0   65 70*   2 10 -11  697  730 17    2 11   5  692  703 13    2 13 -12  286  310 21
 2  7  -1 1994 2006  9    2  8  13  793  824 14    2 10 -10  612  582 13    2 11   6  610  611 14    2 13 -11  119   70 75*
 2  7   0  531  476 13    2  8  14  126  176 45*   2 10  -9 1038 1045 14    2 11   7  249  250 21    2 13 -10  216  181 26
 2  7   1 2418 2391 10    2  8  15  674  670 16    2 10  -8  889  889 13    2 11   8  704  746 14    2 13  -9  100   47 60*
 2  7   2  709  590 11    2  8  16   38  122 77*   2 10  -7 1217 1243 14    2 11   9  182  210 30    2 13  -8    0   80 73*
 2  7   3 1767 1829 10    2  8  17  447  424 15    2 10  -6  918  909 13    2 11  10  259  266 22    2 13  -7   96   92 71*
 2  7   4  111  111 27*   2  8  18    0  147 66*   2 10  -5 1120 1106 13    2 11  11  122  160 72*   2 13  -6  240  296 22
 2  7   5 1487 1497 11    2  8  19  151  206 81*   2 10  -4  796  794 14    2 11  12  137  264 76*   2 13  -5    0   28 71*
 2  7   6  225  180 16    2  9 -20  154   96 78*   2 16  11  238  174 29    2 11  13  196  205 30    2 13  -4  534  539 13
 2 13  -3  174  224 30*   2 15 -14  328  388 22    2 16  12  410  397 18    2 19  -9  140   23 83*   3  0   4 1315 1321  8
 2 13  -2  858  848 17    2 15 -13  111   12 81*   2 16  13    0  126 83*   2 19  -8    0   37 82*   3  0   6 1359 1364  9
 2 13  -1  260  210 20    2 15 -12  338  341 20    2 16  14  296  309 23    2 19  -7  106  115 71*   3  0   8 1767 1771 10
 2 13   0 1340 1321 15    2 15 -11  189   71 33*   2 17 -13    0   19 86*   2 19  -6  164   96 83*   3  0  10 1710 1734 11
 2 13   1  230  210 23    2 15 -10  202  260 33    2 17 -12  119  248 65*   2 19  -5  244  274 30    3  0  12 1228 1236 13
 2 13   2 1180 1189 16    2 15  -9    0  170 80*   2 17 -11    0   23 83*   2 19  -4  197  174 35*   3  0  14  754  776 17
 2 13   3  428  414 16    2 15  -8    0   11 76*   2 17 -10  214  234 32    2 19  -3  425  418 18    3  0  16  333  366 16
 2 13   4 1394 1441 16    2 15  -7  173   21 32*   2 17  -9    0  109 83*   2 19  -2  268  247 27    3  0  18  112  113 74*
 2 13   5   96  233 74*   2 15  -6  178  173 32*   2 17  -8    0   54 82*   2 19  -1  465  456 17    3  0  20    0   21 77*
 2 13   6  890  900 18    2 15  -5    0  102 73*   2 17  -7  156  165 81*   2 19   0  379  355 20    3  1 -21  129   49 86*
 2 13   7   50   32 73*   2 15  -4  415  398 14    2 17  -6  135  174 68*   2 19   1  445  405 18    3  1 -20    0  213 90*
 2 13   8  700  736 15    2 15  -2  693  717 15    2 17  -5  161  149 39*   2 19   2  273  268 27    3  1 -19    0   60 83*
 2 13   9  118  142 49*   2 15  -1   72   19 73*   2 17  -4  432  430 16    2 19   3  378  354 20    3  1 -18  203  238 36*
 2 13  10  449  388 14    2 15   0  994 1004 18    2 17  -3  224  247 30    2 19   4  309  287 25    3  1 -17    0   82 81*
 2 13  11  235  253 26    2 15   1    0   45 74*   2 17  -2  667  666 17    2 19   5  303  293 26    3  1 -16  259  261 25
 2 13  12  146   99 78*   2 15   2 1109 1118 18    2 17  -1  363  334 19    2 19   6   73  187 88*   3  1 -15  112  117 66*
 2 13  13    0  204 82*   2 15   3  219  141 27    2 17   0  641  632 15    2 19   7  271  228 29    3  1 -14    0   76 76*
 2 13  14    0   47 78*   2 15   4 1103 1162 10    2 17   1  319  294 21    2 19   8  186   87 40*   3  1 -13    0   59 73*
 2 13  15  150  103 79*   2 15   5  222  218 27    2 17   2  640  608 14    2 20  -9    0  208 90*   3  1 -12  109  149 73*
 2 13  16  165   69 37*   2 15   6  887  856 20    2 17   3  439  402 17    2 20  -8   29  129 84*   3  1 -11  169   19 26
 2 13  17  161   82 38*   2 15   7  169  115 37*   2 17   4  499  487 15    2 20  -7  440  453 18    3  1 -10  915  929 14
 2 14 -16  104  162 77*   2 15   8  612  574 15    2 17   5  351  336 21    2 20  -6  104  163 86*   3  1  -9  157  137 24
 2 14 -15  108   52 65*   2 15   9    0   95 80*   2 17   6  451  430 16    2 20  -5  371  434 22    3  1  -8 1473 1457 11
 2 14 -14  349  308 19    2 15  10  317  345 22    2 17   7  126  197 86*   2 20  -3  341  364 23    3  1  -7  463  454 10
 2 14 -13    0   67 78*   2 15  11    0   36 80*   2 17   8  399  359 19    2 20  -2   29  173 88*   3  1  -6 1966 1980  9
 2 14 -12  481  465 15    2 15  12    0  102 80*   2 17   9  109  115 85*   2 20  -1  279  246 27    3  1  -5  630  607 10
 2 14 -11    0   48 78*   2 15  13  163  147 38*   2 17  10  126  201 59*   2 20   0  125  119 73*   3  1  -4 2897 2888  8
 2 14 -10  616  625 14    2 15  14    0   30 79*   2 17  11  151   62 47*   2 20   1   18   50 71*   3  1  -3  611  592  9
 2 14  -9  110   26 74*   2 15  15    0   60 79*   2 17  12   26   26 84*   2 20   2  154   28 87*   3  1  -2 2303 2284  7
 2 14  -8  580  572 13                                                                               3  1  -1  845  839  7
```

```
  h  k   l   Fo   Fc   σ        h  k   l   Fo   Fc   σ        h  k   l   Fo   Fc   σ        h  k   l   Fo   Fc   σ        h  k   l   Fo   Fc   σ

Column 1                     Column 2                     Column 3                     Column 4                     Column 5
 2 14  -7  141   39 73*      2 16 -14  262  246 27        2 18 -12  157  129 83*      2 20   3   79    9 87*      3  1   0 1701 1733  7
 2 14  -6  525  541 12       2 16 -13  168  212 42*       2 18 -11  216  267 34       2 20   4    0   91 89*      3  1   1   94   68 18*
 2 14  -5    0  115 73*      2 16 -12  153  302 86*       2 18 -10  119  285 85*      2 20   5    0  119 88*      3  1   2 1869 1877  7
 2 14  -4  727  704 14       2 16 -11   76  219 85*       2 18  -9  390  426 20       2 20   6  161  159 49*      3  1   3  427  438  8
 2 14  -3  126   53 72*      2 16 -10  452  466 16        2 18  -8  350  377 21       2 20   7  165  156 89*      3  1   4 1090 1095  8
 2 14  -2  532  543 12       2 16  -9  299  236 22        2 18  -7  415  414 18       2 21  -4    0    6 86*      3  1   5  543  525 11
 2 14  -1   57   77 73*      2 16  -8  608  630 15        2 18  -6  406  420 18       2 21  -3  243  269 32       3  1   6  619  629 11
 2 14   0  398  389 15       2 16  -7  233  173 26        2 18  -5  451  465 17       2 21  -2  173   24 87*      3  1   7  383  381  9
 2 14   1    0   73 73*      2 16  -6  581  591 13        2 18  -4  302  333 23       2 21  -1  336  340 24       3  1   8  232  225 13
 2 14   2  181  148 30       2 16  -5  221  201 27        2 18  -3  397  421 18       2 21   0  122   43 72*      3  1   9  121  132 26*
 2 14   3  263  235 22       2 16  -4  651  659 16        2 18  -2  172  205 40*      2 21   1  393  380 21       3  1  10  277  216 14
 2 14   4  380  363 16       2 16  -3  229  227 27        2 18  -1  236  271 30       2 21   2  165   61 88*      3  1  11    0   41 62*
 2 14   5   90  211 78*      2 16  -2  366  382 18        2 18   0    0   33 82*      2 21   3  363  364 23       3  1  12  615  617 13
 2 14   6  666  661 16       2 16  -1  310  274 20        2 18   1  152  183 80*      3  0 -20  156  167 89*      3  1  13  222  261 21
 2 14   7  127  210 48*      2 16   0  129  110 76*       2 18   2    0  111 83*      3  0 -18  375  362 20       3  1  14  621  628 14
 2 14   8  668  667 14       2 16   1  187  190 32*       2 18   3    0    2 83*      3  0 -16  652  620 14       3  1  15  202  188 24
 2 14   9  106  203 79*      2 16   2    0   46 76*       2 18   4    0  195 86*      3  0 -14 1020  985 18       3  1  16  649  643 15
 2 14  10  644  639 14       2 16   3  140  104 77*       2 18   5  128   97 84*      3  0 -12 1636 1567 14       3  1  17  113  151 48*
 2 14  11  124  173 50*      2 16   4  202  246 33        2 18   6  203  234 36*      3  0 -10 1947 1940 12       3  1  18  443  460 15
 2 14  12  458  465 16       2 16   5    0   67 79*       2 18   7    0  136 86*      3  0  -8 2072 2072 10       3  1  19  106   91 75*
 2 14  13   93   56 77*      2 16   6  376  366 19        2 18   8  308  247 24       3  0  -6 1190 1138  9       3  1  20  239  251 25
 2 14  14  339  344 20       2 16   7  137  152 69*       2 18   9  291  230 26       3  0  -4  667  679  9       3  2 -21    0   39 87*
 2 14  15  136   17 45*      2 16   8  399  394 18        2 18  10  327  320 25       3  0  -2  394  393  8       3  2 -20  157  112 46*
 2 14  16  203  245 32       2 16   9  220  203 32        2 18  11  256  252 30       3  0   0  298  278  7       3  2 -19   83   83 84*
 2 15 -15    0   10 80*      2 16  10  437  444 18        2 19 -10  161  110 44*      3  0   2 1186 1177  7       3  2 -18  311  335 23
 3  2 -17    0   79 80*      3  3  -4 1379 1387  8        3  4   9  759  793 15       3  6 -20    0   66 84*      3  7  -6    0  123 58*
 3  2 -16  589  602 15       3  3  -3 1286 1262  8        3  4  10  737  734 17       3  6 -19  153  204 85*      3  7  -5 1445 1402 10
 3  2 -15  146  170 40*      3  3  -2 2494 2479  8        3  4  11  628  653 13       3  6 -18    0   12 82*      3  7  -4  358  342  9
 3  2 -14  710  791 15       3  3  -1 1129 1188  8        3  4  12  374  339 13       3  6 -17  414  433 18       3  7  -3 1900 1888 10
 3  2 -13  272  234 20       3  3   0 1770 1784  7        3  4  13  469  490 12       3  6 -16    0   88 80*      3  7  -2  184  144 15
 3  2 -12 1174 1182 14       3  3   1 1269 1308  8        3  4  14  363  322 14       3  6 -15  635  631 14       3  7  -1 1763 1763 10
 3  2 -11  451  454 11       3  3   2 1651 1630  8        3  4  15  252  263 21       3  6 -14  188  192 31       3  7   0    0   16 51*
 3  2 -10 1216 1203 13       3  3   3 1447 1458  8        3  4  16    0  164 75*      3  6 -13  787  779 18       3  7   1 1516 1527 10
 3  2  -9  259  244 14       3  3   4  973  982  9        3  4  17  122   98 75*      3  6 -12  252  286 21       3  7   2   56    3 52*
 3  2  -8 1357 1356 11       3  3   5  573  596 12        3  4  18    0   82 77*      3  6 -11  891  846 16       3  7   3  985 1066 11
 3  2  -7  270  197 11       3  3   6  191  221 15        3  4  19  143   14 77*      3  6 -10  304  279 14       3  7   4  185  205 18
 3  2  -6 1135 1134  9       3  3   7 1046 1034 11        3  4  20    0   13 77*      3  6  -9  867  880 14       3  7   5 1028 1074 12
 3  2  -5  386  360  9       3  3   8  244  253 14        3  5 -21  235  239 30       3  6  -8  304  303 12       3  7   6  485  487 11
 3  2  -4 1242 1249  8       3  3   9  256  246 15        3  5 -20   74  146 84*      3  6  -7  906  913 11       3  7   7  419  438 11
 3  2  -3 1231 1203  8       3  3  10  526  512 13        3  5 -19  308  363 23       3  6  -6  177  119 16       3  7   8  428  413 12
 3  2  -2  380  322  8       3  3  11  122  177 66*       3  5 -18  145  233 48*      3  6  -5  643  639 12       3  7   9   77   30 56*
 3  2  -1  548  550  9       3  3  12  470  441 11        3  5 -17  292  336 24       3  6  -4  256  242 11       3  7  10  296  330 17
 3  2   0  156  165 11       3  3  13  104  221 69*       3  5 -16    0  221 79*      3  6  -3  415  387  9       3  7  11  320  372 17
 3  2   1  143  116 12       3  3  14  482  482 12        3  5 -15  162  190 37*      3  6  -2  114  151 22*      3  7  12  102  145 48*
 3  2   2 1221 1253  7       3  3  15  334  304 16        3  5 -14   80   92 57*      3  6  -1  144  110 17       3  7  13  543  480 12
 3  2   3  609  625  9       3  3  16  378  365 15        3  5 -13  150  112 35*      3  6   0  285  301  9       3  7  14    0   17 74*
 3  2   4 1804 1801  8       3  3  17  289  276 20        3  5 -12  148  134 34*      3  6   1  589  592 12       3  7  15  499  493 13
 3  2   5  404  403 10       3  3  18  367  347 16        3  5 -11  267  230 18       3  6   2  336  326  9       3  7  16  116   56 75*
 3  2   6 1430 1482 10       3  3  19  202  234 30        3  5 -10  201  172 21       3  6   3 1215 1193 10       3  7  17  442  439 16
 3  2   7  630  620 13       3  4 -21  107  121 64*       3  5  -9  579  557 11       3  6   4   75   76 54*      3  7  18  136  177 77*
 3  2   8 1578 1573 11       3  4 -20    0   81 83*       3  5  -8  413  441 10       3  6   5 1261 1286 11       3  7  19  330  338 20
 3  2   9  746  747 14       3  4 -19  139  199 70*       3  5  -7  945  917 11       3  6   6  525  506 12       3  8 -20    0   31 85*
 3  2  10 1316 1373 12       3  4 -18  226  212 29        3  5  -6  495  516 10       3  6   7 1364 1387 12       3  8 -19  143  148 72*
 3  2  11  699  680 16       3  4 -17  334  324 21        3  5  -5 1015 1043  9       3  6   8  269  261 15       3  8 -18  144  105 84*
 3  2  12  775  782 16       3  4 -16  405  411 16        3  5  -4  848  818 10       3  6   9 1153 1127 14       3  8 -17  357  290 21
 3  2  13  226  200 20       3  4 -15  460  487 14        3  5  -3 2106 2148  9       3  6  10    0   99 67*      3  8 -16   18  149 83*
 3  2  14  690  712 13       3  4 -14  412  442 15        3  5  -2 1217 1189  9       3  6  11  742  721 18       3  8 -15  603  581 15
 3  2  15  204  169 24       3  4 -13  744  720 13        3  5  -1 2023 2023  8       3  6  12  208  282 25       3  8 -14  270  203 22
 3  2  16  286  309 20       3  4 -12  578  601 12        3  5   0 1340 1291  8       3  6  13  575  563 13       3  8 -13  670  654 15
 3  2  17   68   49 72*      3  4 -11  643  616 12        3  5   1 2537 2511  9       3  6  14    0   56 71*      3  8 -12  164  124 30*
 3  2  18   70  125 76*      3  4 -10  556  536 13        3  5   2 1414 1420  9       3  6  15  328  316 18       3  8 -11 1050 1068 15
 3  2  19  108   83 57*      3  4  -9  711  695 14        3  5   3 2319 2315  9       3  6  16    0   87 78*      3  8 -10  288  279 16
 3  2  20    0   15 75*      3  4  -8  640  619 13        3  5   4  652  658 12       3  6  17  248  148 23       3  8  -9 1127 1139 13
 3  3 -21    0  172 85*      3  4  -7  595  600 13        3  5   5  920  908 11       3  6  18  111  151 78*      3  8  -8  302  284 14
 3  3 -20  138  199 85*      3  4  -6  484  498  9        3  5   6  426  410 10       3  6  19   57   56 78*      3  8  -7  889  894 13
 3  3 -19  245  256 29       3  4  -5  350  363  9        3  5   7  662  679 15       3  6  20    0   90 78*      3  8  -6  267  257 14
 3  3 -18  254  265 27       3  4  -4  697  679 10        3  5   8  111  108 61*      3  7 -20    0   61 85*      3  8  -5  685  692 14
 3  3 -17  209  233 31       3  4  -3  438  423  8        3  5   9  225  231 19       3  7 -19  279  249 25       3  8  -4  379  386 10
 3  3 -16    0  163 79*      3  4  -2    0   28 45*       3  5  10    0   33 64*      3  7 -18  131   91 82*      3  8  -3   70   58 56*
 3  3 -15  227  226 26       3  4  -1  250  264  9        3  5  11  166  170 27       3  7 -17  272  292 27       3  8  -2  449  475 14
 3  3 -14   38   66 75*      3  4   0  399  393  8        3  5  12  118  139 39*      3  7 -16  211  200 31       3  8  -1    0  245 13
 3  3 -13  270  242 20       3  4   1  637  626 10        3  5  13    0   91 69*      3  7 -15  142  151 81*      3  8   0  112  131 27*
 3  3 -12  355  346 15       3  4   2 1298 1287  8        3  5  14  142  169 36*      3  7 -14  193  168 31       3  8   1  606  627 14
 3  3 -11    0   31 65*      3  4   3 1034 1064  9        3  5  15  324  351 17       3  7 -13  131    8 74*      3  8   2  348  334 11
 3  3 -10  401  411 11       3  4   4 1288 1273  9        3  5  16  216  248 26       3  7 -12  351  373 16       3  8   3  868  845 13
 3  3  -9  411  401 10       3  4   5 1486 1515 10        3  5  17  336  335 19       3  7 -11  216  222 22       3  8   4  528  514 12
 3  3  -8  782  792 12       3  4   6 1391 1377 10        3  5  18  102  168 65*      3  7 -10   86  104 64*      3  8   5 1032 1088 13
 3  3  -7  777  795 12       3  4   7 1181 1197 11        3  5  19  328  314 20       3  7  -9  689  680 15       3  8   6  559  563 13
 3  3  -6 1397 1374  9       3  4   8 1080 1074 12        3  5  20  145  139 42*      3  7  -8  190  205 19       3  8   7 1289 1296 14
 3  3  -5  873  922  9       3 10 -13  604  594 13        3  6 -21  124  123 81*      3  7  -7 1135 1187 12       3  8   8  243  239 19
 3  8   9 1168 1172 15       3 10 -12  509  459 12        3 11   5    0  154 71*      3 13 -11  152  135 77*      3 14  11  154   75 77*
 3  8  10  219  230 24       3 10 -11  798  866 18        3 11   6  502  521 12       3 13 -10  260  217 22       3 14  12  304  323 23
 3  8  11 1041 1101 17       3 10 -10  789  771 17        3 11   7  112  103 61*      3 13  -9   91  163 74*      3 14  13    0   39 82*
 3  8  12  126  267 76*      3 10  -9  945  962 16        3 11   8  228  213 23       3 13  -8  523  507 12       3 14  14  222  254 30
 3  8  13  641  659 16       3 10  -8  588  612 14        3 11   9  242  237 23       3 13  -7  133  110 73*      3 14  15    0   14 83*
 3  8  14  132  234 78*      3 10  -7  791  774 16        3 11  10  115  102 74*      3 13  -6  677  663 14       3 15 -15   74   54 84*
 3  8  15  399  385 16       3 10  -6  451  447 11        3 11  11  385  358 16       3 13  -5  344  361 16       3 15 -14  190  110 36*
 3  8  16  247  234 25       3 10  -5  583  566 13        3 11  12  286  259 21       3 13  -4  925  924 16       3 15 -13    0  122 84*
 3  8  17  208  122 29       3 10  -4  205  176 20        3 11  13  291  298 22       3 13  -3  434  444 13       3 15 -12  130   17 81*
 3  8  18  163  155 38*      3 10  -3  281  289 15        3 11  14  281  300 24       3 13  -2 1115 1078 16       3 15 -11    0  106 83*
 3  8  19  159   14 39*      3 10  -2    0   60 63*       3 11  15  330  299 20       3 13  -1  343  285 16       3 15 -10  211  156 30
 3  9 -19  216  145 35       3 10  -1   70  132 63*       3 11  16  278  285 24       3 13   0 1141 1156 16       3 15  -9  111   20 59*
 3  9 -18    0   25 89*      3 10   0  383  409 11        3 11  17  248  236 27       3 13   1  413  373 14       3 15  -8  421  367 16
 3  9 -17  237  217 32       3 10   1  403  413 11        3 12 -18  210  157 38*      3 13   2 1131 1089 16       3 15  -7   57   21 77*
 3  9 -16   49    9 84*      3 10   2  310  296 14        3 12 -17  136  174 85*      3 13   3    0  118 74*      3 15  -6  539  492 13
 3  9 -15    0  158 82*      3 10   3  795  798 16        3 12 -16  282  290 25       3 13   4  660  691 15       3 15  -5  112   25 75*
 3  9 -14   87   54 78*      3 10   4  357  365 13        3 12 -15  209  269 31       3 13   5   59   36 56*      3 15  -4  785  836 15
 3  9 -13    0   73 75*      3 10   5  882  910 16        3 12 -14  417  403 16       3 13   6  414  401 15       3 15  -3  179  144 32*
 3  9 -12   93  100 69*      3 10   6  488  462 11        3 12 -13  378  364 16       3 13   7    0  231 77*      3 15  -2 1001  971 18
 3  9 -11  316  250 15       3 10   7  912  923 17        3 12 -12  508  517 13       3 13   8    0  181 77*      3 15  -1  133  197 78*
 3  9 -10  320  296 15       3 10   8  817  801 18        3 12 -11  357  396 17       3 13   9  271  240 22       3 15   0 1030 1052 18
 3  9  -9  608  640 13       3 10   9  992  989 18        3 12 -10  569  573 13       3 13  10  133  119 46*      3 15   1  148  151 76*
 3  9  -8  401  370 12       3 10  10  638  603 15        3 12  -9  411  465 14       3 13  11  111  247 81*      3 15   2 1006 1017 19
 3  9  -7 1021  991 13       3 10  11  773  777 19        3 12  -8  515  511 12       3 13  12  117  167 79*      3 15   3  212  225 29
 3  9  -6  497  479 11       3 10  12  592  578 14        3 12  -7  527  529 11       3 13  13    0   69 80*      3 15   4  628  635 14
 3  9  -5 1434 1436 12       3 10  13  487  501 14        3 12  -6  453  441 13       3 13  14  247  219 27       3 15   5  133  114 45*
 3  9  -4  667  679 15       3 10  14  380  342 18        3 12  -5  547  563 13       3 13  15    0  117 83*      3 15   6  333  334 20
 3  9  -3 1548 1527 11       3 10  15   84  278 82*       3 12  -4  193  192 26       3 13  16  252  245 27       3 15   7   40   28 79*
 3  9  -2  465  481 11       3 10  16  172  188 37*       3 12  -3  495  489 12       3 14 -16  258  281 27       3 15   8  204  163 32
 3  9  -1 1078 1085 12       3 10  17    0  121 81*       3 12  -2  246  224 20       3 14 -15   58   24 82*      3 15   9    0   29 81*
 3  9   0  551  553 11       3 11 -18   80  120 90*       3 12  -1    0   92 69*      3 14 -14  383  381 19       3 15  10    0   55 84*
 3  9   1 1248 1228 12       3 11 -17  351  110 84*       3 12   0  417  445 13       3 14 -13    0   43 02*      3 15  11    0   20 85*
 3  9   2  399  412 10       3 11 -16  129  140 70*       3 12   1  104   63 52*      3 14 -12  463  442 16       3 15  12    0  163 85*
 3  9   3  930  932 14       3 11 -15  121   47 51*       3 12   2  388  351 14       3 14 -11   56  104 77*      3 15  13  124   63 84*
 3  9   4  288  260 14       3 11 -14    0   41 77*       3 12   3  684  688 14       3 14 -10  463  421 15       3 15  14  118  175 70*
 3  9   5  634  636 12       3 11 -13  139   20 38*       3 12   4  905  886 17       3 14  -9    0  140 78*      3 16 -14  220  273 34
 3  9   6  218  190 20       3 11 -12   67   67 61*       3 12   5  648  610 15       3 14  -8  317  350 19       3 16 -12  336  351 22
 3  9   7  385  367 13       3 11 -11  249  265 22        3 12   6  648  676 15       3 14  -7   99   63 74*      3 16 -11    0  105 87*
 3  9   8    0   26 70*      3 11 -10  328  296 17        3 12   7  452  461 14       3 14  -6  381  357 16       3 16 -10  416  416 18
 3  9   9  136   87 71*      3 11  -9  382  358 15        3 12   8  816  880 20       3 14  -5    0   69 75*      3 16  -9    0   87 81*
 3  9  10    0    6 59*      3 11  -8  688  648 13        3 12   9  493  528 14       3 14  -4  264  242 21       3 16  -8  312  336 22
 3  9  11  283  319 20                                    3 12  10  676  672 15       3 14  -3    0   54 75*      3 16  -7  154  140 41*
 3  9  12  106  124 57*                                   3 12  11  218  227 28       3 14  -2    0   54 75*
```

h	k	l	Fo	Fc	s
3	9	13	507	490	13
3	9	14	26	154	76*
3	9	15	552	566	14
3	9	16	154	159	41*
3	9	17	366	432	20
3	9	18	139	101	46*
3	10	-19	54	131	90*
3	10	-18	217	124	36*
3	10	-17	274	233	29
3	10	-16	293	251	25
3	10	-15	401	448	18
3	10	-14	393	376	16
3	16	6	555	552	14
3	16	7	250	184	27
3	16	8	562	522	15
3	16	9	198	199	37*
3	16	10	432	420	19
3	16	11	150	156	86*
3	16	12	282	298	27
3	16	13	111	124	86*
3	17	-13	30	101	85*
3	17	-12	124	67	85*
3	17	-11	150	110	86*
3	17	-10	0	103	85*
3	17	-9	229	196	31
3	17	-8	280	305	25
3	17	-7	48	161	84*
3	17	-6	459	441	16
3	17	-5	292	288	24
3	17	-4	573	584	14
3	17	-3	310	324	23
3	17	-2	589	563	13
3	17	-1	314	312	23
3	17	0	518	489	14
3	17	1	362	361	19
3	17	2	394	410	18
3	17	3	215	233	32
3	17	4	336	333	22
3	17	5	164	139	83*
3	17	6	263	253	27
3	17	7	0	41	85*
3	17	8	57	111	61*
3	17	9	0	28	89*
3	17	10	119	108	90*
3	17	11	0	60	86*
3	17	12	264	221	29
3	18	-11	350	326	22
3	18	-10	244	294	31
3	18	-9	284	319	27
3	18	-8	281	290	26
3	18	-7	319	299	22
3	18	-6	138	160	52*
3	18	-5	210	239	35
3	18	-4	0	60	83*
3	18	-3	0	78	84*
3	18	-2	161	70	82*
3	18	-1	159	19	81*
3	18	0	73	170	85*
3	18	1	137	113	81*
3	18	2	239	200	29
3	18	3	247	227	29
3	18	4	205	284	38*
3	18	5	305	283	25
3	18	6	310	294	25
3	18	7	359	333	22
3	18	8	352	350	23
3	18	9	402	363	22
4	4	17	210	191	28
4	4	18	0	125	79*
4	4	19	175	180	36*
4	5	-20	140	101	55*
4	5	-19	0	135	88*
4	5	-18	133	99	56*
4	5	-17	0	15	85*
4	5	-16	0	34	82*
4	5	-15	200	147	32
4	5	-14	104	55	59*
4	5	-13	241	194	24
4	5	-12	111	99	75*
4	5	-11	583	570	12
4	5	-10	439	409	12
4	5	-9	848	824	15
4	5	-8	584	555	12
4	5	-7	1187	1165	12
4	5	-6	751	761	13
4	5	-5	1784	1789	10
4	5	-4	812	789	12
4	5	-3	1911	1884	10
4	5	-2	902	906	11
4	5	-1	1601	1605	10
4	5	0	673	636	12
4	5	1	1233	1244	10
4	5	2	198	193	15
4	5	3	0	79	55*
4	5	4	0	90	55*
4	5	5	242	245	14
4	5	6	230	208	15
4	5	7	492	498	11
4	5	8	340	357	13
4	5	9	592	554	13
4	5	10	210	186	21
4	5	11	450	463	12
4	5	12	367	371	14
4	5	13	635	605	14
4	5	14	320	331	18
4	5	15	527	525	13
4	5	16	175	202	33*
4	5	17	493	456	14
4	5	18	185	183	33*
4	5	19	291	311	23
4	6	-20	172	52	45*
4	6	-19	307	295	26
4	6	-18	123	49	88*
4	6	-17	379	395	21
4	6	-16	0	121	85*
4	6	-15	499	479	15
4	6	-14	0	180	80*
4	6	-13	514	467	13
4	6	-12	198	179	28
4	6	-11	516	499	12
4	6	-10	70	92	70*
4	6	-9	435	436	11
4	12	-13	178	247	38*
3	11	-7	538	500	12
3	11	-6	950	955	16
3	11	-5	621	634	13
3	11	-4	1108	1111	14
3	11	-3	956	952	15
3	11	-2	923	909	15
3	11	-1	799	820	16
3	11	0	953	967	15
3	11	1	816	813	17
3	11	2	614	621	13
3	11	3	630	630	13
3	11	4	659	683	13
3	18	10	303	287	27
3	19	-9	262	253	28
3	19	-8	0	136	89*
3	19	-7	337	336	23
3	19	-6	148	210	86*
3	19	-5	396	435	20
3	19	-4	206	242	36*
3	19	-3	401	425	19
3	19	-2	330	299	22
3	19	-1	388	367	20
3	19	0	190	221	39*
3	19	1	276	273	27
3	19	2	160	220	87*
3	19	3	294	293	26
3	19	4	0	138	88*
3	19	5	218	204	36
3	19	6	110	50	86*
3	19	7	173	151	90*
3	19	8	0	31	90*
3	20	-7	241	258	31
3	20	-6	0	111	86*
3	20	-5	106	184	61*
3	20	-4	0	114	87*
3	20	-3	53	70	86*
3	20	-2	37	69	86*
3	20	-1	0	58	88*
3	20	0	0	23	86*
3	20	1	0	149	88*
3	20	2	129	105	74*
3	20	3	265	233	30
3	20	4	272	179	29
3	20	5	295	284	28
3	20	6	176	155	92*
3	21	-1	379	408	22
3	21	0	118	40	88*
4	0	-20	213	245	39*
4	0	-18	435	444	19
4	0	-16	653	641	15
4	0	-14	868	880	20
4	0	-12	1145	1164	16
4	0	-10	1094	1042	15
4	0	-8	755	748	14
4	0	-6	472	410	11
4	0	-4	155	271	16
4	0	-2	330	346	7
4	0	0	1114	1136	9
4	0	2	1678	1646	9
4	0	4	1989	1978	9
4	0	6	1860	1849	10
4	0	8	1835	1846	11
4	0	10	961	1028	13
4	0	12	487	486	12
4	0	14	73	200	70*
4	0	16	0	38	70*
4	0	18	0	148	75*
4	6	-8	170	151	24
4	6	-7	262	208	15
4	6	-6	194	127	18
4	6	-5	166	132	21
4	6	-4	482	477	12
4	6	-3	866	856	12
4	6	-2	452	427	11
4	6	-1	1510	1536	10
4	6	0	426	423	10
4	6	1	1880	1923	10
4	6	2	255	277	13
4	6	3	1783	1802	10
4	6	4	671	646	14
4	6	5	1494	1492	11
4	6	6	358	368	12
4	6	7	1139	1126	13
4	6	8	237	219	19
4	6	9	563	537	14
4	6	10	86	45	67*
4	6	11	462	428	12
4	6	12	118	91	41*
4	6	13	189	175	28
4	6	14	0	147	76*
4	6	15	71	52	75*
4	6	16	263	243	23
4	6	17	133	124	66*
4	6	18	152	171	41*
4	6	19	193	184	33*
4	7	-20	0	82	91*
4	7	-19	173	110	90*
4	7	-18	184	131	43*
4	7	-17	0	38	88*
4	7	-16	81	117	85*
4	7	-15	238	193	30
4	7	-14	0	165	82*
4	7	-13	303	268	21
4	7	-12	142	113	73*
4	7	-11	700	699	14
4	7	-10	119	93	69*
4	7	-9	1087	1039	14
4	7	-8	103	63	54*
4	7	-7	1242	1234	13
4	7	-6	121	31	31*
4	7	-5	1664	1643	11
4	7	-4	213	195	17
4	7	-3	1645	1621	11
4	7	-2	137	48	24*
4	7	-1	1379	1366	11
4	7	0	119	21	27*
4	7	1	768	781	13
4	7	2	294	300	12
4	7	3	265	294	14
4	7	4	205	195	18
4	7	5	277	237	15
4	7	6	0	148	65*
4	13	9	297	306	23
3	12	12	474	482	15
3	12	13	214	179	30
3	12	14	309	342	22
3	12	15	48	150	80*
3	12	16	185	151	36*
3	12	17	126	66	79*
3	13	-17	0	46	82*
3	13	-16	0	170	83*
3	13	-15	0	18	80*
3	13	-14	0	101	80*
3	13	-13	0	51	79*
3	13	-12	167	60	35*
3	14	10	516	533	15
4	0	20	0	99	75*
4	1	-21	0	31	90*
4	1	-20	139	85	58*
4	1	-19	0	63	87*
4	1	-18	0	57	86*
4	1	-17	0	65	85*
4	1	-16	154	72	82*
4	1	-15	0	8	80*
4	1	-14	253	260	25
4	1	-13	0	138	79*
4	1	-12	799	732	19
4	1	-11	311	309	17
4	1	-10	1046	1055	14
4	1	-9	392	405	12
4	1	-8	1229	1205	12
4	1	-7	640	594	14
4	1	-6	1739	1667	10
4	1	-5	786	774	11
4	1	-4	1382	1382	9
4	1	-3	396	383	10
4	1	-2	1318	1311	8
4	1	-1	429	397	9
4	1	0	1120	1081	9
4	1	1	426	408	9
4	1	2	670	693	10
4	1	3	405	397	10
4	1	4	0	22	50*
4	1	5	296	285	10
4	1	6	554	538	13
4	1	7	50	170	56*
4	1	8	880	850	13
4	1	9	171	174	21
4	1	10	1205	1236	13
4	1	11	413	422	11
4	1	12	902	913	16
4	1	13	0	194	68*
4	1	14	872	857	17
4	1	15	143	215	35*
4	1	16	556	551	13
4	1	17	0	63	75*
4	1	18	294	306	20
4	1	19	0	26	75*
4	1	20	200	181	29
4	2	-21	0	73	89*
4	2	-20	13	221	91*
4	2	-19	0	93	86*
4	2	-18	397	397	19
4	2	-17	189	170	38*
4	2	-16	518	531	15
4	2	-15	0	214	83*
4	2	-14	605	634	14
4	2	-13	394	379	16
4	2	-12	747	767	13
4	2	-11	25	118	72*
4	2	-10	690	677	13
4	7	7	499	485	10
4	7	8	122	64	36*
4	7	9	928	867	16
4	7	10	272	241	19
4	7	11	872	863	18
4	7	12	83	126	61*
4	7	13	822	746	19
4	7	14	0	47	76*
4	7	15	618	584	14
4	7	16	140	57	76*
4	7	17	424	426	16
4	7	18	0	27	80*
4	7	19	289	278	22
4	8	-18	60	234	93*
4	8	-17	443	418	20
4	8	-16	128	162	66*
4	8	-15	517	510	16
4	8	-14	156	96	42*
4	8	-13	682	657	16
4	8	-12	284	267	20
4	8	-11	624	685	15
4	8	-10	250	267	21
4	8	-9	415	408	13
4	8	-8	276	267	17
4	8	-7	222	184	20
4	8	-6	311	265	14
4	8	-5	334	327	13
4	8	-4	255	250	16
4	8	-3	799	766	14
4	8	-2	142	138	26*
4	8	-1	1081	1055	12
4	8	0	145	81	17*
4	8	1	1321	1294	12
4	8	2	328	335	12
4	8	3	1500	1509	12
4	8	4	400	412	11
4	8	5	1467	1471	13
4	8	6	224	250	20
4	8	7	1268	1255	14
4	8	8	243	283	21
4	8	9	1012	1009	16
4	8	11	493	489	13
4	8	13	91	164	76*
4	8	14	342	336	19
4	8	15	165	92	37*
4	8	16	211	203	30
4	8	17	129	130	49*
4	8	18	0	108	81*
4	9	-19	132	73	93*
4	9	-18	126	29	65*
4	9	-17	0	54	91*
4	9	-16	0	105	88*
4	15	4	73	41	67*
3	14	-1	0	131	75*
3	14	0	304	335	19
3	14	1	33	82	56*
3	14	2	687	681	15
3	14	3	0	112	77*
3	14	4	960	1017	19
3	14	5	78	93	65*
3	14	6	817	865	20
3	14	7	65	133	58*
3	14	8	669	667	14
3	14	9	0	72	82*
4	2	-9	101	104	54*
4	2	-8	664	631	15
4	2	-7	257	201	14
4	2	-6	484	494	11
4	2	-5	1056	1056	10
4	2	-4	430	467	10
4	2	-3	792	754	10
4	2	-2	912	856	9
4	2	-1	999	981	9
4	2	0	1644	1618	8
4	2	1	541	491	11
4	2	2	2012	2033	9
4	2	3	651	651	11
4	2	4	1695	1673	9
4	2	5	829	838	11
4	2	6	1545	1559	10
4	2	7	813	791	12
4	2	8	1387	1360	11
4	2	9	663	647	15
4	2	10	718	722	15
4	2	11	0	95	64*
4	2	12	598	586	13
4	2	13	101	30	45*
4	2	14	171	131	27
4	2	15	191	194	27
4	2	16	0	16	73*
4	2	17	173	162	32*
4	2	18	195	128	28
4	2	19	0	100	77*
4	2	20	133	156	76*
4	3	-21	0	113	90*
4	3	-20	131	89	88*
4	3	-19	107	132	89*
4	3	-18	117	27	65*
4	3	-17	0	66	86*
4	3	-16	103	83	58*
4	3	-15	56	23	80*
4	3	-14	330	325	19
4	3	-13	142	165	42*
4	3	-12	385	387	16
4	3	-11	566	523	12
4	3	-10	676	687	13
4	3	-9	880	868	14
4	3	-8	1039	1033	12
4	3	-7	1239	1192	11
4	3	-6	1313	1299	10
4	3	-5	1161	1199	10
4	3	-4	1991	2000	9
4	3	-3	914	852	10
4	3	-2	1467	1424	9
4	3	-1	1224	1229	9
4	3	0	1099	1092	9
4	3	1	955	993	9
4	3	2	373	396	9
4	3	3	335	340	8
4	9	-15	0	92	88*
4	9	-14	92	137	70*
4	9	-13	358	329	19
4	9	-12	307	279	20
4	9	-11	691	677	15
4	9	-10	438	444	14
4	9	-9	946	979	16
4	9	-8	489	448	12
4	9	-7	1095	1095	14
4	9	-6	469	475	11
4	9	-5	1220	1185	13
4	9	-4	374	341	12
4	9	-3	958	947	14
4	9	-2	322	330	14
4	9	-1	734	739	16
4	9	0	255	211	15
4	9	1	507	533	11
4	9	2	252	278	17
4	9	3	343	323	13
4	9	4	193	223	24
4	9	5	95	28	66*
4	9	6	49	72	68*
4	9	7	598	600	15
4	9	8	154	94	34*
4	9	9	773	794	19
4	9	10	171	146	32*
4	9	11	724	754	15
4	9	12	139	216	78*
4	9	13	715	724	16
4	9	14	184	205	34*
4	9	15	480	495	15
4	9	16	165	155	38*
4	9	17	243	296	28
4	9	18	151	92	79*
4	10	-18	104	160	93*
4	10	-17	319	321	27
4	10	-16	283	291	30
4	10	-15	464	469	18
4	10	-14	366	314	20
4	10	-13	598	593	15
4	10	-12	433	414	15
4	10	-11	595	655	14
4	10	-10	377	359	16
4	10	-9	530	570	12
4	10	-8	112	131	61*
4	10	-7	285	256	18
4	10	-6	0	57	70*
4	10	-5	0	37	68*
4	10	-4	0	125	68*
4	10	-3	243	251	19
4	10	-2	223	194	20
4	10	-1	453	447	11
4	10	0	410	415	12
4	10	1	895	840	15
4	10	2	435	462	12
4	17	7	148	119	89*
3	16	-6	338	354	19
3	16	-5	109	190	82*
3	16	-4	0	117	79*
3	16	-3	184	191	34*
3	16	-2	67	173	79*
3	16	-1	88	115	78*
3	16	0	107	222	82*
3	16	1	0	22	79*
3	16	2	466	452	15
3	16	3	232	193	28
3	16	4	511	509	15
3	16	5	181	243	38*
4	3	4	338	315	9
4	3	5	394	396	10
4	3	6	420	423	10
4	3	7	201	149	17
4	3	8	801	765	14
4	3	9	417	404	11
4	3	10	623	633	12
4	3	11	630	583	13
4	3	12	464	632	14
4	3	13	465	437	12
4	3	14	593	581	12
4	3	15	371	381	15
4	3	16	472	472	13
4	3	17	299	278	20
4	3	18	374	340	16
4	3	19	148	194	78*
4	3	20	257	217	23
4	4	-21	69	198	90*
4	4	-20	0	166	89*
4	4	-19	300	256	26
4	4	-18	257	261	29
4	4	-17	321	316	23
4	4	-16	349	321	20
4	4	-15	423	428	17
4	4	-14	309	298	21
4	4	-13	414	459	16
4	4	-12	496	446	12
4	4	-11	398	367	14
4	4	-10	433	407	12
4	4	-9	293	275	15
4	4	-8	252	268	16
4	4	-7	155	80	22
4	4	-6	320	274	11
4	4	-5	272	235	12
4	4	-4	340	329	9
4	4	-3	990	1017	10
4	4	-2	955	916	10
4	4	-1	1334	1310	9
4	4	0	1140	1136	9
4	4	1	1613	1629	9
4	4	2	1410	1425	9
4	4	3	1988	1963	10
4	4	4	1174	1163	10
4	4	5	1115	1115	11
4	4	6	718	740	13
4	4	7	1019	1005	12
4	4	8	682	683	16
4	4	9	545	542	13
4	4	10	250	264	18
4	4	11	232	242	20
4	4	12	267	277	19
4	4	13	168	202	29*
4	4	14	105	60	47*
4	4	15	0	36	55*
4	4	16	156	16	34*
4	10	3	1049	1080	15
4	10	4	570	548	12
4	10	5	986	986	16
4	10	6	849	892	17
4	10	7	929	941	17
4	10	8	645	629	15
4	10	9	662	703	16
4	10	10	603	612	14
4	10	11	302	372	21
4	10	12	282	265	22
4	10	13	0	183	82*
4	10	14	133	107	78*
4	10	15	0	9	81*
4	10	16	0	16	81*
4	10	17	0	60	81*
4	11	-18	129	38	93*
4	11	-17	0	18	92*
4	11	-16	0	55	86*
4	11	-15	96	72	65*
4	11	-14	115	173	83*
4	11	-13	197	211	34*
4	11	-12	349	361	19
4	11	-11	377	381	17
4	11	-10	622	588	15
4	11	-9	456	462	14
4	11	-8	706	702	14
4	11	-7	611	581	12
4	11	-6	759	758	19
4	11	-5	817	796	17
4	11	-4	793	801	17
4	11	-3	728	728	17
4	11	-2	702	698	13
4	11	-1	410	410	13
4	11	0	476	466	12
4	11	1	455	472	12
4	11	2	557	592	13
4	11	3	211	236	24
4	11	4	214	193	24
4	11	5	448	365	13
4	11	6	0	45	72*
4	11	7	341	366	17
4	11	8	249	227	23
4	11	9	575	544	14
4	11	10	491	515	14
4	11	11	391	405	17
4	11	12	396	455	19
4	11	13	349	353	20
4	11	14	424	419	17
4	11	15	296	301	24
4	11	16	0	252	86*
4	11	17	254	208	27
4	12	-17	42	153	92*
4	12	-16	324	275	24
4	12	-15	249	229	29
4	12	-14	307	304	23
5	0	-12	376	334	18

```
 4 12 -12  279  276 24    4 13  10  311  347 22    4 15   5   62   20 80*   4 17   8  285  249 28    5  0 -10   72   55 74*
 4 12 -11  292  280 22    4 13  11    0  196 82*   4 15   6    0   61 82*   4 17   9  179  154 91*   5  0  -8  431  424 12
 4 12 -10  112  233 80*   4 13  12  396  371 19    4 15   7    0   49 81*   4 17  10  346  365 26    5  0  -6 1192 1159 12
 4 12  -9  386  379 17    4 13  13    0  138 83*   4 15   8   74  234 85*   4 17  11  119  149 64*   5  0  -4  750  803 13
 4 12  -8   94   38 76*   4 13  14  380  383 20    4 15   9  150   43 47*   4 18 -10  110  144 63*   5  0  -2 1145 1075 10
 4 12  -7  359  389 17    4 13  15  134  154 83*   4 15  10  275  300 27    4 18  -9  161  153 88*   5  0   0 1936 1935 10
 4 12  -6  121   66 46*   4 14 -15    0    9 88*   4 15  11    0   40 88*   4 18  -8  109   31 86*   5  0   2 1965 1900 10
 4 12  -5  161  196 34*   4 14 -14  265  277 29    4 15  12  308  319 25    4 18  -7    0   88 87*   5  0   4 1770 1745 11
 4 12  -4  387  398 15    4 14 -13  130   63 84*   4 15  13    0   13 85*   4 18  -6    0   59 88*   5  0   6 1374 1426 11
 4 12  -3   23   74 60*   4 14 -12  301  283 24    4 16 -13  137   55 89*   4 18  -5    0   41 87*   5  0   8  751  796 15
 4 12  -2  765  719 19    4 14 -11   80   89 82*   4 16 -12  288  264 27    4 18  -4    0  169 87*   5  0  10  110   33 64*
 4 12  -1  383  377 15    4 14 -10  225  223 30    4 16 -11  142   50 53*   4 18  -3  222  120 32    5  0  12    0   84 67*
 4 12   0  673  715 14    4 14  -9    0   43 81*   4 16 -10  191  162 39*   4 18  -2  257  282 30    5  0  14  274  261 18
 4 12   1  826  789 18    4 14  -8    0  139 80*   4 16  -9   99  101 60*   4 18  -1  223  208 33    5  0  16  181  242 31*
 4 12   2 1049 1029 17    4 14  -7  119  141 79*   4 16  -8  136  107 84*   4 18   0  252  256 30    5  0  18  157  176 36*
 4 12   3  528  555 12    4 14  -6   24   41 66*   4 16  -7    0   99 84*   4 18   1  328  310 23    5  1 -21  153   26 57*
 4 12   4  906  869 18    4 14  -5   57   14 77*   4 16  -6    0  121 85*   4 18   2  401  366 20    5  1 -20  134   78 96*
 4 12   5  425  400 15    4 14  -4  315  297 19    4 16  -5  129   35 81*   4 18   3  430  400 19    5  1 -19    0   30 92*
 4 12   6  966 1000 16    4 14  -3  113   22 74*   4 16  -4  323  360 23    4 18   4  371  351 22    5  1 -18  258  206 34
 4 12   7  393  428 16    4 14  -2  653  678 13    4 16  -3    0   85 82*   4 18   5  374  415 23    5  1 -17   74   29 89*
 4 12   8  670  647 16    4 14  -1    0   22 75*   4 16  -2  448  470 17    4 18   6  350  343 24    5  1 -16  424  382 20
 4 12   9  146  142 77*   4 14   0  797  832 15    4 16  -1   37  134 63*   4 18   7  388  403 23    5  1 -15   88  126 85*
 4 12  10  475  478 15    4 14   1  199   83 30    4 16   0  565  604 14    4 18   8  198  261 45*   5  1 -14  745  722 17
 4 12  11  125  179 79*   4 14   2 1120 1118 18    4 16   1  330  311 21    4 18   9  411  384 22    5  1 -13  149  233 82*
 4 12  12  232  213 28    4 14   3  132   91 78*   4 16   2  631  613 15    4 19  -8    0  186 90*   5  1 -12  997  987 19
 4 12  13   86   91 62*   4 14   4  885  888 20    4 16   3  261  249 27    4 19  -7  301  358 27    5  1 -11  223  147 25
 4 12  14  144   72 82*   4 14   5    0   56 79*   4 16   4  633  622 15    4 19  -6  207  190 37*   5  1 -10 1140 1165 16
 4 12  15    0   28 82*   4 14   6  672  661 16    4 16   5   95  156 85*   4 19  -5  346  348 23    5  1  -9    0  133 70*
 4 12  16  125   32 81*   4 14   7  105   57 56*   4 16   6  550  539 15    4 19  -4  197  225 40*   5  1  -8 1164 1121 14
 4 13 -16   73   21 87*   4 14   8  485  496 16    4 16   7  167  153 86*   4 19  -3  222  275 35    5  1  -7  279  256 15
 4 13 -15    0   21 87*   4 14   9    0   17 82*   4 16   8  429  406 19    4 19  -2  170  163 44*   5  1  -6 1107 1079 12
 4 13 -14  123  141 58*   4 14  10  269  289 26    4 16   9  217  166 35    4 19  -1   37  222 88*   5  1  -5   88   41 59*
 4 13 -13    0   35 85*   4 14  11    0   61 84*   4 16  10  214  218 37*   4 19   0  146  110 87*   5  1  -4  527  545 11
 4 13 -12  326  273 21    4 14  12  151  174 83*   4 16  11    0  160 89*   4 19   1  160  225 89*   5  1  -3  327  294 10
 4 13 -11    0   80 82*   4 14  13  109   83 83*   4 16  12    0   78 86*   4 19   2   77   10 67*   5  1  -2  402  375 10
 4 13 -10  403  394 17    4 14  14  138  116 52*   4 17 -12  146  182 76*   4 19   3   55  140 89*   5  1  -1  204  218 15
 4 13  -9    0   34 78*   4 15 -14    0   78 89*   4 17 -11  119  194 90*   4 19   4  184   65 44*   5  1   0  167  148 17
 4 13  -8  639  651 14    4 15 -13  172  112 42*   4 17 -10  280  325 29    4 19   5    0   38 93*   5  1   1  105   93 55*
 4 13  -7  197  204 31    4 15 -12  257  246 29    4 17  -9  214  192 35    4 19   6  160  158 93*   5  1   2  589  582 14
 4 13  -6  866  837 19    4 15 -11    0   63 86*   4 17  -8  402  415 20    4 19   7    0  113 95*   5  1   3  156  117 20
 4 13  -5  312  297 19    4 15 -10  393  403 20    4 17  -7  309  290 24    4 20  -5    0   24 88*   5  1   4 1045 1041 12
 4 13  -4  839  883 19    4 15  -9    0   94 81*   4 17  -6  475  488 17    4 20  -4  103   41 73*   5  1   5   92   90 58*
 4 13  -3  293  305 20    4 15  -8  549  564 14    4 17  -5  349  312 21    4 20  -3   94  108 90*   5  1   6 1374 1369 11
 4 13  -2  905  897 18    4 15  -7   43   83 82*   4 17  -4  431  457 18    4 20  -2   63   92 90*   5  1   7  423  397 10
 4 13  -1  219  124 25    4 15  -6  767  810 16    4 17  -3  269  294 27    4 20  -1  206  201 39*   5  1   8 1628 1595 12
 4 13   0  824  831 19    4 15  -5  279  197 23    4 17  -2  402  371 18    4 20   0    0  108 89*   5  1   9  479  477 12
 4 13   1   12   21 63*   4 15  -4  860  865 20    4 17  -1  261  261 28    4 20   1  264  287 32    5  1  10 1047 1062 14
 4 13   2  409  419 15    4 15  -3  271  241 24    4 17   0  322  312 22    4 20   2  292  218 28    5  1  11  165  171 27
 4 13   3  230  218 24    4 15  -2  839  804 15    4 17   1   12  101 85*   4 20   3  333  362 27    5  1  12  915  952 16
 4 13   4    0   18 76*   4 15  -1  187  109 33*   4 17   2  153  196 47*   4 20   4   94  161 94*   5  1  13  240  244 21
 4 13   5  411  374 16    4 15   0  701  726 16    4 17   3  142   27 84*   5  0 -20  297  270 31    5  1  14  507  524 12
 4 13   6  154   70 78*   4 15   1  106  136 81*   4 17   4    0   82 84*   5  0 -18  371  405 24    5  1  15    0   31 71*
 4 13   7  267  270 23    4 15   2  350  339 19    4 17   5   78   70 87*   5  0 -16  462  482 19    5  1  16  331  327 17
 4 13   8  385  360 18    4 15   3   72   27 79*   4 17   6  159   62 84*   5  0 -14  463  529 17    5  1  17    0   18 75*
 5  1  18  109  127 76*   5  3  -8  893  867 15    5  4   7  474  483 12    5  6 -17  305  271 28    5  7   0  471  428 12
 5  1  19   87   94 53*   5  3  -7  786  798 15    5  4   8  221  221 20    5  6 -16  112   89 90*   5  7   1   40  144 63*
 5  2 -21   82   84 93*   5  3  -6 1282 1256 12    5  4   9  111   86 56*   5  6 -15  228  249 34    5  7   2  430  426 12
 5  2 -20  214  227 42*   5  3  -5  500  494 10    5  4  10  131  175 67*   5  6 -14  144  131 85*   5  7   3  555  557 13
 5  2 -19   95  122 65*   5  3  -4  531  516 12    5  4  11  125  106 38*   5  6 -13  120  174 82*   5  7   4  149   87 28*
 5  2 -18  237  312 36    5  3  -3  833  770 12    5  4  12   95   95 70*   5  6 -12   69   73 79*   5  7   5  687  674 12
 5  2 -17  114  142 89*   5  3  -2  486  470 11    5  4  13  101  168 75*   5  6 -11    0   30 79*   5  7   6    0   40 68*
 5  2 -16  334  344 24    5  3  -1  728  731 13    5  4  14  198  194 28    5  6 -10  249  222 23    5  7   7  906  929 17
 5  2 -15  125  130 58*   5  3   0  272  278 12    5  4  15  326  326 19    5  6  -9  418  391 14    5  7   8  140  141 71*
 5  2 -14  255  309 28    5  3   1  240  253 14    5  4  16  294  254 21    5  6  -8  268  289 20    5  7   9 1027 1030 17
 5  2 -13    0   51 81*   5  3   2  847  832 12    5  4  17  343  317 18    5  6  -7  691  694 13    5  7  10  169   87 31*
 5  2 -12  268  222 24    5  3   3  114  113 57*   5  4  18  284  307 23    5  6  -6  469  440 11    5  7  11  873  854 19
 5  2 -11  313  289 19    5  3   4  787  763 13    5  4  19  249  273 26    5  6  -5 1428 1452 12    5  7  12    0    7 75*
 5  2 -10  119   25 73*   5  3   5  452  424 11    5  5 -20  129   34 95*   5  6  -4  401  407 11    5  7  13  733  723 15
 5  2  -9  391  427 14    5  3   6  895  854 13    5  5 -19  221   72 38*   5  6  -3 1639 1623 12    5  7  14    0   78 78*
 5  2  -8  328  338 15    5  3   7  645  634 16    5  5 -18    0   50 92*   5  6  -2  478  421 11    5  7  15  428  429 17
 5  2  -7  566  568 13    5  3   8  941  950 14    5  5 -17  127  203 90*   5  6  -1 1832 1803 11    5  7  16    0   52 79*
 5  2  -6  845  862 14    5  3   9  739  752 17    5  5 -16  104  103 62*   5  6   0  337  350 12    5  7  17  311  277 21
 5  2  -5  557  531 11    5  3  10  706  677 17    5  5 -15  352  362 23    5  6   1 1565 1589 12    5  7  18    0   16 81*
 5  2  -4 1456 1490 11    5  3  11  539  538 12    5  5 -14  114  209 85*   5  6   2  551  502 12    5  8 -19  176  276 56*
 5  2  -3  643  664 13    5  3  12  818  811 17    5  5 -13  513  506 15    5  6   3 1283 1285 12    5  8 -18    0   43 96*
 5  2  -2 1785 1742 10    5  3  13  437  468 14    5  5 -12  341  316 19    5  6   4  469  464 12    5  8 -17  309  298 30
 5  2  -1  665  650 12    5  3  14  524  542 12    5  5 -11  855  862 19    5  6   5  861  915 15    5  8 -16  179   52 92*
 5  2   0 1933 1899 10    5  3  15  310  314 19    5  5 -10  507  541 13    5  6   6  290  279 16    5  8 -15  323  321 26
 5  2   1  947  947 11    5  3  16  297  322 21    5  5  -9 1109 1090 15    5  6   7  578  586 14    5  8 -14  160   83 85*
 5  2   2 1529 1543 10    5  3  17  221  215 27    5  5  -8  525  533 12    5  6   8    0    9 48*   5  8 -13  240  220 30
 5  2   3  893  885 12    5  3  18  142  163 77*   5  5  -7 1223 1240 14    5  6   9  348  360 15    5  8 -12    0  192 84*
 5  2   4 1385 1375 11    5  3  19  111  149 65*   5  5  -6  662  621 17    5  6  10  245  280 22    5  8 -11  118   46 60*
 5  2   5  762  765 14    5  4 -20  160  165 93*   5  5  -5 1244 1284 13    5  6  11  105  143 72*   5  8 -10  254  261 24
 5  2   6  974  965 13    5  4 -19  131  200 93*   5  5  -4  572  523 12    5  6  12   86  122 73*   5  8  -9  344  319 17
 5  2   7  417  406 10    5  4 -18    0  175 93*   5  5  -3  692  696 15    5  6  13  162  180 77*   5  8  -8  237  242 23
 5  2   8  615  634 12    5  4 -17    0  232 92*   5  5  -2  270  274 14    5  6  14  306  283 20    5  8  -7  591  615 12
 5  2   9   82   29 65*   5  4 -16  194  157 39*   5  5  -1  350  299 11    5  6  15  310  309 21    5  8  -6  169  184 30*
 5  2  10  282  267 16    5  4 -15  249  220 29    5  5   0    0   56 59*   5  6  16  200  154 31    5  8  -5  903  917 16
 5  2  11  246  268 19    5  4 -14  168  169 41*   5  5   1  237  235 15    5  6  17  370  354 18    5  8  -4  103   30 68*
 5  2  12    0   63 69*   5  4 -13    0  120 82*   5  5   2    0   41 59*   5  7 -19  170   78 95*   5  8  -3 1151 1172 14
 5  2  13  290  287 18    5  4 -12  180  166 34*   5  5   3  492  537 10    5  7 -18    0   47 92*   5  8  -2   85   37 67*
 5  2  14  106  218 73*   5  4 -11  150  109 39*   5  5   4  621  578 16    5  7 -17  254  230 34    5  8  -1 1267 1282 13
 5  2  15  196  226 28    5  4 -10    0   35 74*   5  5   5  648  640 16    5  7 -16    0   43 91*   5  8   0  141  136 31*
 5  2  16  327  298 17    5  4  -9  372  348 15    5  5   6  412  427 11    5  7 -15  437  384 19    5  8   1 1358 1328 13
 5  2  17    0  166 75*   5  4  -8  255  243 19    5  5   7  685  711 17    5  7 -14  121   60 65*   5  8   2  197  194 22
 5  2  18  287  278 21    5  4  -7  599  578 13    5  5   8  434  422 12    5  7 -13  671  651 14    5  8   3 1336 1393 14
 5  2  19  117  114 51*   5  4  -6  480  474 11    5  5   9  683  670 13    5  7 -12  155  106 79*   5  8   4  198  125 23
 5  3 -20  179   62 92*   5  4  -5 1341 1329 12    5  5  10  491  500 12    5  7 -11  875  878 19    5  8   5 1032 1023 15
 5  3 -19    0   13 93*   5  4  -4 1125 1155 12    5  5  11  872  839 17    5  7 -10   95  165 77*   5  8   6  251  193 20
 5  3 -18  149  144 75*   5  4  -3 1221 1223 11    5  5  12  342  384 17    5  7  -9  979  967 17    5  8   7  755  755 19
 5  3 -17  148  121 75*   5  4  -2 1214 1157 11    5  5  13  690  683 14    5  7  -8  232  238 24    5  8   8  195  166 27
 5  3 -16  239  263 33    5  4  -1 1544 1545 11    5  5  14  240  252 25    5  7  -7 1063 1037 15    5  8   9  232  238 24
 5  3 -15  339  275 22    5  4   0 1410 1378 11    5  5  15  590  568 14    5  7  -6  107   34 69*   5  8  10  265  272 21
 5  3 -14  452  429 16    5  4   1 1583 1572 11    5  5  16  156  181 79*   5  7  -5  951  937 15    5  8  11    0   50 74*
 5  3 -13  423  418 16    5  4   2 1024 1038 12    5  5  17  369  346 18    5  7  -4  114   33 66*   5  8  12  234  212 26
 5  3 -12  574  570 14    5  4   3  801  846 13    5  5  18  127   82 50*   5  7  -3  682  624 16    5  8  13  281  298 22
 5  3 -11  624  603 13    5  4   4  704  668 14    5  6 -20    0   74 94*   5  7  -2  310  290 14    5  8  14    0  143 81*
 5  3 -10  783  778 19    5  4   5 1030 1009 12    5  6 -19  262  247 35    5  7  -1    0  135 72*   5  8  15  245  271 28
 5  3  -9  784  749 18    5  4   6  466  460 10    5  6 -18  176   90 48*                              5  8  16  153   48 79*
 5  8  17  227  235 30    5 10   0  533  520 13    5 12 -12    0   24 86*   5 13  11  218  133 33    5 15   8  472  464 18
 5  9 -18  195  106 47*   5 10   1 1030 1043 16    5 12 -11  114  141 86*   5 13  12  421  469 20    5 15   9    0   14 89*
 5  9 -17  137  193 96*   5 10   2  769  800 17    5 12 -10  237  180 29    5 13  14  384  379 21    5 15  10  430  425 21
 5  9 -16  242  147 35    5 10   3  878  865 18    5 12  -9  108  114 82*   5 14 -15    0   44 94*   5 15  11  100   61 89*
 5  9 -15  409  347 22    5 10   4  758  729 14    5 12  -8  326  310 21    5 14 -13   72   52 90*   5 16 -12    0   28 95*
 5  9 -14  266  170 29    5 10   5  748  729 14    5 12  -7  129  115 48*   5 14 -12    0   77 91*   5 16 -11  144   44 90*
 5  9 -13  576  586 15    5 10   6  548  539 14    5 12  -6  582  578 15    5 14 -11   61   15 74*   5 16 -10    0   82 91*
 5  9 -12  357  315 20    5 10   7  531  481 12    5 12  -5  353  369 18    5 14 -10    0   57 90*   5 16  -9    0   55 90*
 5  9 -11  724  706 16    5 10   8  426  448 15    5 12  -4  782  777 14    5 14  -9  111   23 85*   5 16  -8  244  214 32
 5  9 -10  313  288 20    5 10   9    0   81 79*   5 12  -3  445  464 15    5 14  -8  272  204 27    5 16  -7  117   53 73*
 5  9  -9  686  676 15    5 10  10  108   86 65*   5 12  -2  921  939 17    5 14  -7    0   81 84*   5 16  -6  412  411 20
 5  9  -8  288  270 20    5 10  11    0   61 84*   5 12  -1  751  727 14    5 14  -6  543  531 14    5 16  -5  201  124 37*
 5  9  -7  659  642 14    5 10  12   24   18 78*   5 12   0  958  949 18                              5 16  -4  521  511 16
 5  9  -6  229  223 24    5 10  13  187  144 35*   5 12   1  517  510 13
```

```
 5  9  -5  448  424 13    5 10  14  158   74 82*   5 12   2  859  903 19    5 14  -5   69   85 81*   5 16  -3  152  202 87*
 5  9  -4  284  261 18    5 10  15  142  162 83*   5 12   3  313  272 20    5 14  -4  816  767 20    5 16  -2  624  620 14
 5  9  -3  275  295 19    5 10  16    0   56 84*   5 12   4  784  817 15    5 14  -3   63   47 82*   5 16  -1  343  273 22
 5  9  -2    0   34 67*   5 11 -17  184  132 50*   5 12   5  227  214 27    5 14  -2  871  889 21    5 16   0  641  622 16
 5  9  -1    0   39 69*   5 11 -16  166  203 97*   5 12   6  570  608 13    5 14  -1   86  133 80*   5 16   1  316  247 23
 5  9   0  161  173 29*   5 11 -15  242  218 35    5 12   7  155  188 78*   5 14   0  985  973 19    5 16   2  655  616 15
 5  9   1  165  158 28*   5 11 -14  358  329 24    5 12   8  283  304 24    5 14   1  176   24 36*   5 16   3  197  157 38*
 5  9   2    0   40 68*   5 11 -13  291  310 27    5 12   9    0  113 83*   5 14   2  756  753 16    5 16   4  489  493 18
 5  9   3  496  499 11    5 11 -12  488  481 16    5 12  10  167   87 40*   5 14   3  154   47 43*   5 16   5    0  140 87*
 5  9   4  322  329 17    5 11 -11  426  435 18    5 12  11  144   56 82*   5 14   4  494  489 15    5 16   6  319  348 26
 5  9   5 1046 1009 16    5 11 -10  479  497 16    5 12  12    0   69 86*   5 14   5    0    4 81*   5 16   7  231  183 34
 5  9   6  360  413 16    5 11  -9  467  435 15    5 12  13    0   55 84*   5 14   6  402  438 19    5 16   8  128  106 68*
 5  9   7 1094 1084 16    5 11  -8  534  503 13    5 12  14  158  141 86*   5 14   7    0   14 84*   5 16   9   12  196 92*
 5  9   8  316  302 19    5 11  -7  474  512 14    5 12  15    0  122 85*   5 14   8  160  165 45*   5 16  10  112   42 91*
 5  9   9 1015 1060 18    5 11  -6  499  491 13    5 13 -16  217  174 42*   5 14   9    0   69 85*   5 16  11  206  174 41*
 5  9  10  332  331 19    5 11  -5  405  423 16    5 13 -15   98   61 92*   5 14  10  120   79 86*   5 17 -11  275  163 31
 5  9  11  737  710 15    5 11  -4  413  436 15    5 13 -14  226  264 38    5 14  11   63   83 87*   5 17 -10  270  319 33
 5  9  12  137  217 80*   5 11  -3  242  181 23    5 13 -13    0   96 90*   5 14  12    0   27 87*   5 17  -9  242  225 35
 5  9  13  488  509 15    5 11  -2  221  205 25    5 13 -12  416  389 20    5 14  13    0   68 89*   5 17  -8  333  336 26
 5  9  14   76  173 58*   5 11  -1    0   70 74*   5 13 -11    0  122 88*   5 15 -14  138  218 72*   5 17  -7  207  227 40*
 5  9  15  276  284 25    5 11   0  303  317 19    5 13 -10  522  553 17    5 15 -13  129   35 93*   5 17  -6  277  310 30
 5  9  16    0   97 83*   5 11   1  495  489 13    5 13  -9  150  135 47*   5 15 -12  329  364 27    5 17  -5   75  167 88*
 5  9  17    0  143 84*   5 11   2  161  174 34*   5 13  -8  723  685 17    5 15 -11    0   31 90*   5 17  -4  295  273 26
 5 10 -18    0  151 98*   5 11   3  458  495 14    5 13  -7  151  237 81*   5 15 -10  453  448 19    5 17  -3   94  130 86*
 5 10 -17  241  250 39    5 11   4   50  214 76*   5 13  -6  659  692 14    5 15  -9  158   49 88*   5 17  -2  211  214 37*
 5 10 -16  213  167 41*   5 11   5  568  575 14    5 13  -5  116  151 56*   5 15  -8  624  629 15    5 17  -1   97   29 85*
 5 10 -15  281  298 31    5 11   6  513  548 13    5 13  -4  544  541 14    5 15  -7  162  101 88*   5 17   0   93  130 74*
 5 10 -14    0  169 90*   5 11   7  662  648 16    5 13  -3  178   99 34*   5 15  -6  578  603 15    5 17   1    0  105 88*
 5 10 -13  261  257 29    5 11   8  620  618 14    5 13  -2  407  387 16    5 15  -5   92  167 86*   5 17   2   91   70 88*
 5 10 -12  159   86 84*   5 11   9  430  464 17    5 13  -1  253  184 24    5 15  -4  458  467 17    5 17   3  144  138 56*
 5 10 -11  207  172 32    5 11  10  584  580 13    5 13   0  140  157 42*   5 15  -3   99   90 63*   5 17   4  242  223 34
 5 10 -10    0   52 78*   5 11  11  439  420 17    5 13   1  356  373 18    5 15  -2  360  370 20    5 17   5   92  147 89*
 5 10  -9    0   23 65*   5 11  12  481  432 15    5 13   2  294  271 22    5 15  -1    0   67 83*   5 17   6  412  345 21
 5 10  -8  240  216 25    5 11  13  294  317 25    5 13   3  367  354 18    5 15   0    0   51 83*   5 17   7  247  208 34
 5 10  -7  100  227 76*   5 11  14  255  265 28    5 13   4  254  286 26    5 15   1  119   51 57*   5 17   8  456  438 20
 5 10  -6  263  264 22    5 11  15    0  195 83*   5 13   5  203  242 31    5 15   2  252  187 27    5 17   9  281  243 31
 5 10  -5  482  448 13    5 11  16   68  157 87*   5 13   6  505  491 15    5 15   3    0   10 82*   5 18  -9   89   17 91*
 5 10  -4  274  231 19    5 12 -16  215  167 42*   5 13   7  275  285 25    5 15   4  283  285 26    5 18  -8    0  135 93*
 5 10  -3  438  456 13    5 12 -15  227  137 38    5 13   8  487  463 16    5 15   5  102   37 84*   5 18  -7  160  128 92*
 5 10  -2  568  586 12    5 12 -14  171  117 91*   5 13   9  186  175 38*   5 15   6  408  374 20    5 18  -6    0  232 93*
 5 10  -1  748  707 13    5 12 -13    0  119 88*   5 13  10  488  489 16    5 15   7    0    1 87*   5 18  -5  140  175 76*
 5 18  -4  216  302 40*   6  1  -9  114  111 51*   6  2   7   89  198 69*   6  4 -15   89   12 91*   6  5   2  523  508 12
 5 18  -3  258  235 31    6  1  -8  563  555 13    6  2   8  202  167 23    6  4 -14    0   37 89*   6  5   3  672  662 12
 5 18  -2  338  309 24    6  1  -7    0   32 72*   6  2   9  410  382 13    6  4 -13   89  151 86*   6  5   4  372  367 13
 5 18  -1  152  259 91*   6  1  -6  411  312 13    6  2  10  335  305 16    6  4 -12  183  178 39*   6  5   5  893  866 16
 5 18   0  405  398 21    6  1  -5    0  164 68*   6  2  11  262  258 20    6  4 -11  357  330 20    6  5   6  471  475 12
 5 18   1  289  369 30    6  1  -4  164   83 25    6  2  12  511  486 12    6  4 -10  395  435 18    6  5   7  754  766 18
 5 18   2  398  372 22    6  1  -3   96   29 41*   6  2  13  278  279 20    6  4  -9  593  604 14    6  5   8  470  456 13
 5 18   3  377  360 23    6  1  -2  392  434 11    6  2  14  485  486 14    6  4  -8  718  683 14    6  5   9  855  852 18
 5 18   4  349  333 25    6  1  -1  171   85 23    6  2  15  179  188 33*   6  4  -7 1013 1003 16    6  5  10  307  295 18
 5 18   5  330  347 27    6  1   0 1048 1065 13    6  2  16  400  388 16    6  4  -6 1141 1159 15    6  5  11  614  628 13
 5 18   6  154  220 98*   6  1   1  250  245 17    6  2  17    0  141 77*   6  4  -5 1113 1094 15    6  5  12  200  200 30
 5 18   7  314  299 30    6  1   2 1401 1396 12    6  2  18  274  291 23    6  4  -4 1115 1107 14    6  5  13  452  456 15
 5 19  -6    0  151 92*   6  1   3  271  274 16    6  3 -20  116  152 98*   6  4  -3 1221 1225 13    6  5  14  131   90 67*
 5 19  -5   76  143 93*   6  1   4 1655 1632 12    6  3 -19  141   86 82*   6  4  -2 1121 1104 14    6  5  15  256  204 24
 5 19  -4    0   96 90*   6  1   5  438  439 12    6  3 -18   65  231 99*   6  4  -1 1109 1152 14    6  5  16    0   19 80*
 5 19  -3  135  109 60*   6  1   6 1622 1643 13    6  3 -17  183  185 48*   6  4   0  744  760 16    6  5  17  113   36 68*
 5 19  -2  118   12 76*   6  1   7  409  432 13    6  3 -16  349  322 26    6  4   1  585  566 13    6  6 -19  148  118 82*
 5 19  -1    0   65 91*   6  1   8 1166 1148 15    6  3 -15  282  295 31    6  4   2  506  498 11    6  6 -18   11   25 83*
 5 19   0    0   52 91*   6  1   9  137  103 69*   6  3 -14  467  509 18    6  4   3  627  651 12    6  6 -17  181   74 98*
 5 19   1  183    4 92*   6  1  10  767  757 18    6  3 -13  364  340 21    6  4   4  281  242 15    6  6 -16    0   38 93*
 5 19   2    0  154 93*   6  1  11  177  192 24    6  3 -12  593  571 14    6  4   5  218  217 21    6  6 -15  136   72 93*
 5 19   3  139  111 71*   6  1  12  410  429 14    6  3 -11  497  494 15    6  4   6   49   85 67*   6  6 -14  122   38 92*
 5 19   4   84  199 80*   6  1  13  103   20 50*   6  3 -10  592  612 13    6  4   7  160  167 31*   6  6 -13  210  144 36*
 5 19   5  259  249 35    6  1  14   92  209 75*   6  3  -9  570  572 12    6  4   8   74  115 59*   6  6 -12  137  157 86*
 6  0 -20  240  226 42*   6  1  15  137   35 39*   6  3  -8  645  648 15    6  4   9  134  252 73*   6  6 -11  386  360 19
 6  0 -18    0  222 99*   6  1  16   87   21 73*   6  3  -7  440  432 13    6  4  10  345  294 16    6  6 -10    0  158 83*
 6  0 -16    0  178 97*   6  1  17  146   92 39*   6  3  -6  237  160 22    6  4  11  442  429 14    6  6  -9  630  615 14
 6  0 -14  182   39 44*   6  1  18   64   37 65*   6  3  -5  442  403 12    6  4  12  369  377 17    6  6  -8  269  227 23
 6  0 -12  207  163 35*   6  2 -20    0  161 99*   6  3  -4  261  222 18    6  4  13  510  473 13    6  6  -7 1049 1063 17
 6  0 -10  439  416 16    6  2 -19  134   46 69*   6  3  -3  387  355 12    6  4  14  397  405 16    6  6  -6  273  217 21
 6  0  -8  857  876 18    6  2 -18    0  162 98*   6  3  -2  729  704 15    6  4  15  441  426 16    6  6  -5 1353 1320 14
 6  0  -6  795  829 17    6  2 -17    0   25 96*   6  3  -1  160   95 25    6  4  16  379  372 18    6  6  -4  342  308 16
 6  0  -4 1072 1118 14    6  2 -16  164  105 92*   6  3   0 1147 1192 13    6  4  17  354  352 19    6  6  -3 1368 1360 14
 6  0  -2 1627 1540 12    6  2 -15   87   94 90*   6  3   1  515  495 11    6  4  18  214  235 31    6  6  -2  247  239 20
 6  0   0 1709 1693 12    6  2 -14  116   15 88*   6  3   2  968  955 14    6  5 -19    0  143 99*   6  6  -1 1338 1343 14
 6  0   2 1226 1240 13    6  2 -13  116  238 88*   6  3   3  586  574 13    6  5 -18   86  111 97*   6  6   0  280  274 17
 6  0   4  823  782 14    6  2 -12  273  212 25    6  3   4 1026 1045 14    6  5 -17  241  244 38    6  6   1 1028 1033 15
 6  0   6  205  168 21    6  2 -11  389  376 18    6  3   5  777  752 16    6  5 -16   85  139 94*   6  6   2   52  233 70*
 6  0   8  583  537 14    6  2 -10  502  482 14    6  3   6 1001  987 15    6  5 -15  379  337 23    6  6   3  585  596 14
 6  0  10  237  225 21    6  2  -9  500  518 14    6  3   7  708  744 17    6  5 -14  225  273 36    6  6   4    0   41 68*
 6  0  12  595  575 12    6  2  -8  821  810 18    6  3   8  757  786 18    6  5 -13  495  534 18    6  6   5  329  325 16
 6  0  14  373  361 16    6  2  -7  476  487 12    6  3   9  455  455 12    6  5 -12  332  348 23    6  6   6  242  225 21
 6  0  16  301  303 19    6  2  -6 1247 1277 14    6  3  10  857  858 17    6  5 -11  719  741 17    6  6   7   30   24 71*
 6  0  18  312  332 20    6  2  -5  744  662 16    6  3  11  447  453 14    6  5 -10  414  403 17    6  6   8  432  431 14
 6  1 -20  137  232 71*   6  2  -4 1355 1388 13    6  3  12  499  511 13    6  5  -9  826  810 20    6  6   9  255  229 22
 6  1 -19  189   26 98*   6  2  -3  849  869 14    6  3  13  210  273 28    6  5  -8  440  465 15    6  6  10  307  300 19
 6  1 -18  366  366 28    6  2  -2 1532 1488 12    6  3  14  237  239 25    6  5  -7  847  865 18    6  6  11  476  434 14
 6  1 -17    0   70 97*   6  2  -1  961  934 13    6  3  15  143  147 76*   6  5  -6  306  296 19    6  6  12  285  261 22
 6  1 -16  502  533 19    6  2   0 1235 1210 12    6  3  16  120   23 78*   6  5  -5  434  385 13    6  6  13  579  551 13
 6  1 -15  238  158 34    6  2   1  781  785 15    6  3  17  188  129 32*   6  5  -4   88    2 71*   6  6  14  117  122 81*
 6  1 -14  678  694 16    6  2   2  854  828 14    6  3  18    0   95 80*   6  5  -3  141  124 33*   6  6  15  541  521 14
 6  1 -13   50   82 85*   6  2   3  566  528 12    6  4 -19  143   79 98*   6  5  -2   47  117 69*   6  6  16  203  121 33
 6  1 -12  732  732 17    6  2   4  582  561 13    6  4 -18  145   68 97*   6  5  -1  335  319 14    6  6  17  393  390 18
 6  1 -11    0   62 83*   6  2   5  213  184 20    6  4 -17    0   62 72*   6  5   0  199  199 23    6  7 -19    0  199 99*
 6  1 -10  681  712 16    6  2   6  259  257 18    6  4 -16   56   43 78*   6  5   1  563  560 13    6  7 -18  167   13 98*
 6  7 -17  315  281 31    6  8   2   70   87 72*   6 10 -12  180  179 92*   6 11  11  284  295 27    6 13   5  320  288 23
 6  7 -16    0   10 97*   6  8   3  735  738 13    6 10 -11  130  147 88*   6 11  12  235  223 33    6 13   6  576  568 15
 6  7 -15  454  440 21    6  8   4  179  185 30*   6 10 -10  251  263 31    6 11  13  154  131 47*   6 13   7  119  160 66*
 6  7 -14  128    5 91*   6  8   5  292  294 19    6 10  -9  377  327 20    6 11  14  206  133 36*   6 13   8  533  538 17
 6  7 -13  544  573 17    6  8   6  153  175 37*   6 10  -8  358  347 20    6 12 -16  111    9 99*   6 13   9    0  140 89*
 6  7 -12  191   20 38*   6  8   7    0   78 75*   6 10  -7  554  593 14    6 12 -15  124   79 99*   6 13  10  453  465 20
 6  7 -11  604  605 14    6  8   8  249  260 24    6 10  -6  386  399 18    6 12 -14  114   78 98*   6 13  11    0  105 75*
 6  7 -10    0   45 81*   6  8   9  421  383 16    6 10  -5  684  665 16    6 12 -13  147   57 62*   6 13  12  350  379 25
 6  7  -9  645  626 14    6  8  10  127  138 67*   6 10  -4  509  528 16    6 12 -11  153   24 54*   6 13  13   44   19 89*
 6  7  -8    0   73 79*   6  8  11  489  485 15    6 10  -3  667  694 16    6 12 -10  342  366 25    6 14 -14  160   46 83*
 6  7  -7  525  545 13    6  8  12   78   52 81*   6 10  -2  525  542 13    6 12  -9  162  164 89*   6 14 -13   73    7 84*
 6  7  -6  261  240 23    6  8  13  464  423 16    6 10  -1 1023  972 17    6 12  -8  495  484 17    6 14 -12   63  162 97*
 6  7  -5  319  304 18    6  8  14    0   12 82*   6 10   0  812  833 20    6 12  -7  349  358 22    6 14 -11    0   33 96*
 6  7  -4  460  463 13    6  8  15  335  331 22    6 10   1  650  635 16    6 12  -6  660  644 15    6 14 -10  369  344 25
 6  7  -3    0   37 73*   6  8  16   84   44 58*   6 10   2  533  529 13    6 12  -5  440  440 17    6 14  -9   76   47 92*
 6  7  -2  554  544 12    6  9 -17  331  283 31    6 10   3  530  561 13    6 12  -4  759  778 17    6 14  -8  569  574 17
 6  7  -1  481  449 12    6  9 -16  470  420 21    6 10   4  304  317 20    6 12  -3  435  416 18    6 14  -7    0   19 92*
 6  7   0  438  451 13    6  9 -15  306  242 30    6 10   5  179  156 34*   6 12  -2  812  818 15    6 14  -6  774  753 18
 6  7   1  905  919 16    6  9 -14  164  507 23    6 10   6  121  226 80*   6 12  -1  389  432 19    6 14  -5  125   32 87*
 6  7   2  135   79 70*   6  9 -13  172  251 92*   6 10   7    0  127 81*   6 12   0  724  716 13    6 14  -4  788  769 17
 6  7   3 1067 1070 15    6  9 -12  476  476 18    6 10   8  132   87 68*   6 12   1  115  105 82*   6 14  -3  105   75 72*
 6  7   4    0   67 71*   6  9 -11  250  193 28    6 10   9  159  176 42*   6 12   2  526  521 14    6 14  -2  790  799 17
 6  7   5 1107 1121 16    6  9 -10  436  425 17    6 10  10  177  114 38*   6 12   3    0   85 79*   6 14  -1    0   55 83*
 6  7   6  136   11 37*   6  9  -9  146  109 44*   6 10  11  295  271 24    6 12   4  346  360 20    6 14   0  510  518 16
 6  7   7 1076 1063 15    6  9  -8  325  314 20    6 10  12    0  157 86*   6 12   5    0  130 81*   6 14   1    0   58 41*
 6  7   8    0  113 74*                            6 10  13  274  273 27    6 12   6    0   47 82*   6 14   2  296  325 25
 6  7   9  868  877 19                             6 10  14  154  126 85*                            6 14   3   84   22 84*
```

h	k	l	Fo	Fc	σ	h	k	l	Fo	Fc	σ	h	k	l	Fo	Fc	σ	h	k	l	Fo	Fc	σ	h	k	l	Fo	Fc	σ
6	7	10	102	155	78*	6	9	-6	0	39	77*	6	10	15	271	249	28	6	12	7	0	26	84*	6	14	4	307	290	25
6	7	11	666	679	14	6	9	-5	74	127	77*	6	11	-16	135	246	73*	6	12	8	0	128	84*	6	14	5	0	35	85*
6	7	12	120	159	53*	6	9	-4	250	146	23	6	11	-15	268	251	37	6	12	9	166	66	85*	6	14	6	62	26	73*
6	7	13	318	308	21	6	9	-3	111	105	52*	6	11	-14	323	310	30	6	12	10	251	243	32	6	14	7	38	95	88*
6	7	14	18	111	81*	6	9	-2	253	225	22	6	11	-13	352	339	26	6	12	11	0	132	89*	6	14	8	60	83	89*
6	7	15	120	163	69*	6	9	-1	479	463	14	6	11	-12	277	325	32	6	12	12	278	289	30	6	14	9	0	104	92*
6	7	16	0	16	84*	6	9	0	248	193	23	6	11	-11	382	390	23	6	12	13	56	233	92*	6	14	10	174	221	49*
6	7	17	32	44	82*	6	9	1	830	872	19	6	11	-10	250	219	32	6	12	14	337	289	24	6	14	11	116	100	91*
6	8	-18	0	19	99*	6	9	2	417	470	15	6	11	-9	351	355	22	6	13	-15	213	114	46*	6	14	12	265	317	34
6	8	-17	138	101	99*	6	9	3	1129	1144	17	6	11	-8	73	236	86*	6	13	-14	274	278	36	6	15	-12	319	323	32
6	8	-16	0	37	98*	6	9	4	541	531	12	6	11	-7	261	235	27	6	13	-13	129	119	98*	6	15	-11	0	44	97*
6	8	-15	0	45	95*	6	9	5	1224	1201	17	6	11	-6	134	166	69*	6	13	-12	369	384	26	6	15	-10	396	405	25
6	8	-14	0	56	71*	6	9	6	393	396	17	6	11	-5	0	14	61*	6	13	-11	124	140	93*	6	15	-9	103	42	95*
6	8	-13	215	162	38*	6	9	7	1159	1153	17	6	11	-4	0	26	80*	6	13	-10	438	416	21	6	15	-8	309	351	30
6	8	-12	106	57	88*	6	9	8	432	412	16	6	11	-3	184	198	35*	6	13	-9	80	155	90*	6	15	-7	0	42	93*
6	8	-11	338	362	23	6	9	9	636	614	14	6	11	-2	106	117	60*	6	13	-8	462	457	19	6	15	-6	208	208	41*
6	8	-10	127	23	81*	6	9	10	283	252	23	6	11	-1	611	602	14	6	13	-7	127	61	67*	6	15	-5	171	10	88*
6	8	-9	539	533	14	6	9	11	449	427	16	6	11	0	435	409	16	6	13	-6	246	239	32	6	15	-4	53	59	62*
6	8	-8	194	135	32	6	9	12	135	209	82*	6	11	1	583	626	15	6	13	-5	0	82	85*	6	15	-3	139	36	86*
6	8	-7	768	773	14	6	9	13	30	205	84*	6	11	2	498	534	14	6	13	-4	56	54	83*	6	15	-2	92	145	89*
6	8	-6	250	243	24	6	9	14	0	125	84*	6	11	3	706	643	15	6	13	-3	208	190	34	6	15	-1	135	120	73*
6	8	-5	1055	1079	17	6	9	15	126	99	84*	6	11	4	750	771	16	6	13	-2	42	78	83*	6	15	0	258	303	30
6	8	-4	216	184	26	6	9	16	0	79	86*	6	11	5	683	680	17	6	13	-1	365	379	20	6	15	1	0	34	90*
6	8	-3	1150	1167	16	6	10	-17	114	122	99*	6	11	6	658	644	14	6	13	0	442	431	17	6	15	2	398	388	20
6	8	-2	121	42	72*	6	10	-16	72	44	98*	6	11	7	471	503	16	6	13	1	299	310	24	6	15	3	0	7	87*
6	8	-1	1232	1230	15	6	10	-15	0	77	99*	6	11	8	575	574	15	6	13	2	478	477	16	6	15	4	417	423	21
6	8	0	95	38	71*	6	10	-14	0	49	94*	6	11	9	422	437	19	6	13	3	162	220	82*	6	15	5	0	16	88*
6	8	1	1148	1138	16	6	10	-13	120	16	78*	6	11	10	400	379	15	6	13	4	556	557	15	6	15	6	537	518	17
6	15	7	0	42	90*	6	19	-1	191	114	47*	7	2	-19	191	44	55*	7	3	-2	921	965	17	7	5	-18	0	102	99*
6	15	8	391	440	24	7	0	-18	177	40	61*	7	2	-18	108	20	99*	7	3	-1	594	613	15	7	5	-17	192	225	99*
6	15	9	127	122	93*	7	0	-16	0	118	99*	7	2	-17	75	131	77*	7	3	0	907	967	17	7	5	-16	133	158	99*
6	15	10	368	379	26	7	0	-14	266	234	35	7	2	-16	0	84	98*	7	3	1	629	616	14	7	5	-15	296	321	34
6	16	-11	133	23	81*	7	0	-12	343	386	25	7	2	-15	125	223	99*	7	3	2	1090	1033	15	7	5	-14	0	180	99*
6	16	-10	273	253	35	7	0	-10	603	644	15	7	2	-14	112	243	96*	7	3	3	705	725	14	7	5	-13	341	353	28
6	16	-9	0	95	97*	7	0	-8	867	839	20	7	2	-13	317	295	28	7	3	4	922	941	17	7	5	-12	67	156	91*
6	16	-8	335	393	29	7	0	-6	976	959	18	7	2	-12	395	430	22	7	3	5	571	586	13	7	5	-11	318	306	26
6	16	-7	239	177	37	7	0	-4	1057	1049	17	7	2	-11	415	382	19	7	3	6	851	838	18	7	5	-10	192	166	41*
6	16	-6	448	483	21	7	0	-2	1077	1027	16	7	2	-10	591	616	15	7	3	7	257	283	22	7	5	-9	0	180	87*
6	16	-5	214	201	39*	7	0	0	675	630	14	7	2	-9	362	370	20	7	3	8	749	760	14	7	5	-8	87	80	60*
6	16	-4	536	530	17	7	0	2	106	144	72*	7	2	-8	866	879	15	7	3	9	355	323	17	7	5	-7	282	298	25
6	16	-3	310	231	26	7	0	4	259	307	21	7	2	-7	340	341	19	7	3	10	356	365	18	7	5	-6	165	157	39*
6	16	-2	526	542	18	7	0	6	772	754	19	7	2	-6	810	814	20	7	3	11	0	161	78*	7	5	-5	448	458	15
6	16	-1	248	187	33	7	0	8	450	483	14	7	2	-5	644	588	15	7	3	12	0	105	78*	7	5	-4	226	166	26
6	16	0	485	474	18	7	0	10	723	708	15	7	2	-4	913	917	17	7	3	13	0	29	80*	7	5	-3	648	708	16
6	16	1	0	144	91*	7	0	12	491	471	13	7	2	-3	555	616	13	7	3	14	167	131	37*	7	5	-2	0	222	76*
6	16	2	331	327	25	7	0	14	454	470	15	7	2	-2	714	662	14	7	3	15	149	21	80*	7	5	-1	672	679	15
6	16	3	108	135	91*	7	0	16	359	371	19	7	2	-1	452	432	13	7	3	16	257	245	26	7	5	0	363	346	16
6	16	4	0	179	94*	7	1	-19	43	50	79*	7	2	0	366	349	15	7	4	-19	160	37	99*	7	5	1	612	601	12
6	16	5	203	172	42*	7	1	-18	220	325	51*	7	2	1	133	116	71*	7	4	-18	0	12	87*	7	5	2	308	295	18
6	16	6	91	29	92*	7	1	-17	149	86	99*	7	2	2	289	213	18	7	4	-17	190	111	53*	7	5	3	778	777	19
6	16	7	0	181	96*	7	1	-16	370	383	28	7	2	3	204	154	26	7	4	-16	0	59	99*	7	5	4	401	405	15
6	16	8	154	203	80*	7	1	-15	142	53	96*	7	2	4	0	90	72*	7	4	-15	259	230	37	7	5	5	736	746	15
6	16	9	0	151	96*	7	1	-14	392	394	24	7	2	5	436	429	14	7	4	-14	137	202	82*	7	5	6	359	352	17
6	17	-9	0	119	97*	7	1	-13	153	20	92*	7	2	6	493	485	13	7	4	-13	397	432	24	7	5	7	713	703	15
6	17	-8	0	186	98*	7	1	-12	356	335	24	7	2	7	495	500	12	7	4	-12	422	396	20	7	5	8	216	188	28
6	17	-7	0	55	96*	7	1	-11	127	16	86*	7	2	8	504	484	13	7	4	-11	624	618	15	7	5	9	510	485	14
6	17	-6	149	148	92*	7	1	-10	245	170	30	7	2	9	248	243	23	7	4	-10	507	502	16	7	5	10	0	88	79*
6	17	-5	0	13	94*	7	1	-9	147	12	83*	7	2	10	704	683	15	7	4	-9	817	827	16	7	5	11	265	247	25
6	17	-4	136	74	62*	7	1	-8	163	122	40*	7	2	11	333	346	19	7	4	-8	695	745	14	7	5	12	122	67	68*
6	17	-3	97	119	94*	7	1	-7	148	124	41*	7	2	12	599	591	14	7	4	-7	842	837	21	7	5	13	0	8	85*
6	17	-2	51	31	92*	7	1	-6	311	364	20	7	2	13	249	228	25	7	4	-6	597	589	14	7	5	14	145	63	81*
6	17	-1	182	190	48*	7	1	-5	0	36	77*	7	2	14	451	470	16	7	4	-5	792	762	14	7	5	15	0	102	84*
6	17	0	171	219	50*	7	1	-4	825	801	19	7	2	15	74	171	82*	7	4	-4	570	587	14	7	5	16	128	107	82*
6	17	1	272	246	32	7	1	-3	0	74	73*	7	2	16	351	317	19	7	4	-3	561	551	13	7	6	-18	0	14	99*
6	17	2	316	355	29	7	1	-2	1270	1311	15	7	2	17	230	208	25	7	4	-2	421	384	14	7	6	-17	0	72	99*
6	17	3	244	212	37	7	1	-1	278	277	19	7	3	-19	199	131	99*	7	4	-1	101	170	75*	7	6	-16	0	69	37
6	17	4	387	408	25	7	1	0	1454	1455	14	7	3	-18	260	217	41	7	4	0	240	288	22	7	6	-15	196	226	99*
6	17	5	265	260	34	7	1	1	332	313	16	7	3	-17	157	184	99*	7	4	1	158	82	33*	7	6	-14	40	127	98*
6	17	6	408	417	24	7	1	2	1549	1525	14	7	3	-16	358	311	29	7	4	2	131	33	70*	7	6	-13	493	481	20
6	17	7	338	330	28	7	1	3	350	343	16	7	3	-15	91	186	99*	7	4	3	161	148	32*	7	6	-12	0	184	93*
6	18	-7	137	188	81*	7	1	4	1445	1437	14	7	3	-14	321	370	30	7	4	4	0	72	74*	7	6	-11	694	676	16
6	18	-6	275	255	33	7	1	5	317	269	18	7	3	-13	185	183	93*	7	4	5	445	423	14	7	6	-10	224	185	35
6	18	-5	257	209	35	7	1	6	1105	1073	16	7	3	-12	285	274	30	7	4	6	261	192	21	7	6	-9	920	923	22
6	18	-4	316	291	28	7	1	7	0	37	74*	7	3	-11	230	210	33	7	4	7	577	576	14	7	6	-8	277	206	26
6	18	-3	256	262	35	7	1	8	531	523	12	7	3	-10	186	184	41*	7	4	8	488	454	13	7	6	-7	1006	1024	20
6	18	-2	341	336	27	7	1	9	124	52	43*	7	3	-9	159	110	84*	7	4	9	740	730	15	7	6	-6	275	250	24
6	18	-1	314	288	29	7	1	10	400	413	15	7	3	-8	107	95	62*	7	4	10	553	580	13	7	6	-5	830	801	20
6	18	0	328	297	28	7	1	11	0	15	76*	7	3	-7	112	22	57*	7	4	11	631	614	14	7	6	-4	232	152	27
6	18	1	270	299	34	7	1	12	0	58	76*	7	3	-6	420	460	16	7	4	12	541	530	14	7	6	-3	689	651	15
6	18	2	242	226	38	7	1	13	83	57	77*	7	3	-5	104	89	78*	7	4	13	539	542	15	7	6	-2	160	89	37*
6	18	3	161	252	83*	7	1	14	147	64	75*	7	3	-4	644	652	15	7	4	14	399	393	18	7	6	-1	393	376	16
6	18	4	0	79	81*	7	1	15	0	50	79*	7	3	-3	274	274	21	7	4	15	355	386	21	7	6	0	102	17	76*
6	18	5	64	178	98*	7	1	16	112	129	57*	7	9	11	101	59	85*	7	4	16	158	220	83*	7	6	1	65	48	74*
7	6	2	242	252	24	7	8	-11	497	488	19	7	9	12	0	90	73*	7	11	5	526	507	16	7	13	6	514	471	18
7	6	3	123	102	75*	7	8	-10	98	35	69*	7	9	13	0	10	87*	7	11	6	439	500	19	7	13	7	191	134	44*
7	6	4	288	279	20	7	8	-9	618	609	15	7	9	14	0	44	89*	7	11	7	348	364	23	7	13	8	380	424	25
7	6	5	382	386	16	7	8	-8	83	116	66*	7	10	-16	0	72	99*	7	11	8	326	327	24	7	13	9	155	81	55*
7	6	6	534	505	13	7	8	-7	732	753	18	7	10	-15	154	84	69*	7	11	9	268	224	29	7	13	10	318	290	28
7	6	7	594	560	14	7	8	-6	150	129	47*	7	10	-14	0	151	99*	7	11	10	174	186	46*	7	13	11	98	12	93*
7	6	8	415	397	16	7	8	-5	841	801	21	7	10	-13	68	183	99*	7	11	11	150	43	52*	7	14	-12	282	326	41
7	6	9	722	693	16	7	8	-4	147	74	81*	7	10	-12	0	188	99*	7	11	12	220	125	36	7	14	-11	128	30	99*
7	6	10	304	290	22	7	8	-3	699	692	17	7	10	-11	293	271	33	7	11	13	0	94	90*	7	14	-10	471	496	25
7	6	11	710	746	18	7	8	-2	257	143	24	7	10	-10	141	230	94*	7	12	-14	0	215	99*	7	14	-9	180	44	99*
7	6	12	0	117	83*	7	8	-1	614	573	14	7	10	-9	489	441	18	7	12	-13	153	60	99*	7	14	-8	558	560	20
7	6	13	642	641	16	7	8	0	248	248	25	7	10	-8	349	309	24	7	12	-12	306	335	35	7	14	-7	62	22	97*
7	6	14	0	145	86*	7	8	1	188	155	33*	7	10	-7	507	503	18	7	12	-11	180	140	99*	7	14	-6	564	543	18
7	6	15	439	437	18	7	8	2	334	336	20	7	10	-6	440	428	18	7	12	-10	422	421	25	7	14	-5	0	46	93*
7	6	16	150	117	85*	7	8	3	156	159	39*	7	10	-5	538	535	16	7	12	-9	274	275	35	7	14	-4	523	496	18
7	7	-18	169	7	86*	7	8	4	281	230	22	7	10	-4	450	399	17	7	12	-8	502	517	20	7	14	-3	116	10	92*
7	7	-17	0	276	99*	7	8	5	413	401	16	7	10	-3	594	566	14	7	12	-7	0	249	96*	7	14	-2	285	286	30
7	7	-16	0	15	99*	7	8	6	253	264	26	7	10	-2	654	659	15	7	12	-6	633	586	15	7	14	-1	171	23	47*
7	7	-15	406	347	25	7	8	7	648	620	14	7	10	-1	372	380	20	7	12	-5	500	186	27	7	14	0	98	121	90*
7	7	-14	0	37	99*	7	8	8	0	11	81*	7	10	0	369	360	20	7	12	-4	556	552	17	7	14	1	146	66	88*
7	7	-13	347	311	27	7	8	9	582	539	14	7	10	1	166	264	85*	7	12	-3	206	191	38*	7	14	2	0	82	90*
7	7	-12	154	10	56*	7	8	10	51	13	83*	7	10	2	149	151	83*	7	12	-2	489	501	18	7	14	3	91	54	76*
7	7	-11	235	196	36	7	8	11	523	535	16	7	10	3	140	104	82*	7	12	-1	73	29	88*	7	14	4	126	109	91*
7	7	-10	15	14	88*	7	8	12	123	123	64*	7	10	4	136	31	69*	7	12	0	302	208	25	7	14	5	0	106	92*
7	7	-9	171	41	88*	7	8	13	371	379	22	7	10	5	289	305	25	7	12	1	137	3	72*	7	14	6	180	259	96*
7	7	-8	167	65	86*	7	8	14	190	53	39*	7	10	6	77	178	84*	7	12	2	137	98	53*	7	14	7	25	78	93*
7	7	-7	299	286	25	7	9	-17	272	265	42	7	10	7	365	354	21	7	12	3	143	61	72*	7	14	8	401	401	24
7	7	-6	159	129	44*	7	9	-16	0	130	99*	7	10	8	149	205	85*	7	12	4	124	150	61*	7	14	9	138	84	96*
7	7	-5	577	589	13	7	9	-15	273	290	39	7	10	9	380	357	21	7	12	5	0	99	07*	7	14	10	431	462	24
7	7	-4	122	112	53*	7	9	-14	0	126	99*	7	10	11	370	349	22	7	12	6	330	269	24	7	15	-11	140	10	99*
7	7	-3	803	821	20	7	9	-13	122	244	84*	7	10	12	181	193	44*	7	12	7	204	139	38*	7	15	-10	0	143	99*
7	7	-2	61	113	79*	7	9	-12	32	93	98*	7	10	14	0	176	90*	7	12	8	385	372	22	7	15	-9	0	13	99*
7	7	-1	1156	1132	17	7	9	-11	53	163	80*	7	11	-15	212	206	53*	7	12	9	236	221	36	7	15	-8	0	14	99*
7	7	0	128	55	64*	7	9	-10	0	41	92*	7	11	-14	132	168	99*	7	12	10	396	377	22	7	15	-7	85	26	99*
7	7	1	1211	1262	17	7	9	-9	85	66	90*	7	11	-13	215	214	47*	7	12	11	314	283	28	7	15	-6	88	98	96*
7	7	2	198	100	30	7	9	-8	80	43	73*	7	11	-12	0	104	84*	7	13	-13	168	89	65*	7	15	-5	209	35	43*
7	7	3	1047	1081	18	7	9	-7	129	89	66*	7	11	-11	0	150	99*	7	13	-12	172	203	64*	7	15	-4	0	218	99*
7	7	4	110	87	64*	7	9	-6	116	60	85*							7	13	-11	144	72	99*	7	15	-3	54	64	93*
7	7	5	953	934	19	7	9	-5	337	353	22							7	13	-10	147	182	99*	7	15	-2	279	300	32
7	7	6	219	195	27																			7	15	-1	0	33	95*

```
h  k   l   Fo   Fc   q       h  k   l   Fo   Fc   q       h  k   l   Fo   Fc   q       h  k   l   Fo   Fc   q       h  k   l   Fo   Fc   q       h  k   l   Fo   Fc   q
7  7   7   721  750  16      7  9  -4    0  172  84*     7 11 -10   76   62  98*     7 13  -9  121   53  75*     7 15   0  369  366  24      8 12  -1   99   16  86*
7  7   8   198  257  33      7  9  -3  572  550  14      7 11  -9  102   13  92*     7 13  -8   86    5  97*     7 15   1    0   17  93*     9  1  -6  882  909  18
7  7   9   535  542  14      7  9  -2  237  148  28      7 11  -8  168   14  91*     7 13  -7    0  149  97*     7 15   2  365  372  26      9  1  -5  255  223  33
7  7  10    41  118  81*     7  9  -1  943  967  20      7 11  -7  183  188  46*     7 13  -6  185  181  48*     7 15   3  108   74  78*     9  1  -4  913  934  17
7  7  11   234  189  28      7  9   0  410  472  17      7 11  -6    0  104  91*     7 13  -5  252  209  34      7 15   4  483  478  21      9  1  -3  286  222  28
7  7  12   111   91  81*     7  9   1 1030 1004  19      7 11  -5  292  311  28      7 13  -4  322  304  27      7 15   5   35   81  92*     9  1  -2  673  713  16
7  7  13   138   42  81*     7  9   2  434  469  16      7 11  -4  280  324  28      7 13  -3  350  360  24      7 15   6  366  363  27      9  1  -1    0  166  88*
7  7  14     0   24  88*     7  9   3  945  971  20      7 11  -3  578  567  15      7 13  -2  474  499  19      7 15   7  184  166  97*     9  1   0  555  552  16
7  7  15    69   97  72*     7  9   4  432  463  17      7 11  -2  490  490  17      7 13  -1  354  267  23      7 15   8  274  282  37      9  1   1    0  128  89*
7  8 -17     0   67  99*     7  9   5  916  903  21      7 11  -1  612  627  14      7 13   0  512  512  17      7 16  -9  149  145  86*     9  1   2  352  277  22
7  8 -16     0   30  86*     7  9   6  363  406  20      7 11   0  699  699  15      7 13   1  268  225  30      7 16  -8  353  350  31      9  1   3  155   26  86*
7  8 -15   154  213  99*     7  9   7  378  405  19      7 11   1  583  580  14      7 13   2  515  536  17      7 16  -7  171  152  99*     9  1   4   64   84  86*
7  8 -14   108   15  97*     7  9   8  241  224  29      7 11   2  778  754  16      7 13   3  254  251  32      7 16  -6  370  378  28      9  1   5    0   14  88*
7  8 -13   361  371  27      7  9   9  232  257  32      7 11   3  612  626  14      7 13   4  579  592  16      7 16  -5  100  146  98*     9  1   6   49   69  88*
7  8 -12     0   20  95*     7  9  10    0  175  85*     7 11   4  634  624  14      7 13   5   83  211  91*     7 16  -4  354  346  27      9  1   7  103   99  61*
7 16  -3    25  113  96*     8  1  -3  370  314  19      8  3 -16  114  163  81*     8  4   6  651  653  14      8  6  -4  168  182  44*     9  1   8  366  394  23
7 16  -2   287  301  33      8  1  -2 1283 1361  18      8  3 -15   32   60  99*     8  4   7  866  847  21      8  6  -3  260  234  28      9  1   9    0   48  90*
7 16  -1   132  102  95*     8  1  -1  361  322  18      8  3 -14  107   78  99*     8  4   8  631  655  15      8  6  -2    0   27  83*     9  1  10  435  415  20
7 16   0   141  122  96*     8  1   0 1254 1243  17      8  3 -13  204   43  49*     8  4   9  712  713  18      8  6  -1    0   46  83*     9  1  11    0   24  88*
7 16   1     0  113  96*     8  1   1  324  230  20      8  3 -12  193   64  49*     8  4  10  543  570  15      8  6   0  409  226  84*     9  1  12  467  454  19
7 16   2   164   13  94*     8  1   2 1163 1104  18      8  3 -11  136   26  94*     8  4  11  576  580  15      8  6   1  225  287  31      9  1  13  172   41  90*
7 16   3   170  131  96*     8  1   3  115  156  81*     8  3 -10  285  259  31      8  4  12  344  344  23      8  6   2  243  245  28      9  2 -16  235  250  54*
7 16   4   174  172  54*     8  1   4  260  744  15      8  3  -9    0  129  93*     8  4  13  364  349  21      8  6   3  584  603  13      9  2 -15  117  188  99*
7 16   5     0  105  97*     8  1   5  107   24  80*     8  3  -8  506  593  18      8  4  14  119  164  87*     8  6   4  409  355  17      9  2 -14  239  295  52*
7 16   6   368  363  20      8  1   6  182  215  35*     8  3  -7  238  282  33      8  4  15  196  225  38*     8  6   5  785  787  16      9  2 -13  260  239  45*
7 16   7   185   59  99*     8  1   7    0   12  79*     8  3  -6  627  690  14      8  5 -17  131  155  99*     8  6   6  371  362  21      9  2 -12  312  313  37
7 17  -7     0   92  99*     8  1   8  196  205  34*     8  3  -5  445  480  17      8  5 -16    0   76  99*     8  6   7  847  891  16      9  2 -11  238  213  45*
7 17  -6   135   61  84*     8  1   9   47   39  57*     8  3  -4  908  901  20      8  5 -15  127  118  89*     8  6   8  246  249  29      9  2 -10  279  235  38
7 17  -5     0  170  99*     8  1  10  233  204  29      8  3  -3  618  660  15      8  5 -14  128   34  99*     8  6   9  828  819  17      9  2  -9  158  240  99*
7 17  -4     0  149  99*     8  1  11    0   83  84*     8  3  -2  867  923  21      8  5 -13  130   54  99*     8  6  10    0  121  87*     9  2  -8    0  136  99*
7 17  -3   244  227  39      8  1  12  148  221  85*     8  3  -1  585  603  13      8  5 -12   86   13  70*     8  6  11  598  627  15      9  2  -7  149  156  80*
7 17  -2   267  302  38      8  1  13   93   28  84*     8  3   1  634  646  14      8  5 -11    0   54  97*     8  6  12   89  123  86*     9  2  -6    0    8  95*
7 17  -1   351  290  28      8  1  14  288  273  25      8  3   2  830  811  21      8  5 -10  138   47  95*     8  6  13  380  404  23      9  2  -5  159   15  53*
7 17   0   415  417  25      8  1  15   41   28  84*     8  3   3  417  435  17      8  5  -9  299  310  30      8  6  14    0  121  87*     9  2  -4   91  228  94*
7 17   1   260  252  39      8  2 -18  158  116  99*     8  3   4  686  680  16      8  5  -8    0  234  94*     8  7 -16    0   23  99*     9  2  -3  242  254  34
7 17   2   435  429  24      8  2 -17  206  158  99*     8  3   5  156  184  81*     8  5  -7  414  426  20      8  7 -15  178   96  90*     9  2  -2  336  347  24
7 17   3   330  285  31      8  2 -16    0  226  99*     8  3   6  477  480  15      8  5  -6  256  307  31      8  7 -14    0   11  99*     9  2  -1  350  340  23
7 17   4   321  368  32      8  2 -15  148  179  88*     8  3   7  207  198  32      8  5  -5  569  580  15      8  7 -13  198    8  99*     9  2   0  525  540  17
8  0 -18    69  138  99*     8  2 -14  334  340  33      8  3   8  126   89  82*     8  5  -4  342  363  22      8  7 -12  132   38  71*     9  2   1  450  499  19
8  0 -16   101  221  99*     8  2 -13  226  269  45*     8  3   9  151   82  80*     8  5  -2  419  404  18      8  7 -11    0  114  98*     9  2   2  661  685  16
8  0 -14   234  307  46*     8  2 -12  408  466  25      8  3  10    0   88  83*     8  5  -1  638  621  15      8  7 -10    0   90  96*     9  2   3  523  486  16
8  0 -12   378  436  26      8  2 -11  330  313  27      8  3  11   20   61  84*     8  5   0  355  346  20      8  7  -9  325  323  28      9  2   4  696  715  16
8  0 -10   551  552  17      8  2 -10  573  577  17      8  3  12  160  292  87*     8  5   1  722  768  16      8  7  -8    0  129  95*     9  2   5  238  248  33
8  0  -8   693  715  16      8  2  -9  310  282  27      8  3  13    0  106  84*     8  5   2  335  314  20      8  7  -7  557  563  17      9  2   6  654  626  16
8  0  -6   645  674  15      8  2  -8  498  539  18      8  3  14  322  339  24      8  5   3  737  756  16      8  7  -6  127   74  75*     9  2   7  400  422  22
8  0  -4   668  573  14      8  2  -7  379  396  21      8  3  15  134  125  85*     8  5   4  280  257  24      8  7  -5  649  685  14      9  2   8  522  508  17
8  0  -2   249  165  27      8  2  -6  503  510  16      8  4 -17  144  209  99*     8  5   5  587  597  14      8  7  -4   84   30  87*     9  2   9  257  298  33
8  0   0   262  202  25      8  2  -5  368  326  20      8  4 -16    0  197  99*     8  5   6    0  103  84*     8  7  -3  901  940  16      9  2  10  283  298  29
8  0   2   591  572  13      8  2  -4  380  340  19      8  4 -15  198  332  99*     8  5   7  296  284  24      8  7  -2  202   72  36*     9  2  11  147  280  93*
8  0   4   768  810  15      8  2  -3  134   88  82*     8  4 -14  337  295  33      8  5   8  144   44  83*     8  7  -1 1065 1138  21      9  2  12  127  173  89*
8  0   6   689  641  17      8  2  -2  143    6  81*     8  4 -13  466  463  23      8  5   9    0   13  84*     8  7   0    0   81  84*     9  2  13    0  211  92*
8  0   8   615  605  15      8  2  -1  312  287  21      8  4 -12  346  392  29      8  5  10  202  173  36*     8  7   1  911  974  22      9  3 -16  272   37  47*
8  0  10   517  523  15      8  2   0   61  118  80*     8  4 -11  509  554  20      8  5  11   90  208  88*     8  7   2    0   55  84*     9  3 -15  134   20  85*
8  0  12   437  428  18      8  2   1  403  418  17      8  4 -10  465  498  21      8  5  12  209  140  36*     8  7   3  780  788  16      9  3 -14    0  159  99*
8  0  14   271  291  27      8  2   2  407  435  17      8  4  -9  600  597  17      8  5  13  136  244  90*     8  7   4    0  122  84*
8  1 -18   276  173  43      8  2   3  583  610  13      8  4  -8  369  380  23      8  5  14  125  155  87*     8  7   5  585  579  14
8  1 -17     0   14  99*     8  2   4  629  668  14      8  4  -7  508  500  17      8  6 -17  210  226  57*     8  7   6  191  246  38*
8  1 -16   111  137  99*     8  2   5  580  583  13      8  4  -6  269  250  29      8  6 -16    0  117  99*     8  7   7  306  282  24
8  1 -15   145   13  86*     8  2   6  684  691  17      8  4  -5  425  402  18      8  6 -15  343  379  35      8  7   9  130   54  86*
8  1 -14     0   93  99*     8  2   7  316  251  21      8  4  -4   97  110  84*     8  6 -14    0  145  99*     8  7  10    0   30  88*
8  1 -13    92    5  99*     8  2   8  725  699  16      8  4  -3  204  109  33      8  6 -13  500  500  23      8  7  11  124  129  87*
8  1 -12   161   59  57*     8  2   9  423  445  18      8  4  -2  139   62  81*     8  6 -12  197  167  99*     8  7  12  129   41  89*
8  1 -11   171   16  53*     8  2  10  608  591  13      8  4  -1  209   82  30      8  6 -11  603  588  18      8  7  13  287  237  28
8  1 -10   297  283  30      8  2  11  306  299  23      8  4   0  295  259  22      8  6 -10    0  202  99*     8  7  14    0   12  90*
8  1  -9     0   36  91*     8  2  12  400  400  19      8  4   1  249  281  26      8  6  -8  332  286  26      8  8 -16  146   23  99*
8  1  -8   504  514  17      8  2  13  260  257  28      8  4   2  372  396  18      8  6  -6   65  208  89*     8  8 -15  155  274  99*
8  1  -7   113   78  66*     8  2  14  221  263  34      8  4   3  519  522  14      8  6  -5  442  410  19      8  8 -14    0   22  99*
8  1  -6   796  837  17      8  2  15  277  255  21      8  4   4  490  501  15      8 14   4  433  441  24      8  8 -13  364  344  31
8  1  -5   163  171  44*     8  3 -18    0  139  99*     8  4   5  708  735  16      8 14   5    0   64  99*
8  1  -4  1221 1216  18      8  3 -17    0   73  99*     8 12 -10  395  391  30      8 14   6  503  527  22
8  8 -11   382  416  29      8 10 -13    0  186  99*     8 12  -9  183  152  99*     8 14   7    0   32  99*
8  8 -10   172   50  99*     8 10 -12  136  148  99*     8 12  -8  410  371  27      8 15  -8   42  198  92*
8  8  -9   476  506  21      8 10 -11  310  277  35      8 12  -7    0   89  99*     8 15  -7    0   40  99*
8  8  -8     0   52  95*     8 10 -10  285  230  37      8 12  -6  392  349  27      8 15  -6  161  282  99*
8  8  -7   516  509  19      8 10  -9  382  355  28      8 12  -5  103   99  82*     8 15  -5    0   61  99*
8  8  -6   167   17  91*     8 10  -8  254  290  41      8 12  -4  235  278  41*     8 15  -4  322  354  35
8  8  -5   441  403  20      8 10  -7  378  348  26      8 12  -3   27   44  97*     8 15  -3    0   31  99*
8  8  -4   162   39  89*     8 10  -6  269  231  35      8 12  -2  171   34  94*     8 15  -2  370  375  29
8  8  -3   283  257  28      8 10  -5  369  276  25      8 12  -1    0   21  95*     8 15  -1    0   48  97*
8  8  -2     0  100  87*     8 10  -4  319  245  28      8 12   0    0  117  96*     8 15   0  361  359  29
8  8  -1   198  171  37*     8 10  -3  197   64  43*     8 12   1    0   38  93*     8 15   1  125  120  55*
8  8   0   165  106  85*     8 10  -2  133  112  91*     8 12   2  324  296  27      8 15   2  463  405  23
8  8   1   402  421  19      8 10  -1  162   80  91*     8 12   3  293  172  30      8 15   3  181  120  55*
8  8   2   144  177  83*     8 10   0  146  152  75*     8 12   4  416  401  23      8 15   4  244  291  44*
8  8   3   596  579  14      8 10   1  337  301  24      8 12   5  134  184  94*     8 15   5  189  175  99*
8  8   4    93  148  84*     8 10   2  249  256  33      8 12   6  467  443  21      8 15   6  144  143  72*
8  8   5   749  748  17      8 10   3  412  410  21      8 12   7  208  243  45*     8 16  -6  103  220  99*
8  8   6    61   44  85*     8 10   4  306  267  26      8 12   8  430  431  24      8 16  -5  122   38  99*
8  8   7   559  570  15      8 10   5  420  450  20      8 12   9  269  232  36      8 16  -4    0  138  99*
8  8   8     0   32  73*     8 10   6  250  250  31      8 12  10  396  401  26      8 16  -3  121   41  99*
8  8   9   592  584  16      8 10   7  431  378  20      8 13 -11  167   73  99*     8 16  -2    0   39  99*
8  8  10     0   39  92*     8 10   8  220  231  38*     8 13 -10  231  124  50*     8 16  -1  105   48  72*
8  8  11   398  399  22      8 10   9  356  360  26      8 13  -9  196  119  99*     8 16   0  212  183  49*
8  8  12     0   43  89*     8 10  10  159  204  92*     8 13  -8  166  266  68*     8 16   1    0   65  99*
8  8  13   304  344  29      8 10  11  287  289  31      8 13  -7  152  142  70*     8 16   2  338  297  31
8  9 -15   180   75  99*     8 10  12  167  206  96*     8 13  -6  318  366  34      8 16   3   63    7  77*
8  9 -14   189   27  60*     8 11 -14  184   32  99*     8 13  -5  216  208  47*     9  0 -16    0  211  99*
8  9 -13     0    8  99*     8 11 -13    0   31  99*     8 13  -4  485  495  22      9  0 -12  342  280  34
8  9 -12     0   14  99*     8 11 -12  176  165  99*     8 13  -3  250  212  37      9  0 -10  324  305  33
8  9 -11   105   74  99*     8 11 -11   92   79  74*     8 13  -2  512  474  20      9  0  -8  253  210  39
8  9 -10   145   66  77*     8 11 -10  178   68  99*     8 13  -1  270  188  35      9  0  -6    0   41  95*
8  9  -9   267  234  37      8 11  -9  269  252  59*     8 13   0  496  505  20      9  0  -4  299  380  29
8  9  -8   183  180  96*     8 11  -8  184  179  99*     8 13   1  162  210  81*     9  0  -2  533  567  16
8  9  -7   455  473  22      8 11  -7  318  356  33      8 13   2  506  512  20      9  0   0  679  682  16
8  9  -6   263  299  35      8 11  -6  339  351  29      8 13   3   96  196  98*     9  0   2  723  739  15
8  9  -5   647  664  16      8 11  -5  504  495  21      8 13   4  349  369  28      9  0   4  576  589  16
8  9  -4   339  294  25      8 11  -4  425  467  24      8 13   5    0   79  99*     9  0   6  466  448  19
8  9  -3   934  962  17      8 11  -3  598  599  17      8 13   6  299  275  32      9  0   8  566  538  16
8  9  -2   443  470  20      8 11  -2  631  639  16      8 13   7  206   11  45*     9  0  10  320  325  27
8  9  -1   859  887  18      8 11  -1  501  467  19      8 13   8  137  121  75*     9  0  12  242  195  34
8  9   0   322  332  25      8 11   0  513  592  17      8 13   9    0   70  99*     9  1 -16  176   28  99*
8  9   1   805  778  17      8 11   1  516  503  18      8 14 -10  410  381  31      9  1 -15    0    7  85*
8  9   2   259  312  30      8 11   2  475  457  19      8 14  -9  122   17  99*     9  1 -14  227  148  54*
8  9   3   580  562  15      8 11   3  413  380  22      8 14  -8  368  322  32      9  1 -13    0   39  99*
8  9   4   285  244  27      8 11   4  291  344  30      8 14  -7   72   14  88*     9  1 -12  353  336  33
8  9   5   318  268  25      8 11   5  142  222  95*     8 14  -6  242  268  45*     9  1 -10  476  524  24
8  9   6    30  102  86*     8 11   6   36  168  95*     8 14  -5    0   29  99*     9  1  -9    0   87  99*
8  9   7   128   89  67*     8 11   7    0   68  94*     8 14  -4  112  109  99*
8  9   8   124   69  63*     8 11   8  140   91  60*     8 14  -3  141   31  97*
8  9   9     0   57  88*     8 11   9  173   67  93*     8 14  -2    0   43  97*
8  9  10   128   11  91*     8 11  10  140   52  93*     8 14  -1  167   33  97*
8  9  11   140  129  60*     8 11  11    0  217  96*     8 14   0    0  125  97*
8  9  12     0   19  93*     8 12 -13   79  112  99*
```

h	k	l	Fo	Fc	R	h	k	l	Fo	Fc	R	h	k	l	Fo	Fc	R	h	k	l	Fo	Fc	R	h	k	l	Fo	Fc	R
8	9	13	178	179	91*	8	12	-12	348	314	36	8	14	1	0	46	99*	9	1	-8	677	730	17	9	3	-13	134	86	99*
8	10	-14	0	127	99*	8	12	-11	135	166	99*	8	14	2	0	262	98*	9	1	-7	164	163	55*	9	3	-12	259	301	45*
9	3	-11	287	152	38	9	5	-16	0	6	99*	9	6	10	139	67	91*	9	8	10	166	37	91*	9	11	-7	387	357	31
9	3	-10	468	489	23	9	5	-15	0	32	99*	9	6	11	310	290	28	9	8	11	97	289	98*	9	11	-6	357	359	34
9	3	-9	253	244	41	9	5	-14	0	50	99*	9	6	12	121	85	91*	9	9	-13	115	158	99*	9	11	-5	424	402	27
9	3	-8	474	499	22	9	5	-13	118	115	99*	9	7	-15	147	57	86*	9	9	-12	0	123	99*	9	11	-4	434	460	27
9	3	-7	368	389	26	9	5	-12	123	81	99*	9	7	-14	197	80	99*	9	9	-11	127	294	99*	9	11	-3	136	299	80*
9	3	-6	485	578	21	9	5	-11	246	279	46*	9	7	-13	0	151	99*	9	9	-10	175	194	70*	9	11	-2	388	342	27
9	3	-5	386	449	23	9	5	-10	137	184	99*	9	7	-12	0	114	99*	9	9	-9	455	474	28	9	11	-1	316	309	33
9	3	-4	600	579	16	9	5	-9	375	386	29	9	7	-11	285	315	43	9	9	-8	181	248	99*	9	11	0	197	242	99*
9	3	-3	428	388	20	9	5	-8	82	213	99*	9	7	-10	155	111	90*	9	9	-7	609	605	21	9	11	1	238	221	41*
9	3	-2	589	632	15	9	5	-7	459	471	22	9	7	-9	452	514	26	9	9	-6	325	242	34	9	11	2	0	160	98*
9	3	-1	398	385	20	9	5	-6	251	232	38	9	7	-8	194	39	99*	9	9	-5	723	730	17	9	11	3	0	54	98*
9	3	0	518	548	17	9	5	-5	495	534	20	9	7	-7	567	580	20	9	9	-4	328	360	33	9	11	4	0	38	99*
9	3	1	226	252	35	9	5	-4	243	272	36	9	7	-6	64	40	98*	9	9	-3	662	692	17	9	11	5	0	78	98*
9	3	2	415	403	20	9	5	-3	491	500	19	9	7	-5	676	666	16	9	9	-2	278	269	35	9	11	6	79	17	98*
9	3	3	0	64	91*	9	5	-2	209	247	40*	9	7	-4	99	16	81*	9	9	-1	534	519	19	9	11	7	140	204	98*
9	3	4	171	164	45*	9	5	-1	521	496	17	9	7	-3	716	748	18	9	9	0	179	228	95*	9	11	8	0	57	99*
9	3	5	83	28	73*	9	5	0	225	165	35	9	7	-2	184	128	49*	9	9	1	326	308	29	9	11	9	339	317	31
9	3	6	192	166	41*	9	5	1	450	455	19	9	7	-1	598	549	16	9	9	2	218	176	40*	9	12	-10	268	192	49*
9	3	7	0	24	89*	9	5	2	167	148	87*	9	7	0	227	218	38*	9	9	3	236	129	37	9	12	-9	137	17	99*
9	3	8	250	281	33	9	5	3	274	276	29	9	7	1	431	401	20	9	9	4	0	87	96*	9	12	-8	211	117	99*
9	3	9	0	144	91*	9	5	4	117	24	68*	9	7	2	244	196	35	9	9	5	0	25	92*	9	12	-7	208	16	99*
9	3	10	408	408	22	9	5	5	87	1	76*	9	7	3	108	176	94*	9	9	6	0	14	94*	9	12	-6	182	31	99*
9	3	11	189	194	43*	9	5	6	140	125	91*	9	7	4	276	269	30	9	9	7	228	142	39*	9	12	-5	0	103	99*
9	3	12	346	370	25	9	5	7	248	235	34	9	7	5	0	70	91*	9	9	8	195	74	47*	9	12	-4	247	143	45*
9	3	13	153	174	77*	9	5	8	92	218	93*	9	7	6	118	26	93*	9	9	9	170	245	97*	9	12	-3	0	59	99*
9	4	-16	158	223	80*	9	5	9	383	351	23	9	7	7	261	162	32	9	9	10	0	97	99*	9	12	-2	280	265	39
9	4	-15	219	293	99*	9	5	10	116	177	78*	9	7	8	0	19	94*	9	10	-13	145	170	99*	9	12	-1	159	87	99*
9	4	-14	263	240	47*	9	5	11	318	346	28	9	7	9	288	298	31	9	10	-12	207	103	99*	9	12	0	418	390	25
9	4	-13	334	346	37	9	5	12	259	184	32	9	7	10	121	51	99*	9	10	-11	0	175	99*	9	12	1	219	214	47*
9	4	-12	326	268	35	9	5	13	183	266	94*	9	7	11	367	341	25	9	10	-10	210	133	99*	9	12	2	477	441	23
9	4	-11	289	335	39	9	6	-15	0	321	99*	9	7	12	109	15	66*	9	10	-9	213	145	57*	9	12	3	296	228	34
9	4	-10	129	169	99*	9	6	-14	0	108	99*	9	8	-14	0	22	99*	9	10	-8	0	51	99*	9	12	4	471	452	23
9	4	-9	184	246	99*	9	6	-13	308	368	41	9	8	-13	0	291	99*	9	10	-7	0	43	99*	9	12	5	250	236	40
9	4	-8	113	40	97*	9	6	-12	0	137	99*	9	8	-12	0	37	99*	9	10	-6	278	11	39	9	12	6	444	430	25
9	4	-7	0	161	98*	9	6	-11	356	378	34	9	8	-11	102	327	99*	9	10	-5	0	100	99*	9	12	7	181	172	99*
9	4	-6	0	2	95*	9	6	-10	105	173	99*	9	8	-10	39	38	99*	9	10	-4	175	66	60*	9	13	-9	287	122	44
9	4	-5	0	60	93*	9	6	-9	286	222	37	9	8	-9	0	270	99*	9	10	-3	284	251	36	9	13	-8	361	315	36
9	4	-4	123	89	76*	9	6	-8	143	104	99*	9	8	-8	0	44	99*	9	10	-2	337	255	30	9	13	-7	186	145	99*
9	4	-3	129	241	69*	9	6	-7	182	92	98*	9	8	-7	217	114	49*	9	10	-1	303	316	33	9	13	-6	315	380	39
9	4	-2	155	238	89*	9	6	-6	178	57	95*	9	8	-6	177	5	59*	9	10	0	172	284	99*	9	13	-5	0	140	99*
9	4	-1	364	383	23	9	6	-5	0	89	95*	9	8	-5	197	199	99*	9	10	1	364	391	27	9	13	-4	256	353	46*
9	4	0	365	383	23	9	6	-4	87	58	93*	9	8	-4	163	99	99*	9	10	2	190	280	98*	9	13	-3	0	116	99*
9	4	1	559	576	15	9	6	-3	309	320	29	9	8	-3	284	384	36	9	10	3	339	419	29	9	13	-2	341	338	34
9	4	2	503	530	17	9	6	-2	95	239	95*	9	8	-2	183	70	50*	9	10	4	311	270	30	9	13	-1	182	96	99*
9	4	3	692	692	16	9	6	-1	488	539	19	9	8	-1	488	531	21	9	10	5	288	336	33	9	13	0	288	325	39
9	4	4	583	635	16	9	6	0	231	205	36	9	8	0	174	131	93*	9	10	6	165	245	98*	9	13	1	0	96	99*
9	4	5	722	732	16	9	6	1	707	734	16	9	8	1	586	611	17	9	10	7	281	307	34	9	13	2	243	195	44*
9	4	6	595	567	16	9	6	2	218	194	38*	9	8	2	120	37	94*	9	10	8	126	225	75*	9	13	3	156	43	99*
9	4	7	630	633	15	9	6	3	789	825	19	9	8	3	685	691	17	9	10	9	274	235	35	9	13	4	44	92	99*
9	4	8	397	431	22	9	6	4	208	214	40*	9	8	4	137	95	60*	9	10	10	134	226	76*	9	13	5	189	100	99*
9	4	9	494	479	18	9	6	5	831	873	19	9	8	5	521	530	18	9	11	-12	0	126	99*	9	13	6	0	49	99*
9	4	10	278	234	30	9	6	6	240	144	34	9	8	6	127	88	69*	9	11	-11	216	248	61*	9	14	-7	0	20	99*
9	4	11	309	231	27	9	6	7	651	679	16	9	8	7	470	510	21	9	11	-10	208	224	99*	9	14	-6	172	7	99*
9	4	12	129	74	76*	9	6	8	0	112	93*	9	8	8	133	58	93*	9	11	-9	269	299	47*	9	14	-5	0	33	99*
9	4	13	0	137	93*	9	6	9	475	487	20	9	8	9	195	354	99*	9	11	-8	298	330	42	9	14	-4	0	112	92*
9	14	-3	0	79	99*	10	2	-10	204	11	99*	10	4	-7	252	216	45*	10	6	-1	628	662	19	10	9	-11	350	336	42
9	14	-2	224	204	50*	10	2	-9	207	7	57*	10	4	-6	129	164	99*	10	6	0	200	198	52*	10	9	-10	22	194	99*
9	14	-1	0	73	99*	10	2	-8	269	122	41	10	4	-5	310	349	36	10	6	1	740	745	18	10	9	-9	393	410	37
9	14	0	362	313	31	10	2	-7	237	127	46*	10	4	-4	328	310	33	10	6	3	720	744	16	10	9	-8	0	208	99*
9	14	1	99	85	99*	10	2	-6	180	314	99*	10	4	-3	440	463	25	10	6	4	62	123	99*	10	9	-7	418	445	33
9	14	2	446	467	26	10	2	-5	306	288	35	10	4	-2	433	437	24	10	6	5	481	500	22	10	9	-6	246	270	54*
9	14	3	0	62	99*	10	2	-4	403	457	27	10	4	-1	575	604	19	10	6	6	128	144	99*	10	9	-5	391	404	33
9	14	4	435	497	28	10	2	-3	285	302	36	10	4	0	429	502	25	10	6	7	258	327	40	10	9	-4	162	227	92*
9	15	-3	176	64	99*	10	2	-2	593	619	18	10	4	1	597	624	18	10	6	8	0	45	99*	10	9	-3	73	230	93*
9	15	-2	263	271	44*	10	2	-1	348	357	28	10	4	2	560	537	19	10	6	9	44	133	99*	10	9	-2	160	95	99*
9	15	-1	114	133	99*	10	2	0	681	707	16	10	4	3	574	582	19	10	6	10	0	42	99*	10	9	-1	190	55	99*
9	15	0	0	291	99*	10	2	1	309	324	32	10	4	4	381	402	27	10	7	-12	0	58	99*	10	9	0	0	68	99*
10	0	-14	0	106	99*	10	2	2	658	711	17	10	4	5	488	475	21	10	7	-11	360	366	39	10	9	1	119	58	99*
10	0	-12	216	74	99*	10	2	3	170	182	99*	10	4	6	246	206	40	10	7	-10	176	39	74*	10	9	2	65	3	86*
10	0	-10	149	3	99*	10	2	4	555	555	19	10	4	7	335	337	30	10	7	-9	406	381	33	10	9	3	193	187	99*
10	0	-8	0	189	99*	10	2	5	289	292	34	10	4	8	0	90	99*	10	7	-8	0	77	99*	10	9	4	161	75	85*
10	0	-6	429	444	26	10	2	6	424	401	24	10	4	9	0	96	99*	10	7	-7	404	389	32	10	9	5	229	235	47*
10	0	-4	503	599	22	10	2	7	82	221	98*	10	4	10	0	27	82*	10	7	-6	0	72	99*	10	9	6	180	125	58*
10	0	-2	620	655	18	10	2	8	199	184	47*	10	4	11	184	18	96*	10	7	-5	392	410	32	10	9	7	366	344	29
10	0	0	741	728	18	10	2	9	152	196	82*	10	5	-13	0	215	99*	10	7	-4	233	176	48*	10	9	8	0	131	99*
10	0	2	601	602	18	10	2	10	0	50	96*	10	5	-12	79	110	99*	10	7	-3	279	243	40	10	10	-10	0	27	99*
10	0	4	452	427	23	10	2	11	168	95	94*	10	5	-11	0	263	99*	10	7	-2	0	186	99*	10	10	-9	73	57	99*
10	0	6	570	530	19	10	3	-14	166	201	83*	10	5	-10	194	139	99*	10	7	-1	198	143	53*	10	10	-8	0	57	99*
10	0	8	232	216	43*	10	3	-13	210	121	64*	10	5	-9	163	268	96*	10	7	0	0	149	99*	10	10	-7	176	180	97*
10	0	10	186	87	96*	10	3	-12	170	314	99*	10	5	-8	0	141	99*	10	7	1	0	48	99*	10	10	-6	159	112	99*
10	1	-14	0	268	99*	10	3	-11	0	161	99*	10	5	-7	315	311	38	10	7	2	66	131	99*	10	10	-5	307	324	42
10	1	-13	219	41	62*	10	3	-10	388	349	32	10	5	-6	205	190	99*	10	7	3	151	275	99*	10	10	-4	205	266	62*
10	1	-12	379	396	36	10	3	-9	203	232	99*	10	5	-5	172	298	99*	10	7	4	167	14	99*	10	10	-3	352	349	35
10	1	-11	198	69	99*	10	3	-8	385	409	31	10	5	-4	0	145	99*	10	7	5	0	337	99*	10	10	-2	0	255	99*
10	1	-10	471	541	29	10	3	-7	137	237	82*	10	5	-3	316	266	34	10	7	6	166	13	57*	10	10	-1	395	379	30
10	1	-9	0	126	99*	10	3	-6	365	414	31	10	5	-2	235	21	43*	10	7	7	357	417	30	10	10	0	203	255	47*
10	1	-8	626	635	21	10	3	-5	133	138	73*	10	5	-1	263	175	37	10	7	8	0	34	99*	10	10	1	283	350	41
10	1	-7	217	120	51*	10	3	-4	409	394	27	10	5	1	191	16	97*	10	7	9	383	397	28	10	10	2	0	265	99*
10	1	-6	617	665	20	10	3	-3	0	73	99*	10	5	2	0	116	99*	10	8	-12	0	9	99*	10	10	3	260	264	43
10	1	-5	0	67	99*	10	3	-2	288	285	34	10	5	3	143	120	98*	10	8	-11	169	52	99*	10	10	4	247	220	44*
10	1	-4	490	499	23	10	3	-1	67	28	97*	10	5	4	285	246	34	10	8	-10	156	8	99*	10	10	5	158	210	99*
10	1	-3	158	20	98*	10	3	0	121	80	97*	10	5	6	255	247	38	10	8	-9	110	90	99*	10	10	6	149	211	99*
10	1	-2	324	360	31	10	3	1	114	144	97*	10	5	7	375	421	27	10	8	-8	128	19	99*	10	11	-8	320	286	45
10	1	-1	0	20	97*	10	3	2	279	154	32	10	5	9	356	391	28	10	8	-7	234	180	54*	10	11	-7	345	281	41
10	1	0	213	93	44*	10	3	3	0	176	99*	10	5	10	200	194	47*	10	8	-6	36	32	99*	10	11	-6	341	323	40
10	1	1	0	86	96*	10	3	4	384	428	26	10	6	-13	11	109	99*	10	8	-5	388	417	33	10	11	-5	0	205	99*
10	1	2	140	182	74*	10	3	5	137	140	97*	10	6	-12	0	49	99*	10	8	-4	154	50	75*	10	11	-4	169	241	99*
10	1	3	137	59	95*	10	3	6	466	445	22	10	6	-11	0	15	99*	10	8	-3	473	529	26	10	11	-3	0	194	99*
10	1	4	249	266	40	10	3	7	266	255	37	10	6	-10	120	11	99*	10	8	-2	195	26	99*	10	11	-2	0	138	99*
10	1	5	0	46	97*	10	3	8	455	495	23	10	6	-9	156	112	99*	10	8	-1	480	538	25	10	11	-1	103	75	91*
10	1	6	449	486	23	10	3	9	211	254	46*	10	6	-8	32	62	99*	10	8	0	35	74	85*	10	11	0	161	73	88*
10	1	7	0	73	99*	10	3	10	386	362	25	10	6	-7	132	218	99*	10	8	1	518	561	22	10	11	1	86	77	99*
10	1	8	581	567	19	10	3	11	150	215	75*	10	6	-6	82	134	99*	10	8	2	202	84	49*	10	11	2	199	34	99*
10	1	9	136	39	97*	10	4	-14	51	110	99*	10	6	-5	297	366	40	10	8	3	494	463	22	10	11	3	0	194	99*
10	1	10	533	545	21	10	4	-13	0	98	99*	10	6	-4	226	267	49*	10	8	4	91	76	99*	10	11	4	170	102	99*
10	1	11	173	80	98*	10	4	-12	0	78	99*	10	6	-3	517	552	23	10	8	5	381	387	27	10	11	5	0	283	99*
10	2	-14	147	131	99*	10	4	-11	185	15	68*	10	6	-2	193	243	99*	10	8	6	167	29	99*	10	12	-6	217	182	62*
10	2	-13	0	111	99*	10	4	-10	166	24	99*							10	8	7	132	261	99*	10	12	-5	138	104	96*
10	2	-12	0	84	99*	10	4	-9	0	58	99*							10	8	8	0	23	99*	10	12	-4	277	279	48*
10	2	-11	0	104	99*	11	2	0	215	62	54*													10	12	-3	146	140	95*
10	12	-2	378	384	34	11	2	2	210	313	99*	11	5	-2	121	110	99*	11	8	4	184	22	99*	12	3	-3	22	182	99*
10	12	-1	249	249	50*	11	2	3	0	251	99*	11	5	-1	241	222	50*	11	9	-7	155	185	99*	12	3	-2	0	251	99*
10	12	0	417	425	31	11	2	4	255	180	43*	11	5	0	160	167	99*	11	9	-6	0	87	99*	12	3	-1	234	220	58*
10	12	1	278	266	43	11	2	5	177	212	99*	11	5	1	346	363	31	11	9	-5	169	43	99*	12	3	0	299	371	47
10	12	2	343	442	37	11	2	6	18	30	99*	11	5	2	226	257	51*	11	9	-4	0	10	99*	12	3	1	255	209	54*
10	12	3	148	213	92*	11	2	7	0	102	99*	11	5	3	424	475	28	11	9	-3	0	52	99*	12	3	2	361	348	38
10	13	-3	0	100	99*	11	2	8	0	95	99*	11	5	4	0	221	99*	11	9	-2	266	6	51*	12	3	3	224	268	99*
10	13	-2	161	161	86*	11	3	-11	0	141	99*	11	5	5	204	406	99*	11	9	-1	200	143	99*	12	4	-6	252	269	99*
10	13	-1	197	71	63*	11	3	-10	249	248	59*	11	5	6	0	201	99*	11	9	0	0	26	99*	12	4	-5	357	369	45
11	0	-12	0	99	99*	11	3	-9	202	119	99*	11	5	7	356	382	32	11	9	1	118	251	99*	12	4	-4	119	240	99*
11	0	-10	198	246	99*	11	3	-8	0	224	99*	11	6	-10	190	89	99*	11	9	2	196	82	99*	12	4	-3	223	346	99*

h	k	l	Fo	Fc	%
11	0	-8	411	400	34
11	0	-6	479	489	28
11	0	-4	403	452	32
11	0	-2	462	463	27
11	0	0	377	336	33
11	0	2	0	200	99*
11	0	4	238	274	50*
11	0	6	0	26	99*
11	0	8	0	71	99*
11	1	-12	342	356	45
11	1	-11	146	79	99*
11	1	-10	315	378	49
11	1	-9	0	51	99*
11	1	-8	346	331	40
11	1	-7	241	10	55*
11	1	-6	193	183	99*
11	1	-5	213	48	57*
11	1	-4	71	56	99*
11	1	-3	0	25	99*
11	1	-2	96	123	89*
11	1	-1	186	73	99*
11	1	0	254	290	45*
11	1	1	230	72	50*
11	1	2	322	340	37
11	1	3	151	35	90*
11	1	4	411	439	30
11	1	5	0	167	99*
11	1	6	500	531	25
11	1	7	182	113	99*
11	1	8	440	468	27
11	2	-12	0	116	99*
11	2	-11	0	96	99*
11	2	-10	175	215	83*
11	2	-9	220	184	99*
11	2	-8	227	334	99*
11	2	-7	172	247	99*
11	2	-6	309	418	44
11	2	-5	138	233	99*
11	2	-4	387	472	34
11	2	-3	211	270	99*
11	2	-2	457	489	27
11	2	-1	270	278	42
11	2	0	438	442	27
11	2	1	250	219	46*
11	3	-7	94	46	99*
11	3	-6	0	171	99*
11	3	-5	28	28	99*
11	3	-4	110	66	99*
11	3	-3	180	58	99*
11	3	-2	80	78	99*
11	3	-1	195	164	99*
11	3	0	38	248	99*
11	3	1	0	216	99*
11	3	2	364	438	33
11	3	3	234	209	49*
11	3	4	329	433	36
11	3	5	310	312	37
11	3	6	393	427	30
11	3	7	164	206	99*
11	3	8	314	305	36
11	4	-11	227	119	99*
11	4	-10	207	152	99*
11	4	-9	221	234	99*
11	4	-8	255	212	55*
11	4	-7	306	341	47
11	4	-6	223	297	99*
11	4	-5	355	437	39
11	4	-4	0	364	99*
11	4	-3	485	540	28
11	4	-2	354	371	36
11	4	-1	462	534	28
11	4	0	377	380	32
11	4	1	425	443	29
11	4	2	0	271	99*
11	4	3	318	321	36
11	4	4	0	62	99*
11	4	5	0	203	99*
11	4	6	131	14	89*
11	4	7	0	10	99*
11	5	-11	127	177	99*
11	5	-10	0	70	99*
11	5	-9	220	194	99*
11	5	-8	112	78	99*
11	5	-7	0	159	99*
11	5	-6	0	39	99*
11	5	-5	143	84	97*
11	5	-4	174	76	99*
11	5	-3	204	68	99*
11	6	-9	257	221	57*
11	6	-8	235	124	99*
11	6	-7	149	353	99*
11	6	-6	219	218	63*
11	6	-5	491	501	29
11	6	-4	188	188	99*
11	6	-3	508	530	27
11	6	-2	278	160	45
11	6	-1	496	547	27
11	6	0	209	146	99*
11	6	1	444	480	29
11	6	2	186	90	99*
11	6	3	253	257	46*
11	6	4	0	113	99*
11	6	5	162	124	99*
11	6	6	148	29	99*
11	7	-9	174	262	99*
11	7	-8	163	36	92*
11	7	-7	69	246	99*
11	7	-6	0	109	99*
11	7	-5	0	79	99*
11	7	-4	0	134	99*
11	7	-3	141	27	86*
11	7	-2	0	110	99*
11	7	-1	0	165	99*
11	7	0	154	61	83*
11	7	1	301	337	41
11	7	2	0	14	99*
11	7	3	341	407	35
11	7	4	0	8	99*
11	7	5	318	418	38
11	7	6	94	8	89*
11	8	-8	0	11	99*
11	8	-7	173	375	99*
11	8	-6	0	39	99*
11	8	-5	412	457	35
11	8	-4	0	50	99*
11	8	-3	404	423	34
11	8	-2	0	66	99*
11	8	-1	341	419	39
11	8	0	0	71	99*
11	8	1	292	354	43
11	8	2	0	74	99*
11	8	3	303	252	39
11	9	3	314	285	39
11	10	-4	0	155	99*
11	10	-3	312	279	46
11	10	-2	152	141	99*
11	10	-1	182	246	99*
11	10	0	177	170	96*
11	10	1	0	191	99*
12	0	-8	182	288	99*
12	0	-6	293	253	52*
12	0	-4	255	275	58*
12	0	-2	226	199	99*
12	0	0	0	99	99*
12	0	2	174	91	98*
12	0	4	83	124	99*
12	1	-8	0	5	99*
12	1	-7	185	23	83*
12	1	-6	234	82	99*
12	1	-5	166	16	92*
12	1	-4	198	198	99*
12	1	-3	194	54	99*
12	1	-2	166	335	99*
12	1	-1	0	57	99*
12	1	0	392	393	35
12	1	1	0	37	99*
12	1	2	455	448	32
12	1	3	78	134	99*
12	1	4	452	514	32
12	2	-8	276	271	58*
12	2	-7	0	175	99*
12	2	-6	242	296	99*
12	2	-5	203	197	99*
12	2	-4	375	288	39
12	2	-3	0	202	99*
12	2	-2	82	220	99*
12	2	-1	179	143	99*
12	2	0	113	107	99*
12	2	1	151	162	99*
12	2	2	178	22	99*
12	2	3	0	121	99*
12	2	4	0	123	99*
12	3	-7	260	46	60*
12	3	-6	0	28	99*
12	3	-5	231	90	99*
12	3	-4	151	143	99*
12	4	-2	0	217	99*
12	4	-1	300	255	48
12	4	0	139	121	99*
12	4	1	124	141	99*
12	4	2	219	63	99*
12	5	-5	0	194	99*
12	5	-4	143	131	99*
12	5	-3	0	306	99*
12	5	-2	268	182	54*
12	5	-1	339	397	43
12	5	0	115	239	99*
12	5	1	221	443	99*
12	6	-3	326	333	48
12	6	-2	0	82	99*
12	6	-1	54	262	99*

* = reflection not used in the data refinement