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Department of Chemistry

Structural Systematics of Diorganotin Compounds

Veronica J. Hall B.Sc. (Hons)

A thesis submitted for the degree of Doctor of Philosophy.

October 1998

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ADDENDUM

Page 1, line 14: replace affects by effects
Page 5, Figure 1.4: one of the sites *ortho* to the carboxylate is a pyridine-nitrogen atom
Page 14, line 6: replace orgaontin by organotin
Page 20, ref. 35: the Journal is *Inorganica Chimica Acta*
Page 25, the expression for deriving σF_{obs} is:

$\sigma(F_{obs}) = [C + \frac{1}{4}(\frac{t_c}{t_b})^2(b1 + b2) + (P \times I)^2]^{0.5}$ where C = total number of counts for the peak; t_c = time spent counting peak intensity; t_b = time spent counting one side of background; b_1 = high-angle background counts; b_2 = low-angle background counts; p = p-factor; and

$I = C - \frac{1}{2}(t_c/t_b)(b_1 + b_2)$

Page 26, line 17: replace eccentric by acentric
Page 4, Figure 1.2: the caption should read α-$[Hg(S_2COEt)_2]$
Page 14, Figures 1.16 & 1.17: the N and C labels of the central N and C atoms should be reversed
Page 91, Table 4.2: The references [7], [8] and [5] are [6], [7] and [4], respectively
Table 3.1: The value of Z for R = tBu = 4; 2θ values are 8.0, 6.0, 6.0 and 6.0, respectively
Page 125, Table 4.5: R = iPr, *b* = 15.125(3) Å
Page 147, Ref. 2, add Jircitano, A.J. and Takeuchi, K.J. to the author list
Page 5, line 6: From a survey...
Page 13, line 23: To mirror this series...
Page 13, line 26: ...adducts have also been...
Page 15, line 20: methods
Page 24, line 25: Rigaku AFC6R diffractometer
Page 73, line 4: centrosymmetrically related...
Page 93, line 1: replace white by colourless
Page 111, line 7: factor to the size of the Sn-ligand...
Page 113, line 17: the closest Cl...H contacts are...
Page 144, line 12: distances for reduced Lewis acidity
Page 188, line 3: array of diorganotin...

Declaration

Declaration

This thesis contains no material that has been submitted previously for a degree or diploma in any university and to the best of my knowledge contains no material published or written by another person, except where due reference is made.

I consent to this thesis being made available for photocopying and loan.

Veronica J Hall
October 1998

Acknowledgments

Acknowledgements

Compilation of this thesis has been a result of 6 years hard work. There are many people that I would like to thank for all their efforts. Firstly I would like to recognize all the support that my family has offered me in the undertakings of this thesis. My parents and my grandmother are to be acknowledged for all their encouragement and faith in my abilities. I have many supportive friends that have been integral to the completion of this thesis. I would like to thank them all.

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The receipt of a Commonwealth Postgraduate Research Award is gratefully acknowledged.

Abstract

Abstract

This combined crystallographic and theoretical study of selected organotin systems has addressed the question whether crystal packing effects can significantly influence molecular geometry. Attempts at correlating changes in Sn-ligand parameters with the Lewis Acidity of the tin centre and/or the Lewis basicity of the ligand were also undertaken in this study.

The first and foremost observation is that as a general rule, a non-symmetric molecule, in terms of the relative disposition of the ligand donor set and the variation of geometric parameters, found in a crystallographic environment becomes (more) symmetric in the gas phase. The changes in molecular geometry that occur upon the symmetrisation of the structure are generally accompanied by an elongation of the metal-ligand bond distances, however, it is noted that the theoretical model employed also contributes to the elongation of bond distances in the theoretical structures. Noteworthy also is the observation that polymorphs of particular compounds investigated thus far converge to the same geometry and similar observations are found when calculations are performed on systems that crystallise with multiple molecules in the crystallographic asymmetric unit. These key results indicate that there is no inherent chemical reason for the adoption of non-symmetric structures in the solid state and thus, point to the influence of crystal packing effects on molecular geometry.

Systematic crystallographic investigations of the R_2SnCl_2(diimine) series of compounds revealed that the increasing Sn-Cl and Sn-N bond distances could be correlated with decreasing Lewis acidity at the tin atom. Deviations from these correlations could be explained in terms of *intra*molecular Cl...H interactions. Similarly the $R_2Sn(S_2CNR'_2)Cl$ series of compounds were investigated. Attempts at correlating changes in the solid state Sn-ligand parameters with the nature of both R and R' were unsuccessful. The geometry optimisation calculations showed clear and systematic correlations in the Sn-ligand parameters owing to the variation of R' in the dithiocarbamate ligands again pointing to the influence of crystal packing effects on the tin atom geometry. Similarly, consistent trends are found as the Lewis acidity of the tin center is moderated but these can not be correlated directly with the electron withdrawing capability of the tin-bound R groups. This latter result indicates that Lewis acidity at the tin center is also influenced by the steric demands of these substituents.

Abbreviations

Abbreviations

The following abbreviations are used in this thesis.

Me	Methyl
Et	Ethyl
^{i}Pr	iso-propyl
^{n}Bu	normal butyl
^{t}Bu	tertiary butyl
Ph	Phenyl
Cy	Cyclohexyl
Bz	Benzyl
Vin	Vinyl
Å	Angstroms
°C	Degrees Celsius
°	Degrees
K	Kelvin
s	Singlet (NMR Tables)
b	broad
bs	broad singlet
d	doublet
dd	doublet of doublets
ddd	doublet of doublets of doublets
t	triplet
tt	triplet of triplets
q	quartet
sx	sextet
sept	septet
dt	doublet of triplets
m	multiplet (NMR Tables)
IR	Infrared Spectroscopy
sh	shoulder
s	strong (IR tables)
w	weak
m	medium (IR Tables)
NO	not observed
Hz	Hertz
MHz	Mega Hertz
ppm	parts per million
NMR	Nuclear magnetic resonance spectroscopy
^{1}H NMR	proton –1 NMR
^{13}C NMR	broad-band noise proton-decoupled carbon –13 NMR
^{119}Sn NMR	proton-decoupled tin –119 NMR

TMS	Tetramethylsilane
FID	Free induction decays
δ	Chemical shift in ppm
^{x}J	Coupling constant over x bonds in Hz
M. Wt.	Molecular weight
M. Pt	melting point in ° C
R	Alkyl, aryl group
λ	wavelength cm^{-1}
ν	stretching frequency cm^{-1} of the X-Y band
mol	mole
M	Molar
dec.	decomposed
V	Volume
Z	No. molecules in the asymmetric unit
D_{calcd}	Calculated density in g cm^{-3}
$e^{-}/Å^{3}$	Residual electron density per cubic angstroms
kJ mol^{-1}	kilojoules per mol
sec.	seconds

Publications

Publications

(1) Buntine, M.A.; Hall, V.J.; Kosovel, F.J.; Tiekink, E.R.T.: Influence of crystal packing on molecular geometry: a crystallographic and theoretical investigation of selected diorganotin systems. *J. Phys. Chem. A*, **1998**, *102*, 2472.

(2) Tiekink, E.R.T.; Hall, V.J.; Hook, J.; Buntine, M.A.: Examination of the effect of crystal packing forces on geometric parameters: a crystallographic and theoretical Study of 2,2'-bipyridyl adducts of R_2SnCl_2. *J. Phys. Chem. A*, submitted.

(3) Buntine, M.A.; Hall, V.J.; Tiekink, E.R.T.: The crystal and molecular structures of R_2SnCl_2(1,10-phenanthroline), R= ^{i}Pr, Cy, Bz and R_2= Me, Ph: a comparison between solid state and theoretical structures. *Z Kristallogr.*, accepted.

(4) Hall, V.J.; Tiekink, E.R.T.; Buntine, M.A.: An examination of the influence of crystal structure on molecular structure. The crystal and molecular structures of some diorganotinchloro(*N*, *N*-dialkyldithiocarbamate)s, $R_2Sn(S_2CNR'_2)Cl$, R= Me, ^{t}Bu, Cy and R'_2= $(Et)_2$, (CyEt) and $(Cy)_2$: a comparison between solid state and theoretical structures. *Z Kristallogr.*, accepted.

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Chapter 1

Introduction

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1.1 Preamble.

X-ray crystallography is the most powerful tool that can be used in the elucidation of chemical structure for crystalline compounds. There have been a substantial number of molecular structures determined which encompass small molecules, macromolecules and minerals. The information obtained from such studies is used to provide a solid foundation upon which an informed interpretation of the chemical and physical properties of the materials under investigation can be made.

For molecular compounds, i.e. excluding macromolecular and mineral structures, the perennial question remains: how does the solid state structure compare with the solution state structure? In other words, do crystal packing effects influence the structure ultimately adopted in the solid state?

It is probably fair to say that the so-called crystal packing effects *per se* have been largely ignored in structure determinations except for the possible exclusion of hydrogen bonding effects. Thus, it has been largely assumed that crystal packing affects do not influence greatly the adoption of a particular structural motif. A number of recent reviews of the structural chemistry of main group element compounds challenge this assumption for main group element chemistry [1-4]. In the following section, 1.2, a number of main group element systems are discussed in this context.

The structural information reported in the literature is mainly concerned with the elucidation of the molecular structure rather than the crystal structure. Thus, it is not surprising that crystal packing has mostly been seen as unimportant. To date a systematic investigation into the affect of the molecular arrangement in the unit cell of the molecules containing heavy-metal centres has not been undertaken.

1.2 Structural diversity in main group element compounds - a brief survey

A survey of the literature has revealed that some main group metal elements display a rich variety of different structural motifs for compounds of closely related chemical composition [1-4]. It is well known that by changing the steric profiles of ligands one can alter the coordination of the central element; this has been used to great extent in vapor deposition strategies [5]. The following discussion is concerned, however, with the modification in molecular structure when only small changes in the ligand, often remote from the main group element centre, occur. This idea is illustrated in the following descriptions of the structural chemistry of the mercury *bis* xanthates 1.2.1, and particularly in the diorganotin bis picolinates 1.2.2, the tetra-organo distannoxanes 1.2.3, and the diorganotin bis dithiolates 1.2.4.

1.2.1 Structural motifs for the mercury bis xanthates.

A number of crystal structure determinations for mercury(II) *bis* xanthates[a] $Hg(S_2COR)_2$ are known [6-10].

Three structural motifs exist for these compounds as illustrated by R= Me, Et and ^{i}Pr. The common feature of the three motifs is that they are polymeric. The different structures arise as a result of the dissimilar modes of attachment of the xanthate ligands. A segment of the polymeric structure of $[Hg(S_2COMe)_2]$ is shown in Figure 1.1 [1][b]. $[Hg(S_2COMe)_2]$ contains bidentate and bridging as well as monodentate xanthate ligands [6]. Each mercury atom is coordinated by three xanthate ligands resulting in the formation of a helical chain. The mercury atoms in this structure are thus three-coordinate and exist in *T*-shaped geometries.

---

[a] Xanthate is the generic name for O-alkyl (or aryl) dithiocarbonate $^{-}[S_2COR]$.

[b] All of the molecular structures illustrated in this chapter are scanned images taken directly from the literature and are referenced accordingly i.e. Figure 1.1[1]

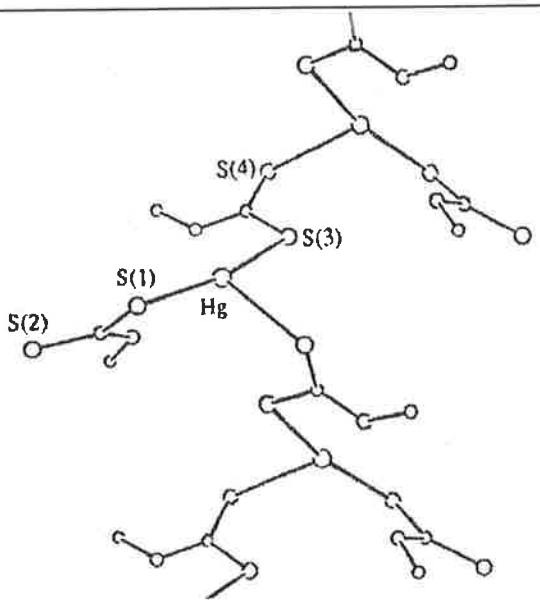


Figure 1.1

$[Hg(S_2COMe)_2]$

A portion of the polymeric structure of $Hg(S_2COR)_2$ where R= Et [7], is shown in Figure 1.2 [1]. All the xanthate ligands are bidentate and bridging, giving rise to tetrahedral mercury centres [7]. The structure can be envisaged to comprise sixteen-membered rings, formed by four $[Hg(S_2COEt)]$ units which are linked to symmetry related mercury centres. This leads to a layered structure with laterally interconnected sixteen-membered rings in which adjacent metal centres are linked by bridging xanthate ligands. Subsequently, four sulfur atoms derived from four different xanthate ligands define the tetrahedral mercury atom geometries.

This structural motif is also seen in the mercury(II) bis *n*-propylxanthate [8]. In this example the mercury atom lies on a crystallographic *2*-fold axis.

Mercury(II) *bis* ethylxanthate has been shown to crystallize in at least two polymorphs. In the α-polymorph [7], Figure 1.2 [1], which crystallizes in the non-centrosymmetric space group $P2_1$, all the successive layers of the 16-membered rings lie in the same orientation. However in the centrosymmetric β-polymorph [9], which crystallizes in the $P2_1/n$ space group, the successive layers are related to each other by centres of inversion [9].

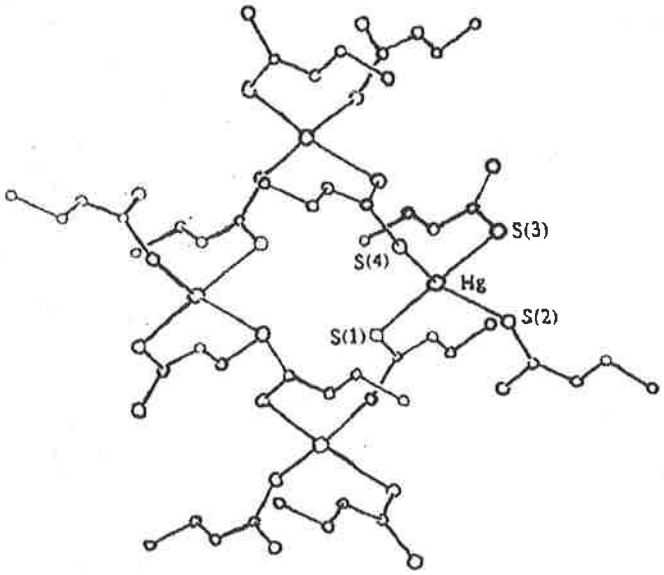


Figure 1.2

α-[Hg(S_2CO^nPr)$_2$]

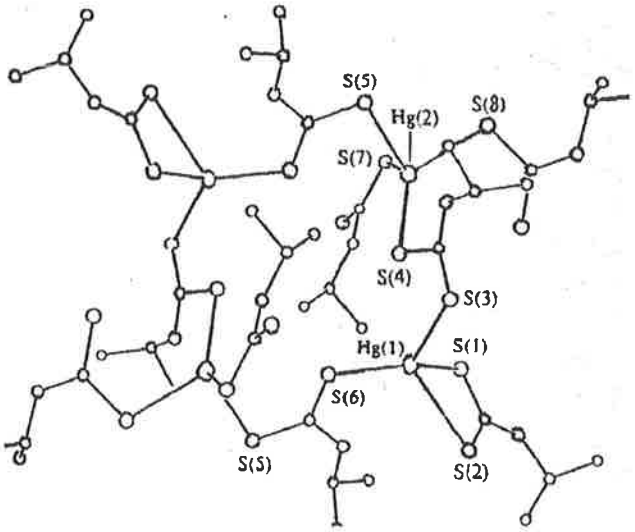


Figure 1.3

[Hg(S_2CO^iPr)$_2$]

Tetrahedral mercury geometries are also found in the structure of Hg(S_2CO^iPr)$_2$ [10] as depicted in Figure 1.3 [1]. As in R= Et sixteen-membered rings are still evident as are the tetrahedral coordinated mercury centres. The difference arises in the mode of attachment of the sixteen-membered rings and the existence of two types of mercury atom environments. Two of the mercury centres in the [Hg(S_2CO^iPr)]$_4$ sixteen membered rings are linked to neighbouring sixteen membered rings via bridging xanthate ligands above and below the original sixteen membered ring. Each of the two remaining mercury atoms are chelated by a xanthate ligand. Thus, there are two different mercury atom environments. Two sulfur atoms derived from bridging xanthate ligands and two sulfur atoms from a chelating xanthate ligand define one of the mercury atoms' geometry. Four sulfur atoms derived from four bridging xanthate ligands define the remaining mercury atoms' geometry.

In the three structural motifs described, where the differences in the chemical composition between the Hg(S_2COR)$_2$ compounds are seemingly minimal, a progression from a linear one dimensional polymer (R= Me) to a two dimensional layer structure (R= Et), and finally to a three dimensional network structure (R= ^{i}Pr) is observed. It is

interesting to note that as the steric profile of the xanthate ligand increases, the degree of polymerization of the structure increases against expectation.

With the expanding interest in the chemistry of tin, in particular organotin compounds due to their increased use in many areas of application e.g. agricultural and industrial chemicals [11-14] and anti-tumor drugs [15-16], a wide variety of organotin compounds have been characterized crystallographically. A survey of the literature it is evident that some organotin systems show a rich variety of coordination geometries, even for very closely related compounds [2]. With minimal variations in the nature of the chemical formulae, it has been observed that organotin carboxylates [17-28] and thiolates [29-40] adopt a large number of structural motifs. Sections 1.2.2, 1.2.3, 1.2.4 examines the structural diversity of some of these compounds in view of the fact that diorganotin systems form the focus of the study reported in this thesis.

1.2.2 Structural motifs for the Diorganotin (IV) *bis* 2-picolinates.

There are three distinct structural motifs for compounds of the formulae $R_2Sn(O_2CC_5H_4N\text{-}2)_2$ where R=Me, Ph and ^tBu [17-19] and [$^-O_2CC_5H_4N$-2] is a mono-anion derived from 2-pyridinecarboxylic acid (Figure 1.4):

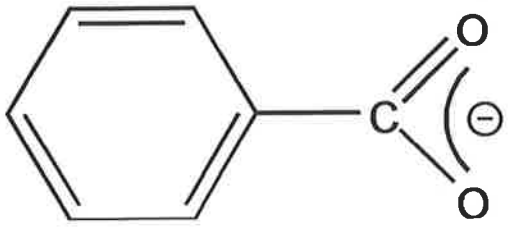


Figure 1.4

2-pyridinecarboxylic acid

For the $[Me_2Sn(O_2CC_5H_4N\text{-}2)_2]$ [17] derivative, Figure 1.5 [20], a seven-coordinate tin atom exists in a distorted pentagonal bipyramidal geometry with the two methyl groups occupying the axial positions. One of the 2-pyridinecarboxylates chelates the tin atom *via* the nitrogen and one of the oxygen atoms, and the other 2-pyridinecarboxylate coordinates in a similar manner, with the exception that it binds a symmetry related tin

atom *via* the second oxygen of the carboxylate group. The bridging mode of the second 2-pyridinecarboxylate ligand leads to a polymeric structure, as shown in Figure 1.5.

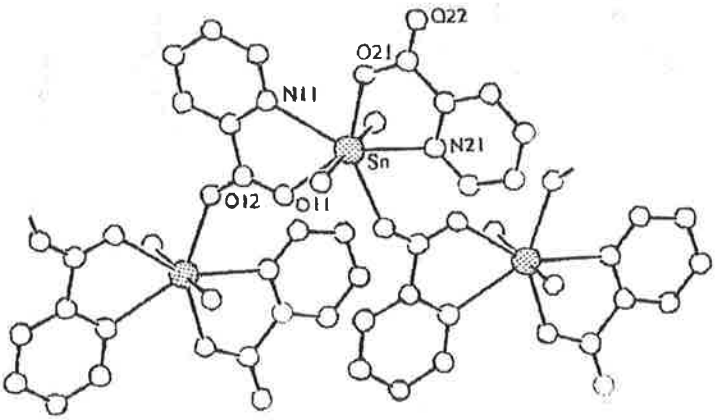


Figure 1.5
$[Me_2Sn(O_2CC_5H_4N\text{-}2)_2]$

By contrast, a monomeric structure is found for the R= Ph [18] analogue, $[Ph_2Sn(O_2CC_5H_4N\text{-}2)_2]$, as shown in Figure 1.6 [20]. For $[Ph_2Sn(O_2CC_5H_4N\text{-}2)_2]$, both the 2-pyridinecarboxylate ligands chelate the tin atom *via* the nitrogen, and one of the oxygen atoms, such that the oxygen atoms occupy positions approximately *trans* to each other. The two phenyl substituents, which occupy positions approximately *cis* to each other, complete a distorted octahedral geometry about the tin atom.

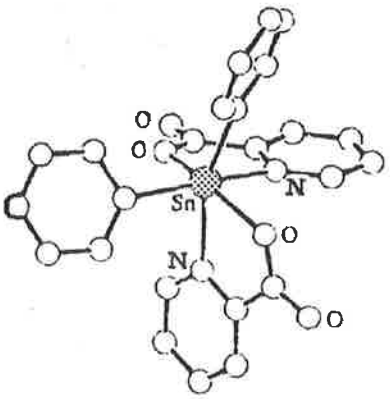


Figure 1.6
$[Ph_2Sn(O_2CC_5H_4N\text{-}2)_2]$

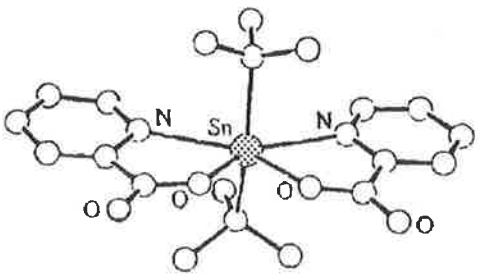


Figure 1.7
$[^tBu_2Sn(O_2CC_5H_4N\text{-}2)_2]$

A monomeric structure is also found in $[^tBu_2Sn(O_2CC_5H_4N\text{-}2)_2]$ [19], as illustrated in Figure 1.7 [20]. In this structure the two 2-pyridinecarboxylate ligands chelate the tin atom as for the R= Ph derivative, however, the two ligands are essentially co-planar with

the oxygen atoms *cis* to each other and the tertiary butyl groups *trans* to each other. Another difference relates to the strength of the Sn-N interactions. In the R= Ph structure the Sn-N distances are both 2.284(5) Å, whereas in [$^{t}Bu_2Sn(O_2CC_5H_4N\text{-}2)_2$], both Sn-N interactions are greater than 2.50 Å. Thus, the SnN_2O_2 plane is skew trapezoidal with the two organic substituents lying over the Sn-N bonds; the overall geometry is thus best defined as being based on a skew-trapezoidal bipyramid. Clearly, there are three different molecular geometries for the $R_2Sn(O_2CC_5H_4N\text{-}2)_2$ compounds, where R= Me, Ph and ^{t}Bu, which may be due to electronic and/or steric factors associated with the tin-bound R groups. This can not be the only rationalization for the diverse coordination geometries as shown by the structures described in 1.2.3 and 1.2.4.

1.2.3 Structural motifs for the Tetra-organo distannoxannes.

The greatest degree of structural diversity found among tin carboxylates is found among the diorganotin derivatives. There are four major structural types of dicarboxylato tetra-organo distannoxanes i.e. compounds of the general formula $\{[R_2Sn(O_2CR')]_2O\}_2$. The dominant form for compounds of this type is structural Type *A*. However, there is a wide representation of carboxylate-bound substituents among the different structural types and similarly, there is a wide variety of tin-bound substituents. There are no apparent trends that may suggest why one structural type may be favoured over another [4].

A common feature to all of the four different structural types is that they are all constructed about a centrosymmetric Sn_2O_2 core. Connected to this core, *via* the oxygen atoms, are two exocyclic tin atoms, Figure 1.8, producing a normally centrosymmetric $R_8Sn_4O_2$ framework. The structures differ from each other in the mode of association of four carboxylate ligands to the $R_8Sn_4O_2$ framework. The framework is quite rigid, with the geometric parameters showing little change among the structures.

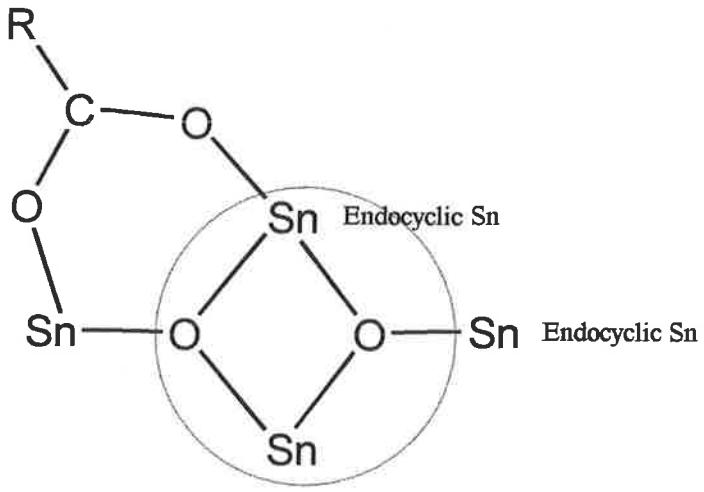


Figure 1.8

Centrosymmetric endocyclic Sn_2O_2 core

Most of the compounds with the general formula $\{[R_2Sn(O_2CR')]_2O\}_2$ adopt the Type *A* motif as illustrated in Figure 1.9A [4]. There are many examples of the Type *A* structures e.g. R= Me, Et, ^{n}Pr, ^{n}Bu and R'= CH_2Cl, ^{t}Bu, CH_2SPh and CCl_3 [21-24] respectively. In Type *A* structures bidentate bridging ligands are observed. Two of the carboxylate ligands bridge a pair of endo- and exo-cyclic tin atoms employing one oxygen atom to each tin atom i.e. bidentate bridging. The bridges are almost symmetrical. Each of the remaining two carboxylate ligands coordinates to one of the exocylic tin atoms *via* only one of the oxygen atoms with the non-coordinating oxygen atom directed away from the rest of the molecule (Figure 1.9A) i.e. monodentate coordination. Although there is evidence for a weak intramolecular interaction involving the endocyclic tin atom and oxygen atom of the monodentate carboxylate ligand, it is considered too long to be a significant interaction. Therefore, both the endo- and exo-cyclic tin atoms are five-coordinate and each exists in a distorted trigonal bipyramidal geometry.

The second structural type, Type *B*, for compounds of the general formula $\{[R_2Sn(O_2CR')]_2O\}_2$ has been observed in three cases for i) R= Me, R'= $(CH_2)_2C(O)Ph$ ii) R= ^{n}Bu, R'= $(CH_2)_2C(O)Ph$ and iii) R= Me, R'= $C_6H_4NH_2$-*p* [25-27]. The diagram for this motif is shown in Figure 1.9B [4]. The basic $R_8Sn_4O_2$ framework is retained. There are two major differences between Type *A* and *B*. Firstly, the bridging carboxylate ligand utilizes only one oxygen atom to link the

two tin atoms rather than two oxygen atoms. Secondly, the carboxylate ligand connected to the exocyclic tin chelates that tin atom asymmetrically, in contrast to the monodentate mode observed for Type *A* structures. The endocyclic tin atoms each exist in distorted trigonal bipyramidal geometries.

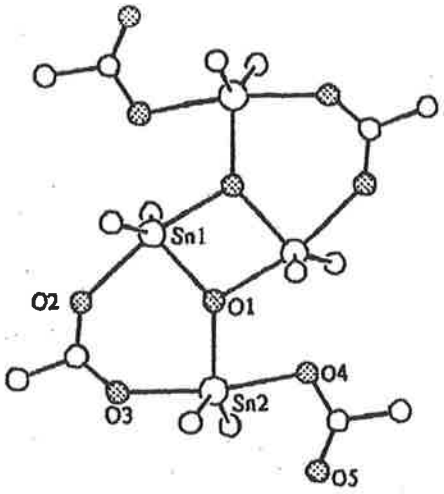


Figure 1.9A
Type A

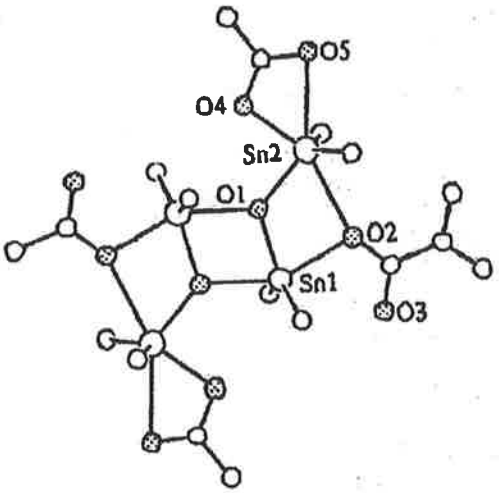


Figure 1.9B
Type *B*

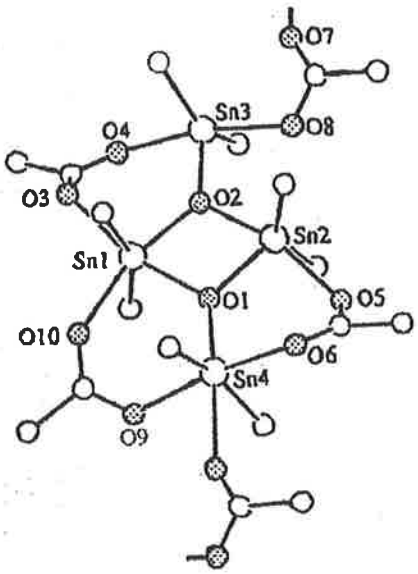


Figure 1.9C
Type *C*

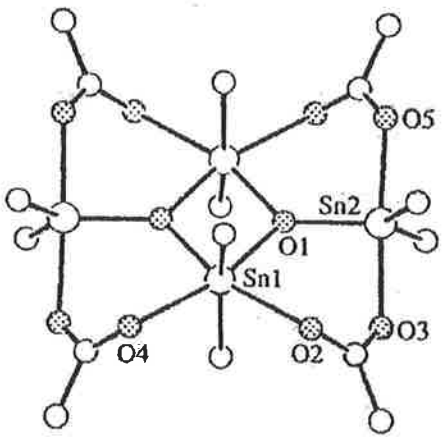


Figure 1.9D
Type *D*

The four different structural types of
$\{[R_2Sn(O_2CR')]_2O\}_2$

In contrast to all the other dicarboxylato tetra-organo distannoxane compounds, the structure of Type *C* $\{[R_2Sn(O_2CR')]_2O\}_2$, R, R'= Me [28] shown in Figure 1.9C [4], has no crystallographically imposed symmetry. Three pairs of endo- and exo-cyclic tin atoms in the $R_8Sn_4O_2$ framework are linked by symmetrically, bridging carboxylate ligands, which employ both oxygen atoms in their coordination. The fourth carboxylate ligand is also bridging, however, it serves to weakly connect (Sn...O' > 2.5 Å) symmetry related tetramers, thereby generating a chain of weakly associated tetramers. The geometries about the five-coordinate tin atoms are based on a distorted trigonal bipyramidal geometry. The six-coordinate tin atom geometries are distorted octahedral.

A fourth structural motif, Type *D* (Figure 1.9D [4]) for compounds with the general formula $\{[R_2Sn(O_2CR')]_2O\}_2$, has been found for two structures, R= Ph , R'= CCl_3 and R= Me and R'= ^tBu [22, 29]. The former has been shown to exist as a Type *A* structure as well. In this structural type, the four carboxylate ligands symmetrically bridge, using both oxygen atoms, each pair of endo- and exo-cyclic tin atoms in the $R_8Sn_4O_2$ framework. This configuration has the result that the endocyclic tin atom is a six-coordinate distorted octahedral, and the exocyclic tin atoms are five-coordinate, distorted trigonal bipyramidal.

1.2.4 Structural motifs for the Diorganotin(II) bis dithiolates.

The structural chemistry of 1,1-dithiolate tin compounds is as diverse as that of the carboxylates. The following survey provides evidence that suggests that there are no correlations between the nature of the tin-bound substituent and the structures found in the solid state [3]. The uni-negative ligands of this series include the dithiocarbamates $^-[S_2CNR_2]$, xanthates $^-[S_2COR]$ and dithiophosphates $^-[S_2P(OR)_2]$, where R= alkyl or aryl. For compounds with the general formula $R_2Sn(S_2Y)_2$ i.e. Y= CNR_2, COR or $P(OR)_2$, there are four major motifs that have been observed. The predominant motif is that shown in Figure 1.10 [3], and is illustrated by $[Me_2Sn(S_2CNMe_2)_2]$ [30].

The geometry about the tin atom is best described as skew-trapezoidal bipyramidal with the basal plane being defined by the four sulphur atoms derived from the asymmetrically chelating dithiolate ligands. For the dithiocarbamate structures that adopt this motif, the tin-bound substituents represented include R= Me, ^{n}Bu, ^{t}Bu and Cy [31-34], for the xanthates R= Me and Ph [35-36], and for the dithiophosphates R= Me and Ph [37-48]. Clearly, there is a broad representation of tin-bound substituents for this motif. Nevertheless, there are three other additional structural motifs found for the $R_2Sn(S_2Y)_2$ compounds.

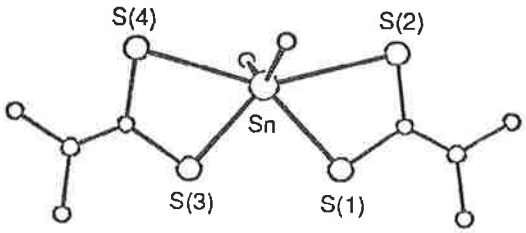


Figure 1.10

$[Me_2Sn(S_2CNMe_2)_2]$

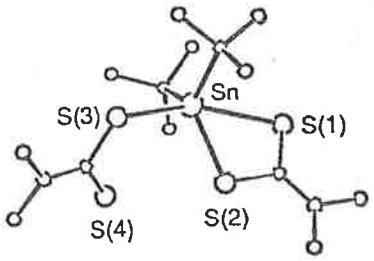


Figure 1.11

$[^{t}Bu_2Sn(S_2CNMe_2)_2]$

In the structure of $[^{t}Bu_2Sn(S_2CNMe_2)_2]$ [39] a five coordinate tin atom is present, as shown in Figure 1.11 [3]. The geometry about the tin atom is based on a distorted trigonal bipyramid with the trigonal plane defined by two carbon atoms and one of the sulphur atoms derived from the chelating dithiocarbamate ligand. The second dithiocarbamate ligand coordinates in the monodentate mode, there being no significant intra- or inter-molecular interaction of the pendant sulphur atom with a tin atom. Whereas for $[^{t}Bu_2Sn(S_2CNEt_2)_2]$ [33], a skew trapezoidal bipyramidal geometry is found, the substitution of ethyl for methyl in the dithiocarbamate ligands results in a distorted trigonal bipyramidal geometry.

A six-coordinate, distorted octahedral geometry is found in the structure of $[Ph_2Sn(S_2CNEt_2)_2]$ [40], as shown in Figure 1.12 [3]. In this structure the two dithiocarbamate ligands chelate the tin atom forming Sn-S distances that are far more symmetrical than those found in the structures that adopt the motif shown in Figure 1.10. The phenyl groups occupy approximately *cis* positions, i.e. C-Sn-C is *ca* 102° compared with the C-Sn-C angles in the range of 125-150° found in the predominant skew trapeziodal bipyramidyl motif, $[Me_2Sn(S_2CNEt_2)_2]$, Figure 1.10, described above.

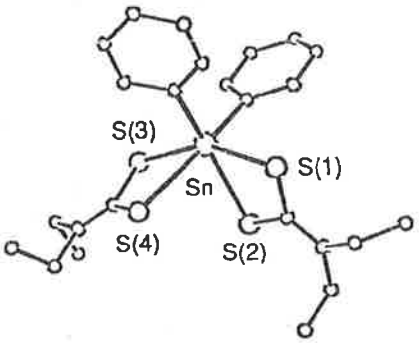


Figure 1.12

$[Ph_2Sn(S_2CNEt_2)_2]$

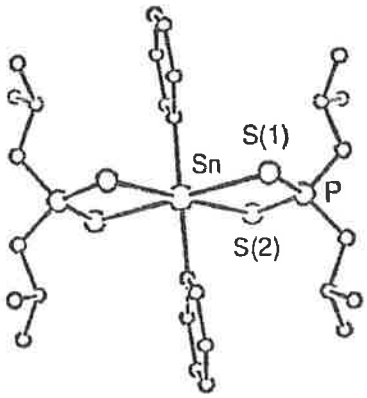


Figure 1.13

$[Ph_2Sn(S_2PO^iPr_2)_2]$

Symmetrical Sn-S distances are also found in the structure of $[Ph_2Sn(S_2P(O^iPr)_2]$ [41] represented in Figure 1.13 [3]. The tin atom in this structure is situated about a crystallographic centre of inversion, which constrains the C-Sn-C angle to 180°. Thus the replacement of the $^-[S_2CNEt_2]$ ligand in $[Ph_2Sn(S_2CNEt_2)_2]$ by the $^-[S_2P(O^iPr)_2]$ ligand results in a change from a *cis* arrangement of the phenyl substituents to a *trans* disposition.

1.3 Aim.

The foregoing survey reveals that major structural changes can be observed for closely related compounds. The aim of the work embodied in this thesis is to determine the reasons behind this observed structural diversity within diorganotin systems. It is possible that this structural diversity may be a consequence of electronic and/or steric effects of the diorganotin metal centre and/or ligand. Crystal packing may also influence the molecular structure of the diorganotin systems. It is understood that internal forces such as dipole/dipole (including hydrogen bonding) may influence the conformation of a particular residue but little is known about the weaker intermolecular forces upon molecular geometry and geometric parameters.

Diorganotin systems were chosen for this study for a number of reasons besides the general importance of these compounds. A number of diorganotin precursors are readily available thus enabling the introduction of small changes in the Lewis acidity of the tin centre whilst maintaining the remaining donor set in a consistent coordination geometry. Similarly, the steric profile of the R_2Sn^+ centres can be modified. The second major reason for this choice of diorgano system was the accessibility of ^{119}Sn nucleus for nuclear magnetic resonance studies in both the solid state and in solution.

As alluded to earlier it is essential that a series of diorganotin compounds without large distortions in tin atom geometry, i.e. compounds with minimal structural diversity be used in the investigations into steric and/or electronic factors that may produce structural diversity. The apparent lack of structural diversity will enable an investigation into the effects of moderating the Lewis acidity of the diorganontin centre (by varying the nature of R coordinated to the tin centre) upon the geometric parameters about the tin centre, (primarily the Sn-N and the Sn-Cl bond lengths) in the crystalline state. The monitoring of this factor is achieved through analysis of the derived interatomic parameters. Consequently, a series of diimine adducts of diorganotin dichloride, namely R_2SnCl_2(2,2'-bipyridyl), have been synthesized and fully characterized. Two R_2SnCl_2(2,2'-bipyridyl), compounds been characterized crystallographically prior to this study, namely R= Et [42] and Ph [43]. These structures feature distorted octahedral geometry with an approximate *trans* disposition of the tin-bound substituents, Figure 1.14 [43]. The apparent lack of structural diversity makes this an ideal series to investigate. To mirror this a series an additional diimine, 1,10-phenanthroline, was also selected and a similar series of, 1,10-phenanthroline dichloride diorganotin adducts, R_2SnCl_2(1,10-phenanthroline) were investigated. Two R_2SnCl_2(1,10-phenanthroline) adducts also been reported in the literature, R= ^nBu [44] and Ph [45] and these conform to the motif found for the R_2SnCl_2(2,2'-bipyridyl) adducts shown in Figure 1.15 [45].

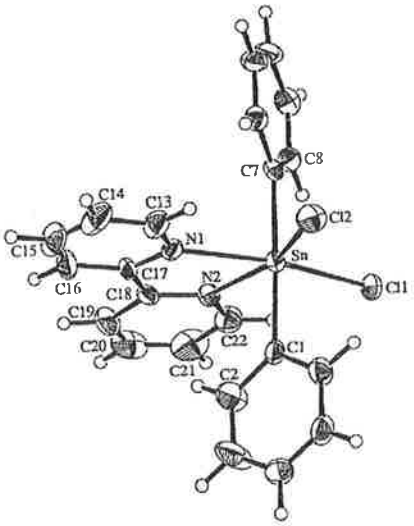


Figure 1.14

$[Ph_2SnCl_2(2,2'\text{-bipyridyl})]$

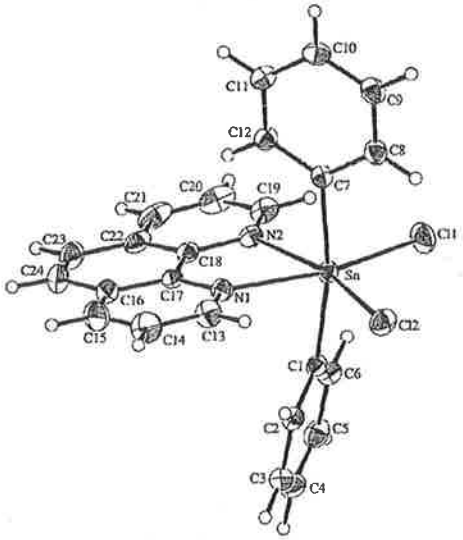


Figure 1.15

$[Ph_2SnCl_2(1,10\text{-phenanthroline})]$

In the literature [31 - 34], dithiocarbamate ligands have been identified to coordinate to metal centres in a variety of ways from monodentate to symmetric/asymmetric bidentate modes, Figures 1.16 and 1.17. The variation of the Lewis acidity of the diorganotin centre should influence the symmetry of the mode of coordination of the dithiocarbamate ligand.

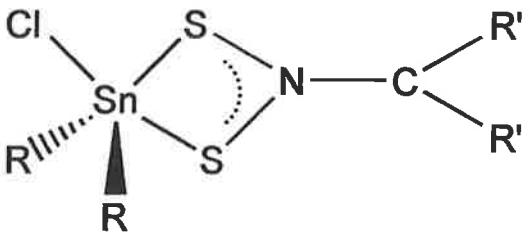


Figure 1.16

$R_2SnCl(S_2CNR'_2)$

Bidentate mode of coordination

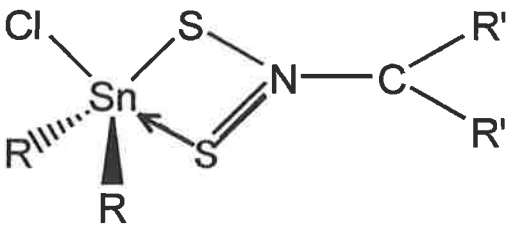


Figure 1.17

$R_2SnCl(S_2CNR'_2)$

Monodentate mode of coordination

The orgaontin dithiocarbamate system chosen for study was $R_2Sn(S_2CNR'R'')Cl$. Substitution of a dithiolate ligand in the $R_2Sn(S_2Y)_2$ compounds, described in section 1.2.4, by a Cl atom results in compounds of the general formulae $R_2Sn(S_2Y)Cl$. There are four instances of structurally characterized compounds in this category i.e.

R= Me [46], $(CH_2)_2CO_2Me$ [47], ^tBu [33] and Ph [33]. A representation of the $[Me_2Sn(S_2CNMe_2)Cl]$ [46] compound is given in Figure 1.18 [3]. The dithiolate ligands chelate the tin atom with disparate Sn-S bond distances although the degree of asymmetry is less than that found in the $R_2Sn(S_2Y)_2$ structures. The Sn atom exists in a distorted trigonal bipyramidal geometry in each case in which the trigonal plane is defined by the two organic substituents and the S atom forming the shorter Sn-S bond. The axial positions are occupied by the weakly coordinating S atom and the Cl atom.

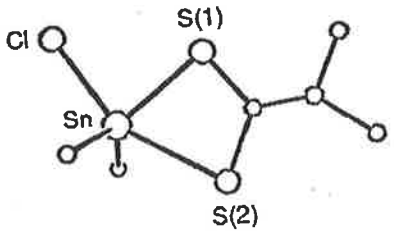


Figure 1.18

$[Me_2Sn(S_2CNMe_2)Cl]$

The mode of coordination of the dithiocarbamate ligand(s) i.e. the degree of symmetry can be monitored as the Lewis acidity is altered in diorganotin system. The dithiocarbamate system also allows an examination of the effect of the nitrogen-bound substituents upon molecular geometry.

The Lewis acidity of the tin centres of the chosen series of compounds i) R_2SnCl_2(2,2'-bipyridyl) ii) R_2SnCl_2(1,10-phenanthroline) iii) $R_2Sn(S_2CNR'R'')Cl$ can be moderated by varying the nature of R. If no extraneous factors are evident, the changes in interatomic parameters about the tin atom, at least, should mirror changes in the Lewis acidity of that centre.

The primary tool of investigation is single crystal X-ray diffraction. This will give, for the solid state, precise geometric information for molecular structures existing in a lattice. Correlations between the solid state and solution structure will be sought employing ^{119}Sn nuclear magnetic resonance (NMR) method wherever possible.

Compounds for which crystallographic data are available will be subjected to an *ab initio* geometry optimization. The availability of powerful computing resources now enables

calculations to be performed on once intractable metal-containing systems. For example, *ab initio* calculations have been employed recently to examine the nature of metal cation interactions with nucleobases [48], gold species with thionucleobases [49], zinc dithiophosphates [50], and bonding in transition metal systems [51]. Thus, while the influence of crystal packing on conformation has been investigated for organic systems [52], in particular with reference to polymorphism and crystal engineering through supramolecular associations, analogous studies involving the heavier elements is an emerging field.

The use of such calculations will enable an examination and correlation of geometric parameters of idealized structures, i.e. gas phase structures in the absence of intermolecular forces. The calculations reported here have been performed at the HF/LanL2DZ level of theory. This approach incorporates the use of the Effective Core Potential (ECP) [53] approximation in the treatment of the tin atoms. The Harteee-Fock (HF) theoretical approach makes no account of electron correlation in the reported geometry optimisations.

Cotton and Feng [54] have undertaken a Density Functional Theory (DFT) study focusing on geometry optimisations of a variety of transition metal-containing dinuclear compounds. The DFT approach includes some account of electron correlation. Cotton and Feng have shown that the ECP approximation within the DFT calculations predicts molecular geometries in good agreement with both experiment and theory, where the more conventional double zeta all electron basis sets are commonly employed. Maduara et al [55] have reported all electron DFT calculations that make structural predictions of Rh-containing species that are in good agreement with X-ray diffraction data.

The previous studies cited give us confidence that the ECP approximation is a valid approach for reporting molecular geometries of transition metal-containing species. It needs, however, to be ascertained that the lack of electron correlation in our treatment does not cast some doubt on the validity of the geometric results reported here. To this end, a series of calculations were performed to compare predicted geometries for two simpler Sn-containing compounds, [$MeSnCl_3$] and [Me_3SnCl], using both HF and DFT

levels of theory [56]. The results of the comparative study show that there is very good agreement in the geometric predictions generated by each theoretical approach and that there is no need to include electron correlation in predictions of molecular geometry for metal-containing compounds, particularly Sn-containing compounds.

The comparisons of the crystallographically determined structures with those employing *ab initio* geometry optimisations will enable firstly an examination of the influence of the solid state effects upon molecular geometry of systems with different packing arrangements, systems with solvent interactions and systems with high symmetry. Secondly the influence of solid state effects upon the molecular geometry of systems of varying tin centre Lewis acidity and minimal structural diversity can be examined.

It is known that the most stable crystal is the one in which molecules pack with the highest 'coordination number' i.e. to maximise forces of attraction. Do these intermolecular forces i.e. the crystal field of the van der Waals forces, modify molecular geometries? How likely is it that different structures arise as a result of a subtle combination of steric and/or electronic factors related to both main group element centre and/or the coordinating ligand? These are questions that will be examined in this thesis by employing a combined crystallographic/theoretical study.

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Chapter 2

Experimental Details

General Information:

All solvents used for recrystallisation and spectroscopy were dried over molecular sieves to ensure the absence of water.

Instrumentation:

2.1 Infrared Spectroscopy (IR).

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

2.2 Nuclear Magnetic Resonance Spectroscopy (NMR).

Solution NMR. Proton (^{1}H) and carbon-13 proton decoupled (^{13}C) NMR spectra were recorded on a Bruker ACP - 300 NMR spectrometer (The University of Adelaide) using a 5 mm ^{1}H and ^{13}C probe at 295K. 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 Me_4Si (TMS). Samples of approximately 60 - 100 mg were dissolved in approximately 0.6 ml of deuterated chloroform, $CDCl_3$, in 5 mm o.d. tubes. Composite pulse decoupling was used to remove any ^{1}H-^{13}C coupling. ^{1}H and ^{13}C spectra were acquired with spectral widths of 4 and 20 kHz and an acquisition time of 2 sec. A relaxation delay of 0 sec. was used together with a pulse width of 4 μsec (~90° pulse) respectively. Accumulation of 32 scans (^{1}H) and between 19000-30000 scans (^{13}C) was necessary before a high signal to noise ratio was achieved. Free induction decays (FID's) were multiplied by an exponential line broadening function (1 Hz) prior to Fourier transformation and processed using standard Bruker software.

Tin-119 proton decoupled (^{119}Sn) NMR spectra were measured in $CDCl_3$ solution on a Bruker ACP - 300 NMR spectrometer (The University of New South Wales) using a 10 mm broad band probe at 300K tuned to 111.92 MHz using tetramethyltin Me_4Sn as the external standard. Samples of approximately 60 - 100 mg were dissolved in

approximately 0.6 ml of $CDCl_3$ in 5 mm o.d. tubes. Composite pulse decoupling was used to remove any ^{1}H-^{119}Sn coupling. ^{119}Sn spectra were acquired with spectral widths of 45 kHz and an acquisition time of 0.18 sec. A relaxation delay of 1.2 sec. was used together with a pulse width of 24 μsec pulse width (90° pulse). These conditions were more than adequate to prevent saturation since the ^{119}Sn T_1 values were less than 2 seconds in solution. Between 100 - 3000 scans were accumulated before a high signal to noise ratio was achieved. Free induction decays (FID's) were multiplied by an exponential line broadening function (1 - 2 Hz), zero-filled to 32 K data points prior to Fourier transformation. T_1 data were acquired using an inversion-recovery sequence (-180-*t*-90-acquire), and processed using standard Bruker software.

The results from the ^{1}H and ^{13}C solution NMR studies for each compound are described in this chapter. ^{119}Sn solution NMR studies were performed on discrete samples of compounds. The results of the solution ^{119}Sn NMR of the selected compounds studied here are described in section 2.6.1 of this chapter.

2.3 Melting Points.

All melting points were determined using a Gallemkamp melting point apparatus calibrated with benzil (m. pt. 94 - 95 °C).

2.4 Crystallography.

Crystal data and refinement details for each structure determined for this thesis are listed in the appendices following the chapters in which the molecular structures are first presented. This section serves only to outline the general procedures for each analysis.

All crystals were mounted on a glass fiber using cyanoacrylate glue. All data collections were performed at room temperature (293 K) unless stated otherwise.

Intensity data were measured on a Rigaku diffractometer fitted with either Mo$K\alpha$ radiation (graphite monochromator; λ= 0.71073 Å), or Cu$K\alpha$ radiation, (Ni-filtered; λ= 1.5418 Å). In each case the unit cell dimensions were determined from the

least - squares refinement of the setting angles of 25 (20 for Cu radiation) carefully centered reflections. The ω:2θ scan technique was employed to measure data up to a maximum Bragg angle θ_{max} of 27.5° for Mo$K\alpha$ or 60° for Cu$K\alpha$ radiation. The net intensity values of three standard reflections, remeasured after every 400 intensity measurements, generally showed no significant change in any of the data collections indicating crystal and machine stability. The specific cases where the data sets were corrected for decay are indicated in the relevant sections where the molecular structure is first described. The data sets were corrected for Lorentz and polarization effects [1] and for absorption effects employing an empirical correction [2]. Of the reflections measured, only those that satisfied the $I \geq 3.0\sigma(I)$ criterion of observability were used in the subsequent analysis.

All structures were solved by direct-methods [3-5], and each refined by a full-matrix least-squares procedure based on F [1]. The function minimised was

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

where n is the number of reflections used and (generally)

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

i.e. a sigma weighting scheme; in some refinements, unit weights were applied.

Non-hydrogen atoms were refined with anisotropic thermal displacement parameters (where possible) and hydrogen atoms were included in their calculated positions (C-H 0.97 Å). A sigma weighting scheme (above equation) was applied and the refinement was continued until convergence in each case. The values of R and R_w are calculated as,

$$R = \frac{\sum_{i=1}^{n} (|F_{obs}|_i - |F_{calc}|_i)}{\sum_{i=1}^{n} |F_{obs}|_i} \qquad \text{and} \qquad R_w = \left\{ \frac{\sum_{i=1}^{n} w_i(|F_{obs}|_i - |F_{calc}|_i)^2}{\sum_{i=1}^{n} w_i(|F_{obs}|_i^2} \right\}^{\frac{1}{2}} .$$

The analysis of variance for each refinement revealed no special features indicating that an appropriate weighting scheme had been applied.

In some cases where necessary, a correction was applied for secondary extinction effects [6] (instances where this correction was applied are indicated in the section where the relevant molecular structure is first described). All scattering factors were as incorporated in the teXsan software package [1] which was installed on a Silicon Graphics Iris Indigo Workstation. Tables of bond distances and bond angles, fractional atomic coordinates, anisotropic thermal parameters, hydrogen-atom parameters, and structure factors for all determinations are located in the Appendices following the chapter where the molecular structure is first described. The expression for the anisotropic thermal parameter used is

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

and the expression for B_{eq} is

$$B_{eq} = \frac{8\pi^2(U_{11} + U_{22} + U_{33})}{3} \quad .$$

All diagrams were drawn utilizing the ORTEP program [7] with variable probability levels as specified in the relevant sections.

The expression for Goodness-Of-Fit (S, the standard deviation of an observation of unit weight) is

$$S = \frac{\Sigma(|F_{obs}|_i - |F_{calc}|_i)/\sigma_i}{(n - m)}$$

where n is the number of reflections used in the refinement and m is the number of variables.

2.5 *Ab initio* Calculations.

All geometry optimisations were performed using the GAUSSIAN 94 suite of programs [9] run on Silicon Graphics Indigo^{2}xZ Workstation and Silicon Graphics Power Challenge computers. All calculations were performed at the Hartree-Fock SCF level of theory using the LanL2DZ basis set [9]. The LanL2DZ basis set employs the Dunning/Huzinaga double zeta descriptor [10] for all first row elements and replaces the core electrons of sulphur (up to 2*p*), chlorine (up to 2*p*), and tin (up to 4*p*) with the effective core potentials (ECPs) of Hay and Wadt [11]

Synthetic Summary:

2.6 Chemicals.

The chemicals used in the syntheses of the complexes and their sources were:

Sodium hydroxide (Ajax), carbon disulfide (Ajax), dicyclohexyl-, diethyl- and cyclohexylethyl-amine (Aldrich), 1,10-phenanthroline (Ajax), 2,2'-bipyridyl (BDH), diphenyl- and dibutyl- (Aldrich), dimethyl-tindichlorides and divinyltindichloride (Strem). All chemicals were used without further purification. Dibenzyl-, dicyclohexyl-, phenylmethyl- and diisopropyl-tindichlorides were gifts from Professor Klaus Jurkschat, Universitat Dortmund (Germany), and were also used without further purification. All solvents employed were of analytical grade.

2.6.1 ^{119}Sn NMR Spectroscopic characterisation of R_2SnCl_2.

Details of solution ^{119}Sn NMR spectroscopic characterization of R_2SnCl_2 are provided below Table 2.6.1. ^{119}Sn chemical shifts (δ, ppm) for R_2SnCl_2 in chloroform solution are given. No coupling constants were observed.

Table 2.6.1: ^{119}Sn NMR data for R_2SnCl_2 where: R_2= (Ph, Me) and R = Me, ^{n}Bu, ^{i}Pr, ^{t}Bu, Cy, Bz, Ph and Vin.

R_2SnCl_2	
R_2 =	δ_{Sn} (ppm)
Me_2	141.9
$^{n}Bu_2$	126.6
$^{i}Pr_2$	92.8
Cy_2	72.2
(Ph, Me)	56.5
$^{t}Bu_2$	54.3
Bz_2	34.7
Ph_2	-27.9
Vin_2	-31.5

2.7 Preparation of Starting Materials.

2.7.1 Sodium N, N-dicyclohexyldithiocarbamate: $Na[S_2CN(Cy)_2]$.

The sodium salt of $^-S_2CN(Cy)_2$ anion was prepared from the slow addition of CS_2 (15.2 gm, 0.2 mol) into an ice-cold solution of $(Cy)_2NH$ (39.9 cm^3, 0.2 mol) and 10 M NaOH (20 cm^3, 0.2 mol). After 30 minutes of stirring, the volume of solution was reduced under vacuum and filtered producing a yellow powder. The resulting yellow powder was washed with diethyl ether and with chloroform. The compound was stored under an inert atmosphere and used without further purification; m. pt. 235 - 237 °C (dec.).

2.7.2 Sodium N-ethyl, N-cyclohexyldithiocarbamate: $Na[S_2CNCyEt]$.

The sodium salt of the $^-S_2CNCyEt$ anion was prepared from the slow addition of CS_2 (15.2 gm, 0.2 mol) into an ice-cold solution of CyEtNH (25.0 cm^3, 0.2 mol) and 10 M NaOH (20 cm^3, 0.2 mol). After 30 minutes of stirring, the volume of solution was reduced under vacuum and filtered producing a yellow powder. The resulting yellow powder was washed with diethyl ether and with chloroform. The resulting compound was stored under an inert atmosphere and used without any further purification; m. pt 101 - 103 °C (dec.).

2.7.3 Sodium N, N-diethyldithiocarbamate: $Na[S_2CN(Et)_2]$.

The sodium salt of the $^-S_2CN(Et)_2$ ligand was prepared as reported in the literature [12].

2.8 Preparation of diimine adducts of diorganotindichlorides [R_2SnCl_2(diimine)].

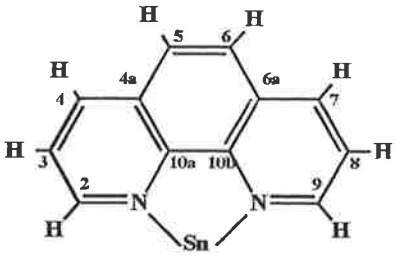
The diimine adducts of the diorganotindichlorides, R_2SnCl_2(1,10-phenanthroline) and R_2SnCl_2(2,2'-bipyridyl), were all prepared in an analogous manner. Hence, the preparation of only one adduct is described below. Methods for the recrystallisation of the adducts to produce single crystals suitable for X-ray diffraction studies are specific to the individual adduct and are detailed in the relevant chapters where the molecular structure is first described. Physical appearance, yields and melting points are listed in Tables 2.8.1a (for the 1,10-phenanthroline adducts) and 2.8.1b (for the 2,2'-bipyridyl adducts). The compounds prepared had R= Me, ^{n}Bu, ^{i}Pr, Cy, Bz and Vin and R_2= (Me, Ph).

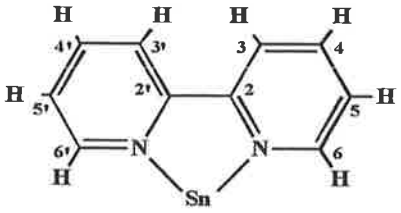
2.8.1 Preparation of [Me_2SnCl_2(1,10-phenanthroline)].

Dimethyltindichloride, Me_2SnCl_2, (0.2 gm, 1 mole equivalent) was dissolved in hot benzene (200 cm^3) and added dropwise to 1,10-phenanthroline (0.19 gm, 1.1 mole equivalent), which is dissolved in a hot, stirred benzene/chloroform mixture (9:1 *v/v*, 100 cm^3). After the addition of Me_2SnCl_2 was completed, the mixture was stirred at room temperature for a further hour. The volume of the solution was reduced under vacuum. The crude product, a white solid, was recrystallised from a warm chloroform/acetonitrile (8:2 *v/v*, 5 cm^3) mixture. Physical data for all adducts can be found in Table 2.8.1*a*, and 2.8.1*b*.

Details of spectroscopic characterization for the 1,10-phenanthroline (*a*) and 2,2'-bipyridyl (*b*) compounds: FTIR (Tables 2.8.2*a, b*) and ^{1}H solution NMR (Tables 2.8.3*a, b*) and ^{13}C solution NMR (Tables 2.8.4*a, b*); are provided below. Coupling constants are quoted only when observed.

Examples of tin-bound ligands are schematically shown below in Figure 2.1 in order to illustrate the numbering scheme employed for the interpretation of spectroscopic results. Examples of the FTIR, ^{1}H, and ^{13}C solution NMR spectra for these compounds are provided in Figures 2.2, 2.3 and 2.4 respectively.

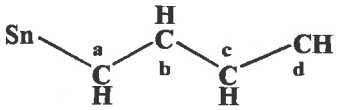


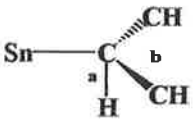


Diimine ligands

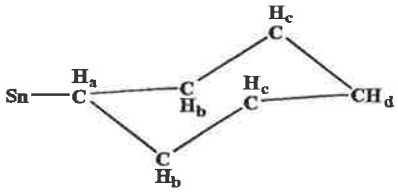
1,10-phenanthroline *2,2'-bipyridyl*

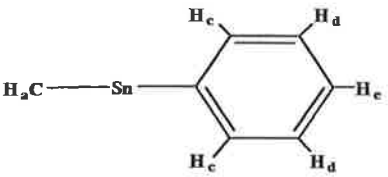




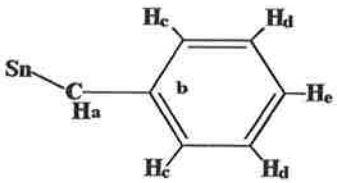


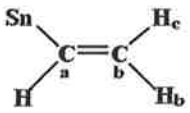
$R_2 = Me$ $R_2 = {}^{n}Bu$ $R_2 = {}^{i}Pr$





$R_2 = Cy$ $R = Me, Ph$





$R_2 = Bz$ $R_2 = Vin$

Sn-bound substituents of R_2SnCl_2

Figure 2.1
Numbering scheme for R_2SnCl_2(2,2'-bipyridyl) and R_2SnCl_2(1,10-phenanthroline)

Table 2.8.1a: Physical data for the 1,10-phenanthroline dichlorodiorganotin adducts:
R_2SnCl_2(1,10-phenanthroline); R_2 = (Me, Ph) and
R =Me, ^{i}Pr, Cy and Bz.

	R_2SnCl_2(1,10-phenanthroline)		
R =	**Yield (%)**	**Appearance**	**Melting point (°C)**
Me	42.1	Colourless crystals	264 (dec)
^{i}Pr	66.0	Colourless crystals	228-230
Cy	70.8	Yellow crystals	271-272
(Ph, Me)	70.7	Colourless crystals	207-209
Bz	29.6	Orange crystals	220-221

Table 2.8.1b: Physical data for the 2,2'-bipyridyl dichlorodiorganotin adducts:
R_2SnCl_2(2,2'-bipyridyl); R_2 = Me, Ph and
R = Me, ^{n}Bu, ^{i}Pr, Bz, and Vin.

	R_2SnCl_2(2,2'-bipyridyl)		
R =	**Yield (%)**	**Appearance**	**Melting point (°C)**
Me	67.3	Colourless crystals	235-237
^{n}Bu	39.7	Colourless crystals	180-181
^{i}Pr	63.5	Colourless crystals	201-202
(Ph, Me)	72.6	Colourless crystals	253-254
Bz	71.1	Yellow crystals	215-217
Vin	90.8	Colourless crystals	202-203

Table 2.8.2a: Selected infrared absorptions (cm^{-1}) for the 1,10-phenanthroline dichlorodiorganotin adducts: R_2SnCl_2(1,10-phenanthroline); R_2 = (Me, Ph) and R = Me, ^{i}Pr, Cy and Bz.

	R_2SnCl_2(1,10-phenanthroline)		
R=	**ν(C= N)**	**ν(C= C)**	
Me	1623(m)	1520(s)	1435(s)
^{i}Pr	1626(w)	1516(s)	1426(s)
Cy	1622(m)	1519(s)	1429(s)
(Ph, Me)	1623(m)	1520(s)	1426(s)
Bz	1617(m)	1521(s)	1428sb

s= strong, m= medium, w= weak, sb= shoulder broad.

Table 2.8.2b: Selected infrared absorptions (cm^{-1}) for the 2,2'-bipyridyl dichlorodiorganotin adducts: R_2SnCl_2(2,2'-bipyridyl); R_2= Me, Ph and R= Me, ^{n}Bu, ^{i}Pr, Bz and Vin.

	R_2SnCl_2(2,2'-bipyridyl)			
R =	**ν(C= N)**		**ν(C= C)**	
Me	1574(m)	1566(m)	1441(s)	1411sh
^{n}Bu	1575(m)	1564(m)	1442(s)	1414sh
^{i}Pr	1575(m)	1564(m)	1440(s)	NO
(Ph, Me)	1574(m)	1564(m)	1440(s)	NO
Bz	1574(s)	1565sh	1440(s)	1411(w)
Vin	1575(m)	1566(m)	1441(s)	NO

s= strong, m= medium, w= weak, sh= shoulder and NO= not observed.

Table 2.8.3a: ^{1}H NMR data for the 1,10-phenanthroline dichlorodiorganotin adducts: R_2SnCl_2(1,10-phenanthroline); R_2= (Me, Ph) and R= Me, ^{i}Pr, Cy and Bz.

	1,10-phenanthroline				R_2Sn-				
R_2 =	H_{29}	H_{47}	H_{56}	H_{38}	H_a	H_b	H_c	H_d	H_e
Me	9.81 dd (4.64^a, 1.21^b)	8.67 dd (8.09^a, 1.50^b)	8.12 s	8.03 dd (8.13^a, 4.78^b)	1.15 s (108.4^c, 103.6^d)				
^{i}Pr	9.77 dd (4.82^a, 1.50^b)	8.62 dd (8.22^a, 1.48^b)	8.07 s	7.95 dd (8.18^a, 4.84^b)	2.02 sept (7.18^a)	1.06 d (7.22^a			
Cy	9.79 dd (4.86^a, 1.46^b)	8.72 dd (8.13^a, 1.59^b)	8.16 s	8.04 dd (8.21^a, 4.86^b)	2.12 tt (11.7^a, 3.1^b)	← 0.90 – 2.02 m →			
(Ph, Me)	9.86 m	8.56 d (8.37^a)	8.00 s	7.64 m	1.21 s		← 6.85 – 7.19 m →		
Bz	9.28 dd (4.90^a, 1.54^b)	8.32 dd (8.23^a, 1.48^b)	7.78 s	7.67 dd (8.04^a, 4.91^b)	3.24 bs (146.3^c, 139.7^d)		6.17 - 6.28 m	← 6.05 - 6.16 m →	

coupling constants (Hz) are in parentheses: a= ^{3}J(HH), b= ^{4}J(HH), c= ^{2}J(^{119}SnH), d= ^{2}J(^{117}SnH)
s= singlet, d= doublet, dd= doublet of doublets, t= triplet, tt= triplet of triplets, sept= septet, sx= sextet, bs=broad singlet m= multiplet.

Table 2.8.3b: ^{1}H NMR data for the 2,2'-bipyridyl dichlorodiorganotin adducts: R_2SnCl_2(2,2'-bipyridyl); R_2= (Me, Ph) and R= Me, ^{n}Bu, ^{i}Pr, Bz and Vin.

	2,2'-bipyridyl				R_2Sn-				
R_2=	$H_{66'}$	$H_{33'}$	$H_{44'}$	$H_{55'}$	H_a	H_b	H_c	H_d	H_e
Me	9.32 d (4.48[a])	8.37 d (8.17[a])	8.12 dt (7.84[a] 1.66[b])	7.64 dt (7.10[a] 0.89[b])	1.10 s (100.3[d] 96.2[e])				
^{n}Bu	9.12 d (4.54[a])	8.49 d (8.03[a])	8.11 dt (7.84[a] 1.76[b])	7.61 ddd (7.57[a] 5.18[b] 0.95[c])	1.61 - 1.67 m	1.48-1.54 m	1.20 sx (7.25[a])	0.75 t (7.31[a])	
^{i}Pr	9.35 d (4.95[a])	8.38 d (8.27[a])	8.13 m	7.62 m	2.05 sept (7.23[a])	1.16 bs			
(Ph, Me)	8.93 d (5.07[a])	8.59 d (8.13[a])	8.08 m	7.74 m	1.17 s	← 7.52 - 8.53 m →			
Bz	9.12 d (5.19[a])	8.40 d (8.10[a])	7.97 dt (8.12[a] 1.70[b])	7.45 ddd (7.56[a] 5.34[b] 0.97[c])	3.23 bs (146.3[d] 139.7[e])		6.55 - 6.60 m (33.7[f] 27.0[g])	6.37- 6.41 m (37.6[h])	1.11 - 1.40 m
Vin	9.43 bs	8.33 d (8.12[a])	8.20 dt (7.82[a] 1.65[b])	7.72 ddd (7.35[a] 5.41[b] 1.0[c])	6.53 bs	← 5.88 bs →			

coupling constants are in parentheses: a= ^{3}J(HH), b= ^{4}J(HH), c= ^{5}J(HH), d= ^{2}J(^{119}SnH), e= ^{2}J(^{117}SnH), f= ^{3}J(^{119}SnH), g= ^{3}J(^{117}SnH), h= ^{4}J(^{119}SnH),
s= singlet, bs=broad singlet, d= doublet, dd= doublet of doublets, ddd= doublet of doublets of doublets, t= triplet, dt= doublet of triplets, tt= triplet of triplets, sx= sextet, m= mu

Table 2.8.4a: ^{13}C NMR data for 1,10-phenanthroline dichlorodiorganotin adducts: R_2SnCl_2(1,10-phenanthroline); R_2 = (Me, Ph) and R= Me, ^{i}Pr, Cy and Bz.

	1,10-phenanthroline						R_2Sn-				
R_2 =	C_{29}	$C_{10a,10b}$	C_{47}	$C_{4a,4b}$	C_{56}	C_{38}	C_a	C_b	C_c	C_d	C_e
Me	148.7	**NO**	139.5	129.9	127.5	125.3	29.7 (930.2[a] 910.6[b])				
^{i}Pr	150.0	140.9	139.8	129.7	127.5	125.0	45.2 (933.8[a] 977.7[b])	21.4 (34.7[c])			
Cy	149.6	**NO**	140.0	129.7	127.5	125.0	54.2	31.0 (36.5[c])	29.0 (132.4[e])	26.4 (15.5[g])	
(Ph, Me)	148.7	**NO**	139.4	129.9	127.5	125.2	29.7	145.2	135.9	127.9	129.7
Bz	148.4	140.2	139.4	139.1	126.7	124.9	51.3 (958.1[a] 914.3[b])	138.4 (93.4[c])	127.4 (59.5[e])	123.8 (47.6[g])	126.6 (40.2[h])

coupling constants are in parentheses: a= $^{1}J(^{119}SnC)$, b= $^{1}J(^{117}SnC)$, c= $^{2}J(^{119}SnC)$, d= $^{2}J(^{117}SnC)$, e= $^{3}J(^{119}SnC)$, f= $^{3}J(^{117}SnC)$, g= $^{4}J(^{119}SnC)$, h= $^{5}J(^{119}SnC)$, NO= not observed.

Table 2.8.4b: ^{13}C NMR data for the 2,2'-bipyridyl dichlorodiorganotin adducts: $[R_2SnCl_2(2,2'\text{-bipyridyl})]$; R_2 = Me, Ph and R_2= Me, ^{n}Bu, ^{i}Pr, Bz and Vin.

	2,2'-bipyridyl					R_2Sn-				
R_2 =	$C_{22'}$	$C_{66'}$	$C_{44'}$	$C_{55'}$	$C_{33'}$	C_a	C_b	C_c	C_d	C_e
Me	**NO**	147.8	141.3	126.7	123.4	24.6				
^{n}Bu	149.7	148.1	140.7	126.2	122.9	39.3	27.6 (41.2[c])	26.1 (182.0[e])	13.5 (9.88[g])	
^{i}Pr	151.9	149.6	139.4	125.5	121.8	41.0	20.9 (30.0[c])			
(Ph, Me)	150.4	**NO**	140.1	126.7	123.5	29.1	144.8	136.7	**NO**	128.9
Bz	161.6	148.2	140.4	139.5	120.9	51.1 (934.5[a] 913.5[b])	139.5 (97.1[c])	127.7 (59.5[e])	124.0 (46.6[g])	127.3 (39.8[h])
Vin	150.9	147.2	140.5	128.3	122.2	148.0 (884[c])	129.7			

coupling constants are in parentheses: a= $^{1}J(^{119}SnC)$, b= $^{1}J(^{117}SnC)$, c= $^{2}J(^{119}SnC)$, d= $^{2}J(^{117}SnC)$, e= $^{3}J(^{119}SnC)$, f= $^{3}J(^{117}SnC)$, g= $^{4}J(^{119}SnC)$, h= $^{5}J(^{119}SnC)$, NO= not observed

Figure 2.2: FTIR Spectra of [$^{n}Bu_2SnCl_2$(2,2'-bipyridyl)].

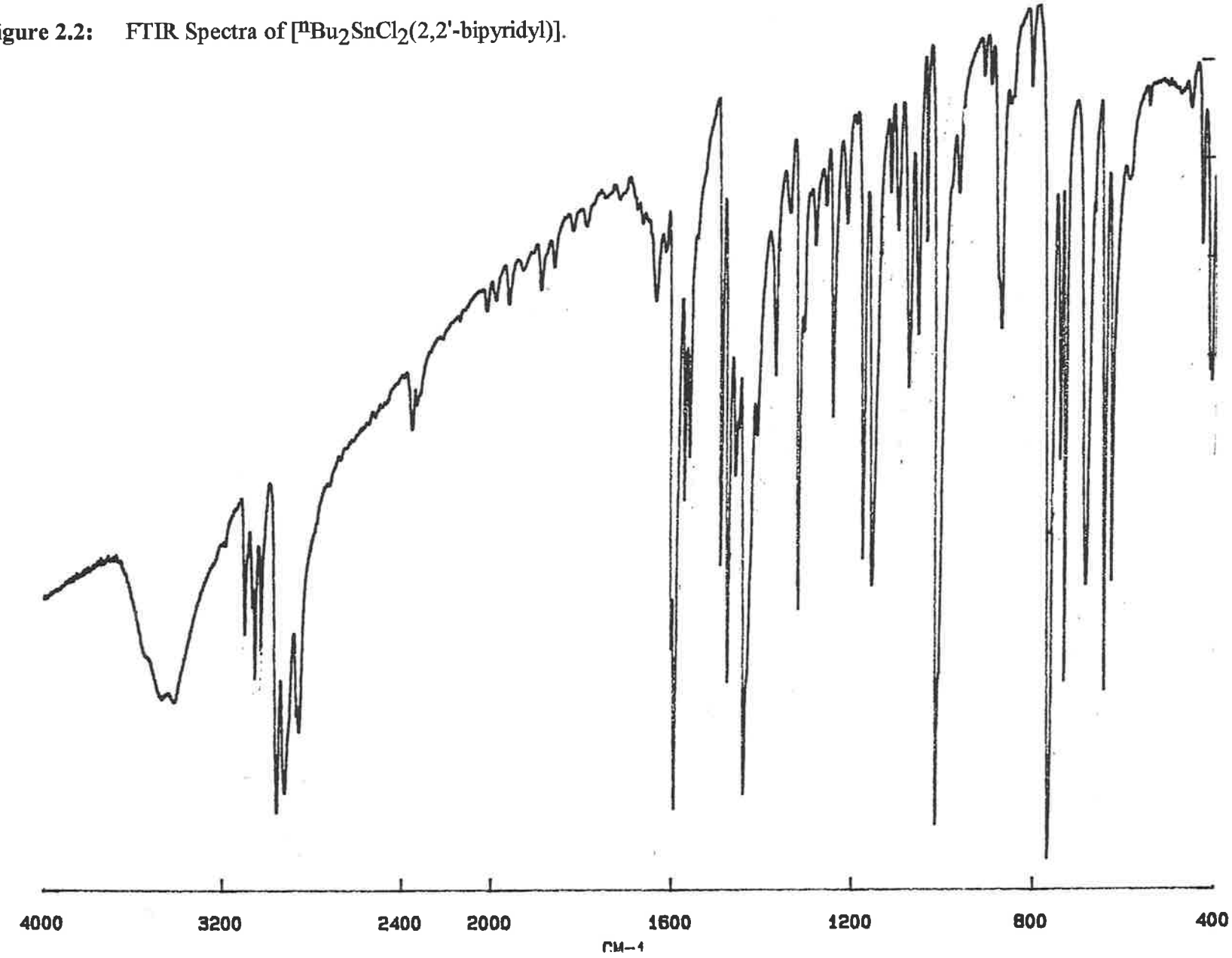


Figure 2.3: ^{1}H NMR Spectra of [$^{i}Pr_2SnCl_2$(1,10-phenanthroline)].

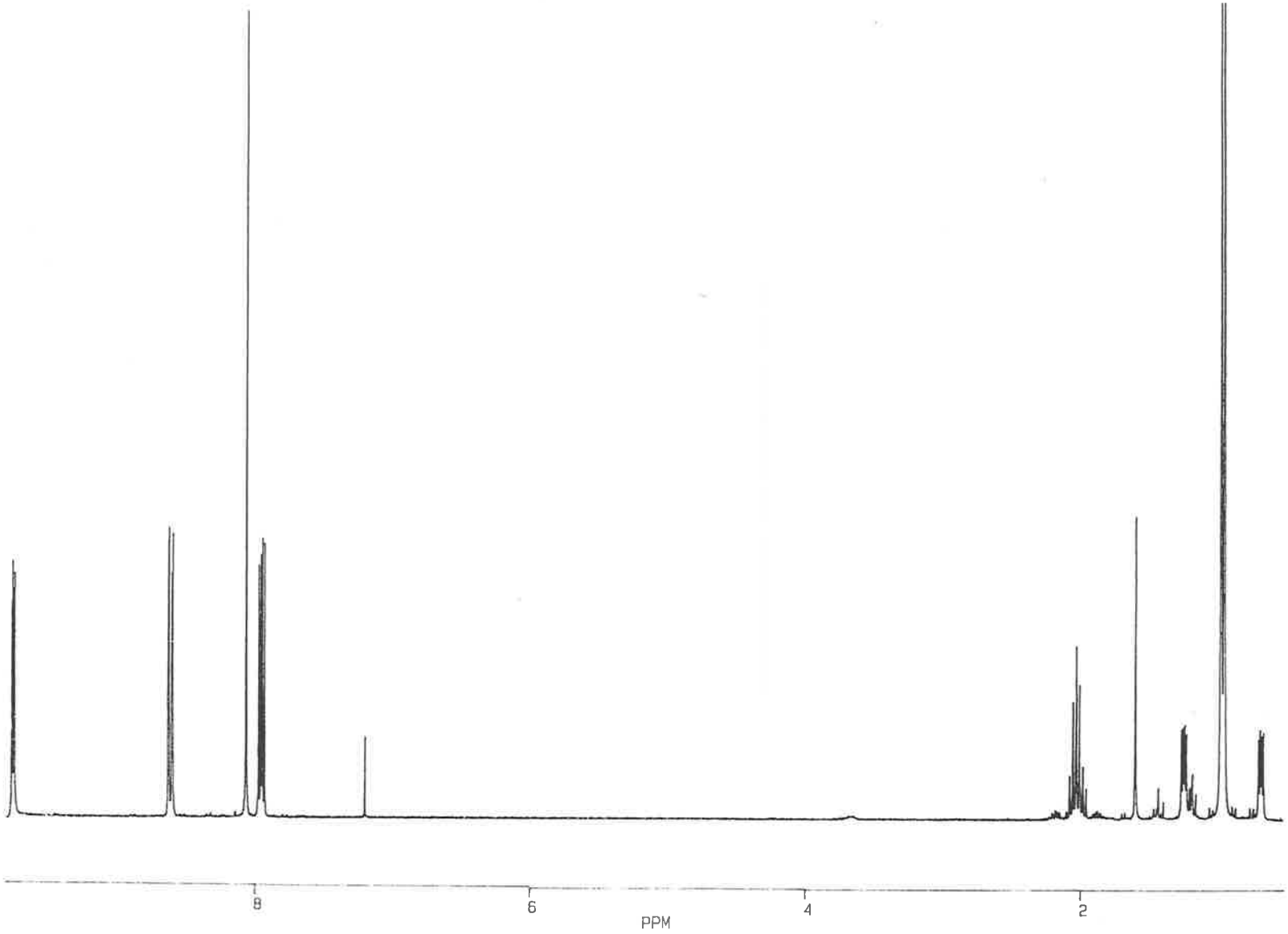
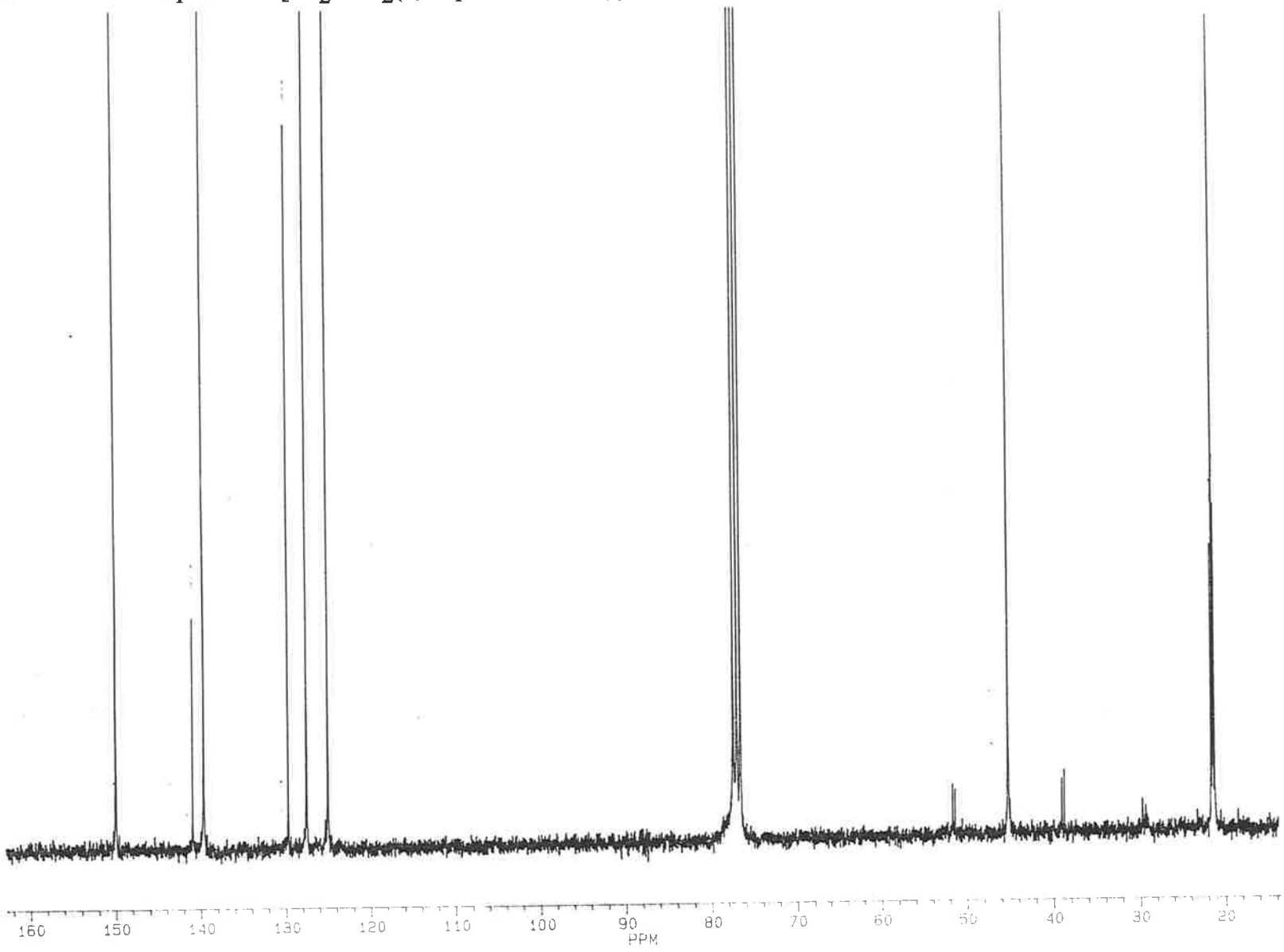


Figure 2.4: ^{13}C NMR Spectra of $[^{i}Pr_2SnCl_2(1,10\text{-phenanthroline})]$.



2.9 Preparation of diorganotinchloride *N, N*-diorganodithiocarbamates $R_2Sn(S_2CNR'_2)Cl$.

The synthesis of diorganotinchloride *N, N*-diorganodithiocarbamates involved the (1:1) reaction of the appropriate diorganotindichloride species with either *N N*-diethyldithiocarbamate, *N, N*- dicyclohexyldithiocarbamate or *N*- cyclohexyl, *N*- ethyldithiocarbamate. Since the method of preparation is analogous for the three types of compounds, irrespective of the nature of organo groups, only a description of the preparation of one of the complexes is described below. Methods of recrystallisation of adducts to produce single crystals suitable for X-ray diffraction are specific to the individual compound and are detailed in the relevant chapters where it's molecular structure is described. Physical appearance, yields and melting points are listed in Tables 2.8.1a, 2.8.1b and 2.8.1c. The compounds prepared had R= Me, Cy or ^{t}Bu and R'= Et, Cy and R'_2 = (Et, Cy).

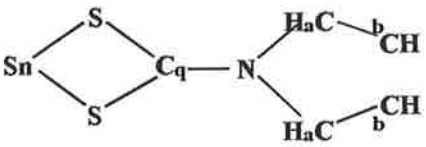
2.9.1 Preparation of $Me_2Sn(S_2CN(Et)_2)Cl$.

The reaction involved the dropwise addition of dimethyltindichloride Me_2SnCl_2 (0.20 gm, 1 molar equivalent) which was dissolved in hot ethanol (20 cm^3) to a hot solution of sodium diethyldithiocarbamate (0.17 gm, 1.1 molar equivalent) dissolved in ethanol (20cm^3) with stirring for an hour to allow for complete reaction. The solvent was reduced under vacuum and a powder precipitated. The powder was filtered off and recrystallised from chloroform.

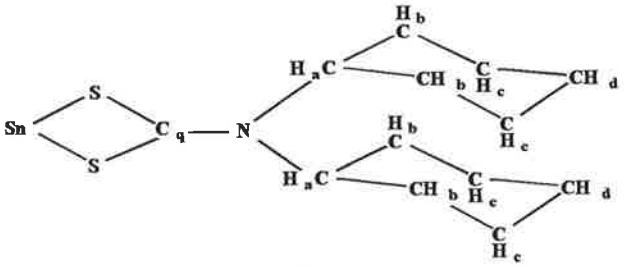
Details of spectroscopic analysis of the *N N*-diethyldithiocarbamate (*a*), *N, N*- dicyclohexyldithiocarbamate (*b*) or *N*- cyclohexyl, *N*- ethyldithiocarbamate (*c*) compounds: FTIR (Tables 2.9.2*a,b,c*), ^{1}H solution NMR (Tables 2.9.3*a,b,c*) and ^{13}C solution NMR (Tables 2.9.4*a,b,c*); are provided below. Coupling constants are quoted where observed.

Examples of tin-bound ligands are schematically shown below in Figure 2.4 in order to illustrate the numbering scheme employed for the interpretation of spectroscopic results.

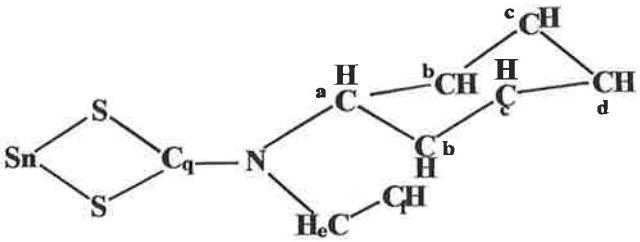
Examples of the FTIR, ^{1}H and ^{13}C NMR spectra for these compounds are provided in Figures 2.5, 2.6 and 2.7, respectively.



N,N-diethyl dithiocarbamate

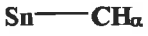


N,N-dicyclohexyldithiocarbamate

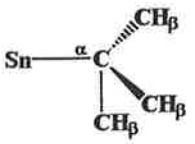


N-ethyl, N-cyclohexyl dithiocarbamate

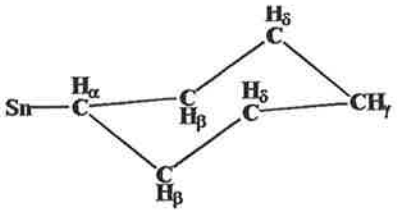
Dithiocarbamate ligands



R = Me



R = tBu



R = Cy

Sn-bound substituents of R_2SnCl_2

Figure 2.4.
Numbering scheme for $R_2Sn(S_2CN(Et)_2)Cl$, $R_2Sn(S_2CN(Cy)_2)Cl$ and $R_2Sn(S_2CN(Et)Cy)Cl$

Table 2.9.1a: Physical data for the diorganotinchloride *N,N*-diethyldithiocarbamates: $R_2Sn(S_2CN(Et)_2)Cl$; R= Me and Cy.

	$R_2Sn(S_2CN(Et)_2)Cl$		
R=	**Yield**	**Appearance**	**Melting point (°C)**
Me	73.2	Colourless crystals	97-99
Cy	68.4	Colourless crystals	114-115

Table 2.9.1b: Physical data for the diorganotinchloride *N,N*-dicyclohexyldithiocarbamates: $R_2Sn(S_2CN(Cy)_2)Cl$; R= Me or Cy.

	$R_2Sn(S_2CN(Cy)_2)Cl$		
R=	**Yield**	**Appearance**	**Melting point (°C)**
Me	69.6	Colourless crystals	203-204
Cy	34.3	Colourless crystals	232-234

Table 2.9.1c: Physical data for the diorganotinchloride *N*-cyclohexyl, *N*-ethyldithiocarbamates: $R_2Sn(S_2CNCyEt)Cl$; R= ^tBu.

	$R_2Sn(S_2CNCyEt)Cl$		
R=	**Yield**	**Appearance**	**Melting point (°C)**
^tBu	40.1	Colourless crystals	127-128

Table 2.9.2a: Selected infrared absorptions (cm^{-1}) for the diorganotinchloride *N, N*-diethyldithiocarbamates: $R_2Sn(S_2CN(Et)_2)Cl$; R= Me or Cy.

	$R_2Sn(S_2CN(Et)_2)Cl$			
R=	ν(C= N)	ν(C= S)		
Me	1513 b (s)	1002 sh	992 (m)	NO
Cy	1509 (s)	NO	992 b (m)	NO

s= strong, m= medium, sh= shoulder and b= broad, NO= not observed.

Table 2.9.2b: Selected infrared absorptions (cm^{-1}) for the diorganotinchloride *N, N*-dicyclohexyldithiocarbamates: $R_2Sn(S_2CN(Cy)_2)Cl$; R= Me or Cy.

	$R_2Sn(S_2CN(Cy)_2)Cl$				
R=	ν(C= N)		ν(C= S)		
Me	1482(s)	1464(s)	1030(ms)	981(m)	991(m)
Cy	NO	1467 b(s)	NO	1003(m)	990(m)

s= strong, m= medium, ms=medium to strong and NO= not observed..

Table 2.9.2c: Selected infrared absorptions (cm^{-1}) for the diorganotinchloride *N*-cyclohexyl, *N*-ethyldithiocarbamates: $R_2Sn(S_2CNCyEt)Cl$; R= ^tBu.

	$R_2Sn(S_2CNCyEt)Cl$			
R=	ν(C= N)		ν(C= S)	
^tBu	1484 b(s)	NO	1013(m)	997(m)

s= strong, m= medium and NO =Not Observed.

Table 2.9.3a: ^{1}H NMR data for diorganotinchloride *N,N*-diethyldithiocarbamates: $R_2Sn(S_2CN(Et)_2)Cl$; R= Me or Cy.

	$^-S_2CN(Et)_2$		R_2Sn-			
R=	H_a	H_b	H_α	H_β	H_γ	H_δ
Me	3.75 q (7.17^a)	1.36 t (7.14^b)	1.29 s (75.6^d 72.3^e)			
Cy	3.79 q (7.16^a)	1.34 t (7.20^b)	2.31 tt (11.8^a 3.47^b)	← 2.15 - 1.40 m →		

coupling constants are in parentheses: a= $^3J(HH)$, b= $^4J(HH)$, d= $^2J(^{119}SnH)$, e= $^2J(^{117}SnH)$, s= singlet, t= triplet, tt= triplet of triplets, q= quartet, m= multiplet.

Table 2.9.3b: ^{1}H NMR data for diorganotinchloride *N,N*-dicyclohexyldithiocarbamates: $R_2Sn(S_2CN(Cy)_2)Cl$; R= Me or Cy.

	$^-S_2CN(Cy)_2$				R_2Sn-			
R=	H_a	H_b	H_c	H_d	H_α	H_β	H_γ	H_δ
Me	4.65 bs	← 1.90 - 1.09 m →			1.27 s ($78.1d^d$ 73.6^e)			
Cy	4.69 bs	← 2.13 - 1.21 m →			2.48 bs	← 2.26 - 0.85 m →		

coupling constants are in parentheses d= $^3J(^{119}SnH)$, e= $^3J(^{117}SnH)$; bs= broad singlet, s= singlet, m= multiplet

Table 2.9.3c: ^{1}H NMR data for diorganotinchloride *N*-cyclohexyl, *N*-ethyldithiocarbamates: $R_2Sn(S_2CNCyEt)Cl$; R= ^{t}Bu.

	$^-S_2CNCyEt$						R_2Sn-			
R=	H_a	H_b	H_c	H_d	H_e	H_f	H_α	H_β	H_γ	H_δ
^{t}Bu	4.59 s	1.97 - 1.11 m			3.74 q (7.13^a)	1.32 t (7.18^a)		1.50 s (118.8^d 113.5^e)		

coupling constants are in parentheses: a= $^3J(HH)$, d= $^3J(^{119}SnH)$, e= $^3J(^{117}SnH)$ s= singlet, t= triplet, q= quartet, m= multiplet.

Table 2.9.4a: ^{13}C NMR data for diorganotinchloride *N, N*-diethyldithiocarbamates: $R_2Sn(S_2CN(Et)_2)Cl$; R= Me or Cy.

	$^-S_2CNEt_2$			R_2Sn-			
R=	C_a	C_b	C_q	C_α	C_β	C_γ	C_δ
Me	50.0	11.9	195.5	9.9 (561.4[a])			
Cy	49.9	12.1	196.5	44.7 (494.3[a] 472.3[b])	30.4 (24.7[c])	28.7 (97.9[d])	26.5 (12.0[e])

coupling constants are in parentheses: a= $^1J(^{119}SnC)$, b= $^1J(^{117}SnC)$, c= $^2J(^{119}SnC)$, d= $^3J(^{119}SnC)$, e= $^4J(^{119}SnC)$, f= $^4J(^{117}SnC)$.

Table 2.9.4b: ^{13}C NMR data for diorganotinchloride *N,N*-dicyclohexyldithiocarbamates: $R_2Sn(S_2CN(Cy)_2)Cl$; R= Me or Cy.

	$^-S_2CN(Cy)_2$					R_2Sn-			
R=	C_a	C_b	C_c	C_d	C_q	C_α	C_β	C_γ	C_δ
Me	68.8, 61.9	29.4, 28.7	26.2	25.2, 24.9	194.4	9.4 (572.3[a])			
Cy	68.2, 61.9	29.7	26.3	25.4, 25.0	195.9	44.0	30.4 (25.1[b])	28.7 (98.2[e])	26.5

coupling constants are in parentheses: a= $^1J(^{119}SnC)$, b= $^2J(^{119}SnC,)$ c= $^3J(^{119}SnC)$, d= $^3J(^{117}SnC)$, e= $^4J(^{119}SnC)$.

Table 2.9.4c: ^{13}C NMR data for diorganotinchloride *N*-cyclohexyl, *N*-ethyldithiocarbamates: $R_2Sn(S_2CNCyEt)Cl$; R= ^{t}Bu.

	$^-S_2CNCyEt$							R_2Sn-			
R=	C_a	C_b	C_c	C_d	C_e	C_f	C_q	C_α	C_β	C_γ	C_δ
^{t}Bu	65.6	30.1	25.5	25.1	44.6	13.9	196.4	43.0 (483.4[a] 461.5[b])	30.5 (34.5[c])		

coupling constants are in parentheses: a= $^1J(^{119}SnC)$, b= $^1J(^{117}SnC)$, c= $^2J(^{119}SnC)$, d= $^3J(^{119}SnC)$, e= $^4J(^{119}SnC)$.

Figure 2.5: FTIR Spectra of $Cy_2Sn(S_2CN(Et)_2)Cl$.

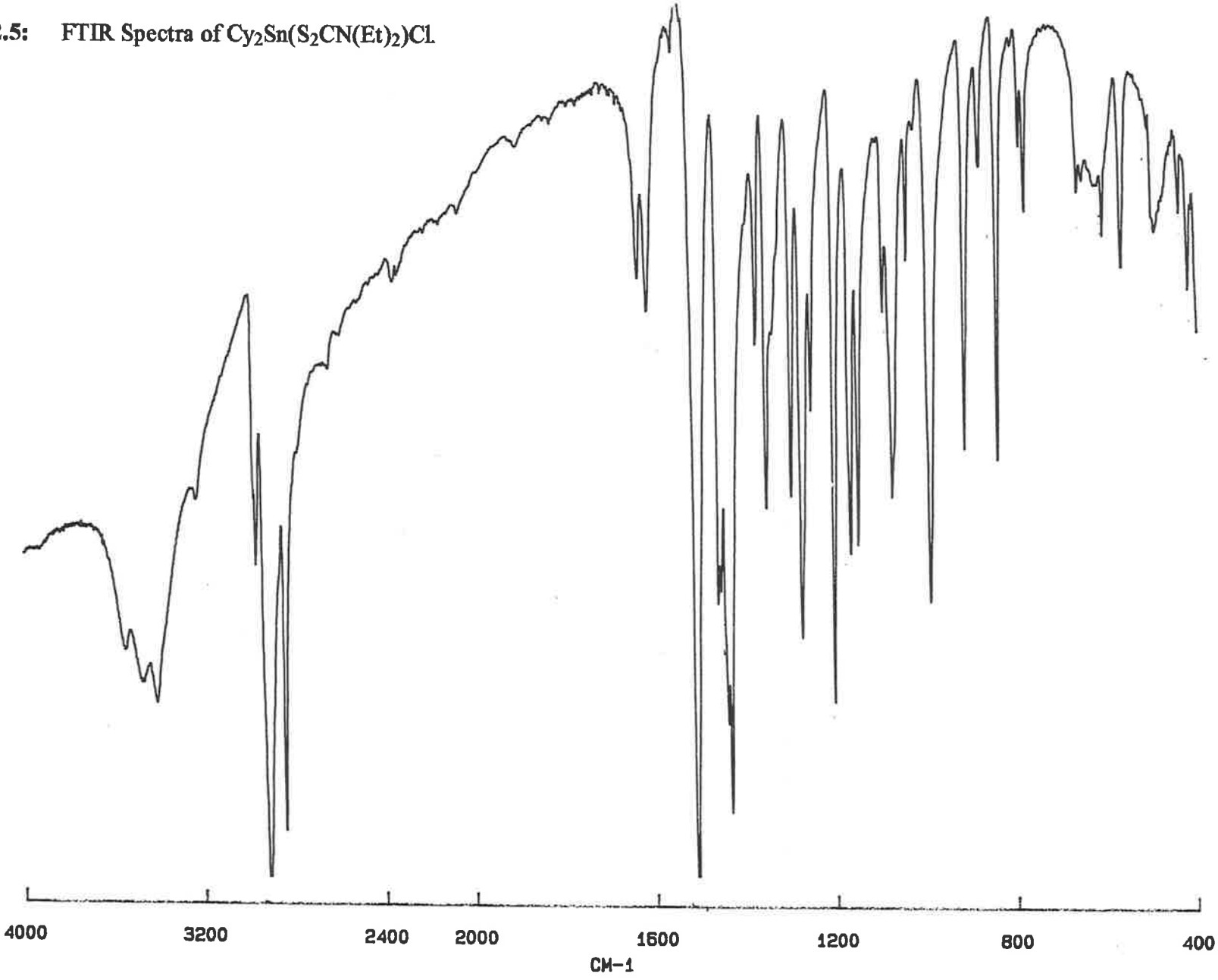


Figure 2.6: ^{1}H NMR Spectra of $^{t}Bu_2Sn(S_2CN(Et)Cy)Cl$.

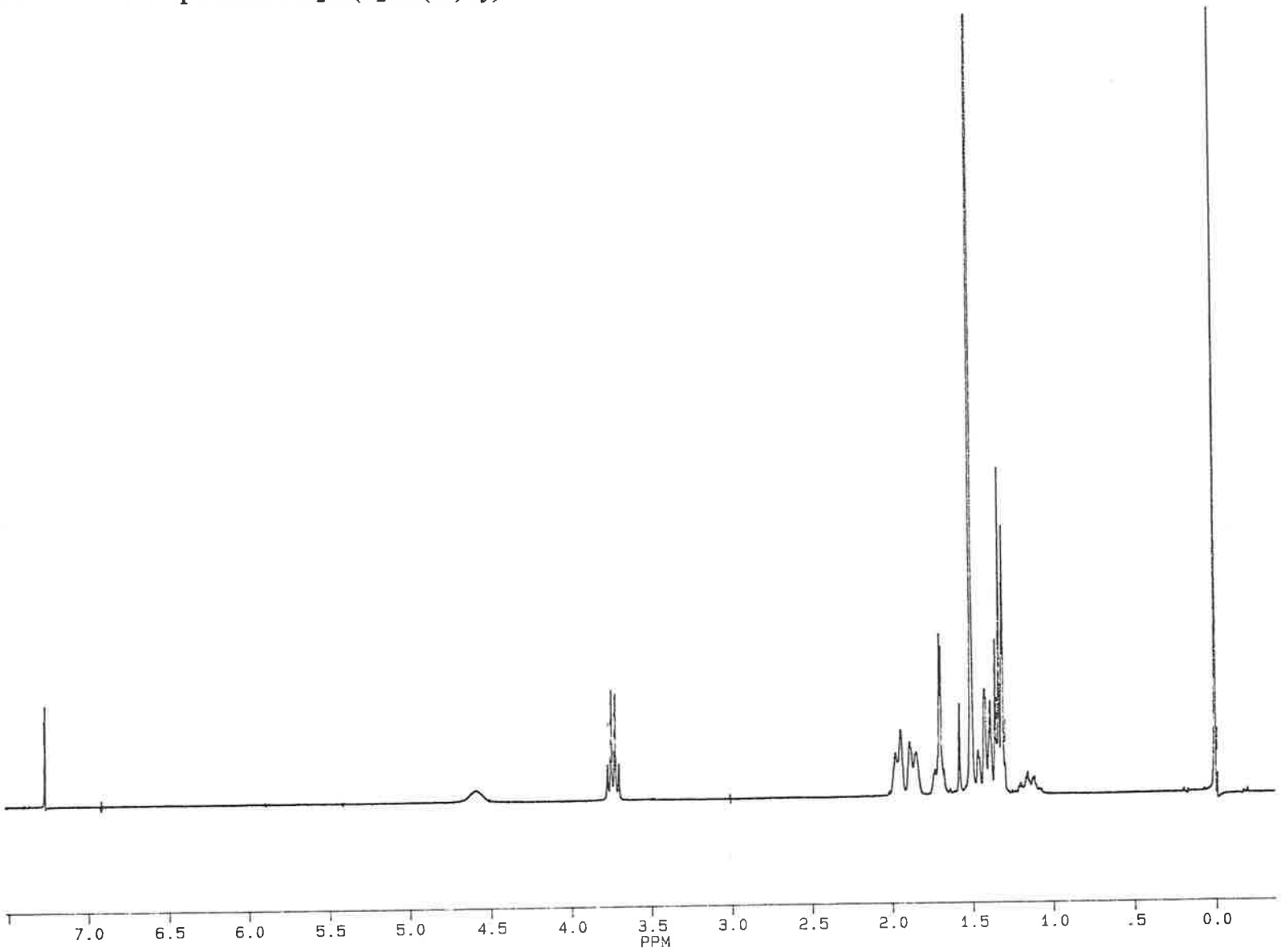
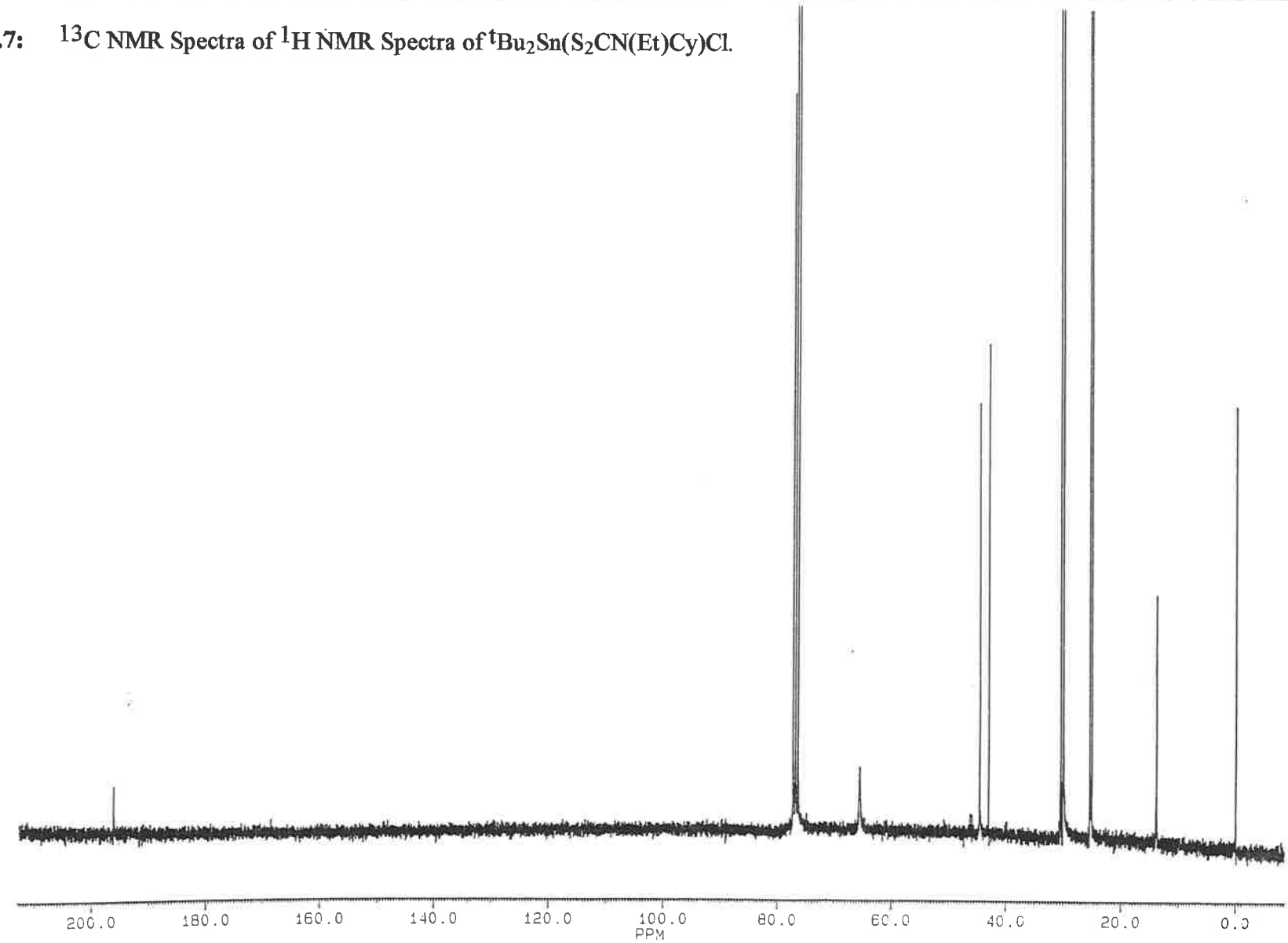


Figure 2.7: ^{13}C NMR Spectra of ^{1}H NMR Spectra of $^{t}Bu_2Sn(S_2CN(Et)Cy)Cl$.



2.10 References

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Chapter 3

The Influence of Crystal Packing on Molecular Geometry: A Crystallographic and Theoretical Investigation of Selected Diorganotin Systems.

3.1 Introduction

As discussed in Chapter 1, a number of recent surveys of the structural chemistry of main group element compounds have highlighted that quite significant changes in the immediate environment of the central element may be found for compounds with similar chemical formulae [1]. The reason(s) for the adoption of diverse motifs in the solid state for many organotin systems are not known, however, electronic and steric factors of the organotin entities and/or ligands may play significant roles. Less tangible is the influence of crystal packing on molecular structure. While it is well known that in the crystalline state intermolecular forces, such as dipole/dipole interactions (including hydrogen bonding), may influence the conformation for a particular residue, less well understood is the role of weaker intermolecular forces on molecular geometry. This particular chapter investigates the influence of crystal packing effects on organotin molecular geometry, using a combination of crystallographic analysis and theoretical modeling.

The diorganotin systems chosen as the focus of this chapter encompass a range of crystallographic circumstances. The first system to be investigated crystallises as two polymorphs, indicating different packing arrangements. Geometry optimisations have also been performed for examples where: i) two molecules comprise the crystallographic asymmetric unit, ii) a molecule has co-crystallised solvent, iii) a solvate has two molecules in the asymmetric unit, and finally iv) a structure has high symmetry (i.e. *m2m*). The comparison of the crystallographically determined structures with those calculated employing *ab initio* geometry optimisations will enable an examination of the influence that solid state effects have on molecular geometry.

The *ab initio* geometry optimisation calculations have been performed at the HF level of theory employing the LanL2DZ basis set. As indicated in Chapter 1 and in earlier work [2], the HF theoretical approach makes no account of electron correlation in the reported geometry optimisations where the DFT level of theory does. Recent Work indicates that generally there is very good agreement in calculations of molecular geometries by each approach. Subsequently electron correlations have not been included in the predictions of molecular geometry for these tin-containing compounds.

The chapter aims to compare geometric parameters derived from crystallographically determined structures with those calculated from *ab initio* geometry optimisations for a number of organotin systems in order to investigate the influence of crystal packing (or solid state effects) on molecular structure.

3.2. Results

Details of the experimental procedure employed in the synthesis of the compounds reported in this chapter are provided in Chapter 2. Spectroscopic characterizations are also provided in Chapter 2.

3.2.1 Crystallographic Studies

The experimental procedure employed in the data collection and the structure determinations are described in Chapter 2. Presented below are the experimental details unique to the diorganotin systems: $[^tBu_2Sn(S_2CNCy_2)Cl]$, $[Vin_2SnCl_2(2,2'\text{-bipyridyl})]\cdot 0.5C_6H_6$, $[Ph(Me)SnCl_2(2,2'\text{-bipyridyl})]\cdot 0.25CHCl_3$ and $[Me_2SnCl_2(1,10\text{-phenanthroline})]$, which are examined in this chapter. Details specific to each structure determination are presented in Table 3.1. The crystal data and refinement details for these molecular structure determinations are provided in Appendix of this chapter. All diagrams are drawn with ORTEP [3] at the 35% probability level.

In section 3.3, the crystal and molecular structure of the above organotin systems are described and brief comments on the literature structures are also made.

3.2.1a $[^tBu_2Sn(S_2CNCy_2)Cl]$

Crystals suitable for X-ray diffraction studies were obtained from the slow evaporation of an ethanol solution of the compound; melting point 172 - 173 °C. Two molecules of this compound comprise the asymmetric unit, labeled *a* and *b*. Owing to the decrease in the net intensity values for a set of three standard reflections (approximately 11 %), a correction was made to the data set assuming a linear decay. High thermal motion was noted for some of the methyl groups, however, no evidence was found for split sites.

3.2.1b [Vin$_2$SnCl$_2$(2,2'-bipyridyl)]·0.5C$_6$H$_6$

Colorless crystals, as a hemi-benzene solvate, were obtained from the slow evaporation of an acetonitrile/benzene (9/1 *v/v*) solution of the compound; melting point 202 - 203 °C.

3.2.1c [Ph(Me)SnCl$_2$(2,2'-bipyridyl)]·0.25CHCl$_3$

Colorless crystals were obtained from the slow evaporation of an acetonitrile/chloroform (9/1 *v/v*) solution of the adduct; melting point 253 - 254 °C. The asymmetric unit comprises two independent molecules of [Ph(Me)SnCl$_2$(2,2'-bipyridyl)]·0.25CHCl$_3$, labeled *a* and *b*, and half a chloroform molecule. The single residual electron density peak of 1.84 eÅ^{-3} was located in the vicinity of the chloroform molecule, however, attempts to refine this as a disordered site did not improve the model.

3.2.1d [Me$_2$SnCl$_2$(1,10-phenanthroline)]

Colorless crystals were obtained from the slow evaporation of an acetonitrile solution of the adduct; melting point 264 (dec) °C. The choice of space group as *Cmcm*, as opposed to non-centrosymmetric *Cmc*2$_1$, was confirmed by the distribution of *E*-statistics and the successful refinement. Thus, the tin atom lies on a site of symmetry *m2m*. Some disorder in the structure is evident as can be seen from the shapes of the thermal displacement parameters of atoms comprising the 1,10-phenanthroline ligand; these were not considered sufficient, however, to reduce the symmetry of the space group.

TABLE 3.1: Crystallographic Data For the diorganotin Systems: [$^{t}Bu_2Sn(S_2CNCy_2)Cl$], [Vin_2SnCl_2(2,2'-bipyridyl)]·0.5C_6H_6, [Ph(Me)$SnCl_2$(2,2'-bipyridyl)]·0.25$CHCl_3$ and [Me_2SnCl_2(1,10-phenanthroline)].

	Diorganotin System			
Crystallographic Data	**[$^{t}Bu_2Sn(S_2CNCy_2)Cl$]**	**[Vin_2SnCl_2(2,2'-bipyridyl)]·0.5C_6H_6**	**[Ph(Me)$SnCl_2$(2,2'-bipyridyl)]·0.25$CHCl_3$**	**[Me_2SnCl_2(1,10-phenanthroline)]**
Formula	$C_{21}H_{40}ClNS_2Sn$	$C_{17}H_{17}Cl_2N_2Sn$	$C_{17.25}H_{16.25}Cl_{2.75}N_2Sn$	$C_{14}H_{14}Cl_2N_2Sn$
Formula weight	524.8	438.9	467.8	399.9
Crystal system	triclinic	triclinic	monoclinic	orthorhombic
Space group	$P\bar{1}$	$P\bar{1}$	$P2_1/n$	*Cmcm*
a, Å	12.761(3)	9.260(1)	14.039(3)	11.321(2)
b, Å	18.329(6)	13.253(3)	16.525(2)	18.889(1)
c, Å	12.191(3)	7.8702(8)	17.174(1)	7.537(1)
α, (°)	97.73(3)	95.21(1)	90.0	90.0
β, (°)	98.85(2)	90.792(9)	91.34(1)	90.0
γ, (°)	107.90(2)	69.76(1)	90.0	90.0
V, $Å^3$	2630(1)	902.3(3)	3983(1)	1611.6(3)
Z	2	2	8	4
D_{calcd}, g cm^{-3}	1.325	1.615	1.560	1.648
Radiation, Å	Cu, 1.5418	Mo, 0.7107	Mo, 0.7107	Cu, 1.5418
μ, cm^{-1}	101.79	17.09	16.50	155.80
Trans coeff	0.798 - 1	0.974 – 1	0.978 - 1	0.843 - 1
2θ range, (°)	3.0 - 120.0	3.0 - 55.0	3.0 - 55.0	3.0 - 120.0
No. reflns meas	8247	4413	9889	3280
No. unique reflns	7838	4157	9516	3280
No of reflns used [a]	5293	3261	5888	1391
No. of variables	469	199	413	59
R	0.059	0.029	0.048	0.046
R_w	0.062	0.030	0.051	0.057
Residual $e^-/Å^3$	1.12	0.41	1.84	0.56

a $I \geq 3.0\sigma(I)$

3.2.2 Computational Details

Experimental details pertaining to the geometry optimisation calculations performed on the structures presented below are discussed in Chapter 2. The results of the optimisations are discussed below. All geometry optimisations were performed by the author unless stated otherwise.

3.3 Discussion

An examination of the relationship between solid state structures of certain diorganotin systems, as determined by X-ray crystallographic techniques, and their gas phase structures employing *ab initio* geometry optimisation calculations are presented below. It is noted that geometric changes are evident once a molecule's structure was calculated in the gas phase and hence, free from the influence of crystal packing. The major observation was that the molecules became more symmetric in the gas phase. In terms of interatomic parameters, significant differences were noted in Sn-ligand parameters, which were found to generally increase. Notable also was the observation that, generally, bond angles did not alter significantly. From the above, clearly, crystal packing effects can influence molecular geometry in diorganotin systems. Alternatively, it can be stated that the magnitude of energy associated with intermolecular interactions can be such as to induce changes in *intra*molecular interactions. The comparison between the crystallographically determined and theoretically calculated structures for five diorganotin systems is presented below.

3.3.1a $[Ph_2Sn(S_2CNEt_2)_2]$

The first study examines the relationship between two polymorphic forms of $[Ph_2Sn(S_2CNEt_2)_2]$ [4, 5], Figure 3.1, and their theoretically-optimised structures. In this context, a polymorph is defined as a material with essentially the same molecular structure but existing in a distinct crystal environment, i.e. a different (at least) arrangement of intermolecular forces.

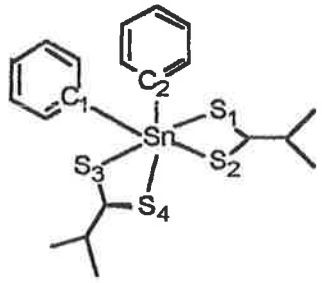


Figure 3.1

$[Ph_2Sn(S_2CNEt_2)_2]$

$[Ph_2Sn(S_2CNEt_2)_2]$ crystallises as two polymorphs, namely monoclinic $P2_1/c$ [4] and tetragonal $P4_12_12$ [5]. The monoclinic form has been the subject of two independent crystal structure determinations on samples recrystallised from methylethylketone [4a] and ethanol/dichloromethane [4b] solutions of the compound, respectively, and the more contemporary results [4b] are employed here; similar unit cell data have been obtained for crystals obtained from recrystallisation from acetone and $CHCl_3$ solutions of $[Ph_2Sn(S_2CNEt_2)_2]$ [5]. The tetragonal form of $[Ph_2Sn(S_2CNEt_2)_2]$ requires the molecule to possess crystallographically imposed two-fold symmetry; crystallisation of $[Ph_2Sn(S_2CNEt_2)_2]$ from an acetonitrile/dichloromethane (1/1 *v/v*) solution gave similar unit cell data [5]. The structure of $[Ph_2Sn(S_2CNEt_2)_2]$ is unusual among compounds of the general formula $R_2Sn(S_2CNR'_2)_2$ which generally adopt skew-trapezoidal bipyramidal geometries owing to the presence of asymmetrically chelating dithiocarbamate ligands (i.e. Sn-S distances of approximately 2.5 Å and 3.0 Å) and in which the R substituents are disposed over the weaker Sn-S bonds [1e, Chapter 1]. In $[Ph_2Sn(S_2CNEt_2)_2]$, a more symmetrical arrangement is found owing to the relatively near equivalence of the Sn-S bonds. Thus, the tin atom in each polymorphic form of $[Ph_2Sn(S_2CNEt_2)_2]$ exists in a distorted octahedral geometry defined by two *ipso* carbon atoms of the phenyl groups that occupy approximately *cis* positions and four sulfur atoms derived from the two ligands.

There are no significant intermolecular contacts in the respective crystal lattices. In tetragonal $[Ph_2Sn(S_2CNEt_2)_2]$, the closest contact involving non-hydrogen atoms of 3.59(1) Å occurs between carbon atoms derived from the dithiocarbamate ligands and in

monoclinic $[Ph_2Sn(S_2CNEt_2)_2]$, there are no non-hydrogen contacts < 3.6 Å. There are some significant differences in the geometric parameters about the tin centers in each polymorphic form of $[Ph_2Sn(S_2CNEt_2)_2]$ as can be evinced from the selected interatomic parameters collected in Table 3.2.

TABLE 3.2: Geometric parameters (Å, deg.) and calculated energies (Hartrees) for $[Ph_2Sn(S_2CNEt_2)_2]$

	$[Ph_2Sn(S_2CNEt_2)_2]$		
Parameter	Solid State tetragonal polymorph *[5]	Solid State monoclinic polymorph [4b]	Optimised Structure(LanL2DZ)
Sn-S(1)	2.556(2)	2.607(3)	2.633
Sn-S(2)	2.659(2)	2.632(3)	2.840
Sn-S(3)	2.556(2)	2.558(3)	2.633
Sn-S(4)	2.659(2)	2.777(3)	2.840
Sn-C(1)	2.148(7)	2.155(9)	2.134
Sn-C(2)	2.148(7)	2.166(8)	2.134
S(1)-Sn-S(2)	67.91(6)	68.2(1)	66.9
S(1)-Sn-S(3)	150.08(7)	155.3(1)	149.6
S(1)-Sn-S(4)	88.67(7)	96.0(1)	89.5
S(1)-Sn-C(1)	95.4(2)	93.9(2)	96.5
S(1)-Sn-C(2)	103.5(2)	98.9(2)	102.0
S(2)-Sn-S(3)	88.67(7)	90.7(1)	89.5
S(2)-Sn-S(4)	78.72(9)	81.0(1)	80.8
S(2)-Sn-C(1)	160.9(2)	158.0(2)	160.6
S(2)-Sn-C(2)	92.2(2)	93.9(2)	89.4
S(3)-Sn-S(4)	67.91(6)	67.0(1)	66.9
S(3)-Sn-C(1)	103.5(2)	103.0(2)	102.0
S(3)-Sn-C(2)	95.4(2)	95.2(2)	96.5
S(4)-Sn-C(1)	92.2(2)	88.6(2)	89.4
S(4)-Sn-C(2)	160.9(2)	161.2(2)	160.6
C(1)-Sn-C(2)	101.1(4)	101.8(3)	104.5
C(1)/Sn/C(2)/C(21)	122.0(6)	-83	-39.5
C(1)/Sn/C(2)/C(26)	-58.2(7)	91	140.3
C(2)/Sn/C(1)/C(11)	122.0(6)	65	140.3
C(2)/Sn/C(1)/C(16)	-58.2(7)	-110	-39.5
Calculated energies	-1001.6459	-1001.5889	-1002.0139

* molecule has crystallographic two-fold symmetry

The dithiocarbamate ligands in tetragonal $[Ph_2Sn(S_2CNEt_2)_2]$ form slightly asymmetric Sn-S distances such that ΔSn-S (i.e. $Sn\text{-}S_{long}$ - $Sn\text{-}S_{short}$) is 0.103 Å, with an average Sn-S bond distance of 2.608 Å [5]. By contrast, in monoclinic $[Ph_2Sn(S_2CNEt_2)_2]$ one

dithiocarbamate ligand forms effectively symmetric Sn-S distances (ΔSn-S is 0.027 Å) and the other is more asymmetric with ΔSn-S of 0.219 Å; the average Sn-S distance is 2.644 Å [4b]. There is a high degree of agreement between the bond angles in the two polymorphs with the notable exception of a few angles involving the S(1) atom where differences of up to 7.3° exist. The geometry optimisations of tetragonal and monoclinic $[Ph_2Sn(S_2CNEt_2)_2]$, starting with the crystallographically determined fractional atomic coordinates, were performed by Dr M Buntine, The University of Adelaide [2], in order to determine whether the different molecular structures found in the polymorphs of $[Ph_2Sn(S_2CNEt_2)_2]$ arose as a result of crystal packing effects.

The geometry optimisations converged to the same structure as illustrated in Figure 3.2; interatomic parameters are listed in Table 3.2. The tetragonal form of $[Ph_2Sn(S_2CNEt_2)_2]$ was determined to be i) 966.2 kJ mol^{-1} higher in energy than the optimised structure, and ii) more stable than the monoclinic form by 175.8 kJ mol^{-1}. The result that there is only one optimised, i.e. gas phase structure, indicates that there is no intrinsic reason for $[Ph_2Sn(S_2CNEt_2)_2]$ to exist as two distinct molecular structures and hence, any differences between the solid state polymorphs can be related to intermolecular forces.

The optimised structure has effective two-fold symmetry as is crystallographically imposed in the crystal structure of tetragonal $[Ph_2Sn(S_2CNEt_2)_2]$ [5]. The average Sn-S distance has expanded to 2.737 Å, ΔSn-S is 0.207 Å, and the angles show a high level of agreement with those of tetragonal $[Ph_2Sn(S_2CNEt_2)_2]$, reflecting the two-fold symmetry in the tetragonal polymorph (crystallographically imposed) and the optimised gas phase structure. The Sn-C distances appear to be shorter in the optimised structure, however, the relatively high errors with the crystallographically determined Sn-C bond distances must be noted. It is noteworthy that the dihedral angles between the phenyl groups are twisted in the following order: optimised structure > tetragonal $[Ph_2Sn(S_2CNEt_2)_2]$ > monoclinic $[Ph_2Sn(S_2CNEt_2)_2]$, see Table 3.2. The reason for the elongation of the Sn-S distances in monoclinic $[Ph_2Sn(S_2CNEt_2)_2]$, over those in

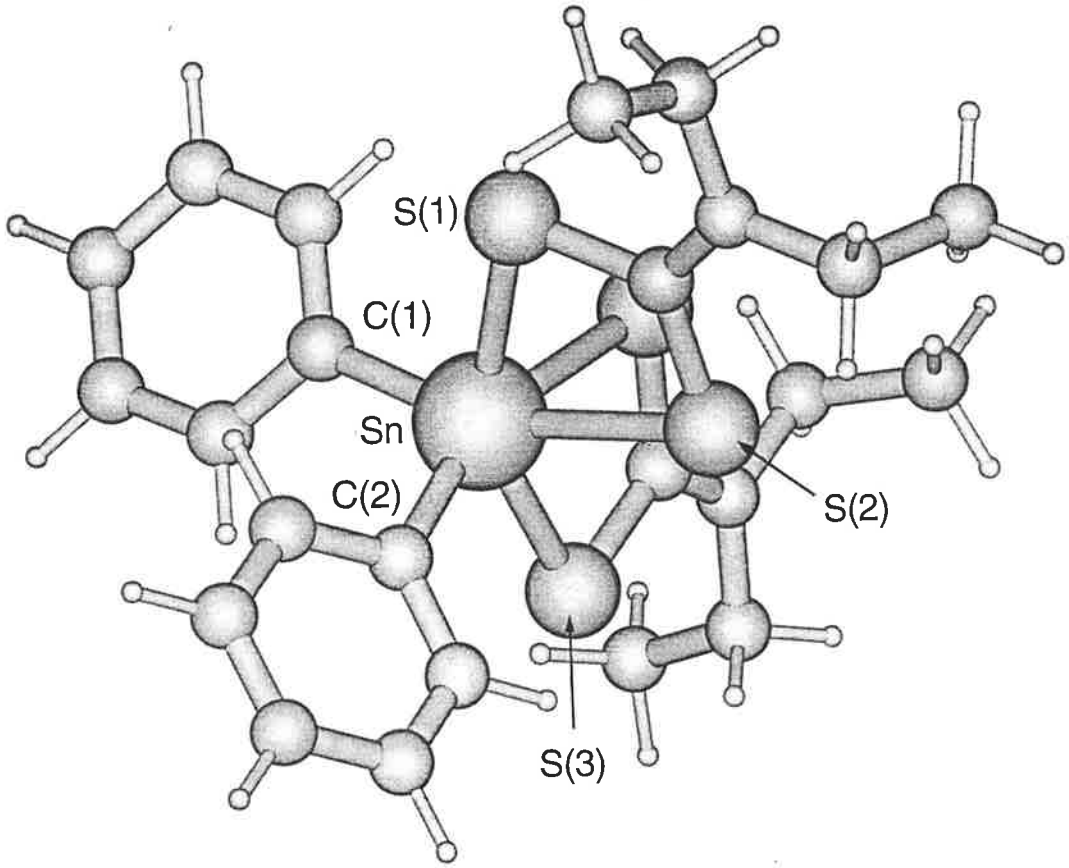


Figure 3.2
The optimised structure of $Ph_2Sn(S_2CNEt_2)_2$

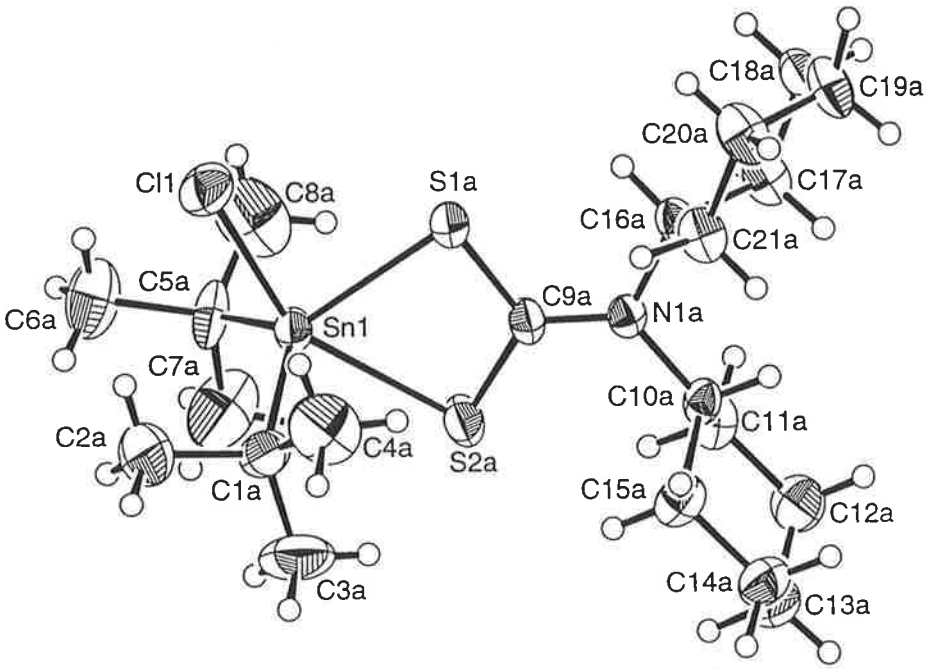
tetragonal $[Ph_2Sn(S_2CNEt_2)_2]$ can be rationalised in terms of the magnitude of the π-interactions between the phenyl groups. In the monoclinic polymorph, the phenyl groups are almost anti-parallel, with an average twist of approximately 13°, indicating a relatively small interaction between the two π -systems. This contrasts to a larger twist of approximately 32° as observed in the structure of tetragonal $[Ph_2Sn(S_2CNEt_2)_2]$. An increase in the interaction between the phenyl π -systems reduces the electron density available to the tin atom and consequently results in the formation of stronger Sn-S interactions. Hence, it may be concluded that the chief influence of the crystal packing in the two polymorphs of $[Ph_2Sn(S_2CNEt_2)_2]$ is to alter the relative positions of the phenyl groups, which in turn influences the geometric parameters about the tin atom. The dihedral angles are quite similar for the optimised structure (approximately 40°) and

tetragonal [$Ph_2Sn(S_2CNEt_2)_2$] and thus, the expansion in the Sn-S bond distances between the two solid state structures reflects the influence of the different intermolecular forces operating in the polymorphs of [$Ph_2Sn(S_2CNEt_2)_2$].

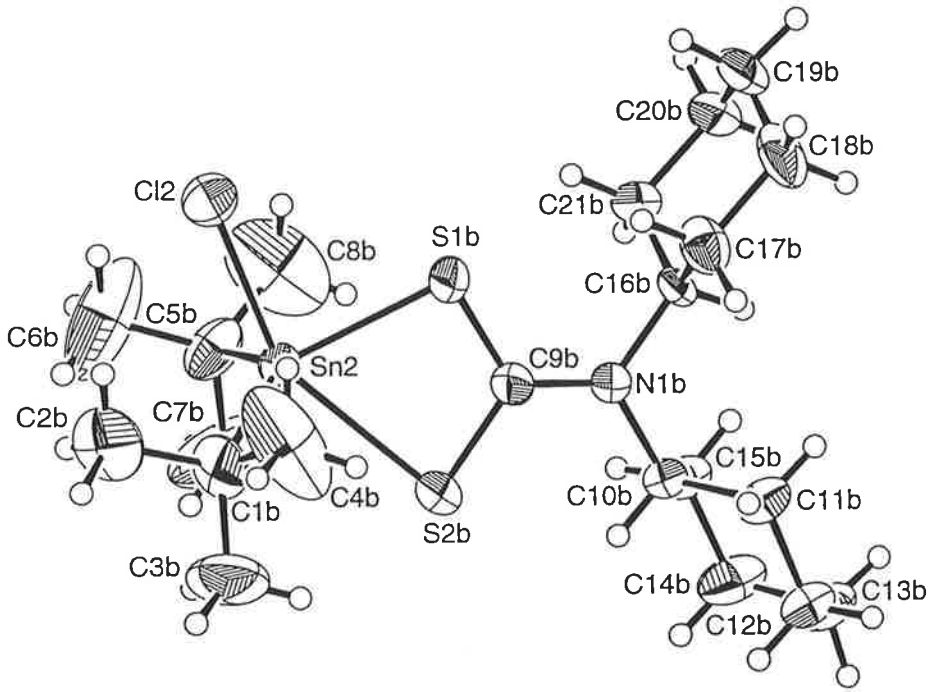
3.3.1b [$^tBu_2Sn(S_2CNCy_2)Cl$]

The structure of [$^tBu_2Sn(S_2CNCy_2)Cl$] is an example of a compound with two formula units comprising the crystallographic asymmetric unit. Thus, while there will be different intermolecular interactions operating on each molecule, as found for the polymorphs of [$Ph_2Sn(S_2CNEt_2)_2$], the molecules are constrained within a single unit cell.

The molecular structures for the two formula units that comprise the crystallographic asymmetric unit of [$^tBu_2Sn(S_2CNCy_2)Cl$], labeled molecules *a* and *b*, are shown in Figure 3.3 and selected interatomic parameters are collected in Table 3.3. The tin atom is five-coordinate being bonded to two *tert*-butyl groups, a chloride and two sulfur atoms derived from an asymmetrically chelating dithiocarbamate ligand. The geometry is distorted trigonal bipyramidal with the axial sites being defined by the chloride and the less-tightly bound S(2) atom. The tin atom lies 0.1270(6) Å (0.1191(7) Å for molecule *b*) out of the trigonal $C_2S(1)$ plane in the direction of the chloride atom. As can be seen from the listed parameters in Table 3.3, there are only minor differences between the two independent molecules with the greatest difference in bond distances involving the Sn-S(2) interactions. The difference between the molecules relates to the relative positions of the cyclohexyl groups.



Molecule a



Molecule b

Figure 3.3

The molecular structure of [^{t}Bu$_2$Sn(S$_2$CNCy$_2$)Cl]

TABLE 3.3: Geometric parameters (Å, deg.) and calculated energies (Hartrees) for [^{t}Bu$_2$Sn(S$_2$CNCy$_2$)Cl]

	[^{t}Bu$_2$Sn(S$_2$CNCy$_2$)Cl]			
Parameter	Solid State Structure (molecule *a*)	Solid State Structure (molecule *b*)	Optimised Structure (molecule *a*)	Optimised Structure (molecule *b*)
Sn-Cl(1)	2.482(3)	2.492(3)	2.485	2.486
Sn-S(1)	2.471(3)	2.477(3)	2.556	2.557
Sn-S(2)	2.722(3)	2.743(3)	2.960	2.957
Sn-C(1)	2.19(1)	2.19(1)	2.177	2.177
Sn-C(5)	2.16(1)	2.21(1)	2.177	2.177
S(1)-C(9)	1.740(9)	1.73(1)	1.814	1.805
S(2)-C(9)	1.71(1)	1.72(1)	1.771	1.779
N(1)-C(9)	1.31(1)	1.31(1)	1.318	1.318
Cl-Sn-S(1)	83.9(1)	85.0(1)	85.7	85.6
Cl-Sn-S(2)	152.0(1)	152.3(1)	151.1	151.0
Cl-Sn-C(1)	96.4(3)	96.3(4)	99.6	99.9
Cl-Sn-C(5)	98.6(3)	96.9(3)	99.9	99.6
S(1)-Sn-S(2)	68.04(8)	67.50(9)	65.4	65.4
S(1)-Sn-C(1)	115.3(4)	120.1(4)	116.0	115.9
S(1)-Sn-C(5)	119.8(4)	113.5(4)	115.9	116.0
S(2)-Sn-C(1)	95.1(3)	95.2(4)	93.4	93.2
S(2)-Sn-C(5)	96.0(3)	96.6(3)	93.2	93.5
C(1)-Sn-C(5)	123.9(5)	125.6(6)	125.4	125.4
Sn-S(1)-C(9)-S(2)	9.6(5)	-8.9(6)	0.1	0.1
Sn-S(1)-C(9)-N(1)	-170.5(8)	173.1(9)	0	179.9
Sn-S(2)-C(9)-N(1)	171.3(4)	-173.9(9)	0	0
C(9)-N(1)-C(10)-C(11)	73(1)	-130(1)	65.2	-116.5
C(9)-N(1)-C(10)-C(15)	-57(1)	102(1)	-65.2	116.4
C(9)-N(1)-C(16)-C(17)	-134.1(9)	75(1)	-116.4	65.4
C(9)-N(1)-C(16)-C(21)	98(1)	-56(1)	116.4	-65.4
Calculated Energies	-910.0397	-910.0337	-910.51223	-910.51253

Molecular models of the two independent molecules shows that the ^{t}Bu$_2$SnCl(S$_2$CN) portions of each molecule are virtually superimposable, however, the cyclohexyl portions are not, as they are approximate mirror images of each other. Hence, the differences

between the two molecules relate to conformation, rather than to disparate interatomic parameters. In the lattice the closest contact occurs between symmetry related C(19) atoms of 3.60(2) Å (symmetry operation: 2 - *x*, - *y*, 1 - *z*). Both molecules that comprise the crystallographic unit in [^{t}Bu$_2$Sn(S$_2$CNCy$_2$)Cl] were subjected to a geometry optimisation.

Geometry optimisations of the two crystallographically independent molecules of [^{t}Bu$_2$Sn(S$_2$CNCy$_2$)Cl], i.e. *a* and *b*, were performed in order to ascertain whether the distinct structures were in fact isomers or were due to crystal packing effects. The energy minimised structures determined for [^{t}Bu$_2$Sn(S$_2$CNCy$_2$)Cl] are illustrated in Figure 3.4 and show that the two molecules are indeed isomers. The geometry optimisations converged to different structures, i.e. molecule *a* (upper view of Figure 3.4) and molecule *b*. The energy difference between the two computed structures is negligibly small. As such, it is possible that normally acceptable criteria describing geometric convergence masked the identity of a single, globally minimised molecular geometry. Accordingly, geometry optimisations were repeated with tighter convergence criteria. The additional calculations confirmed the presence of two distinct structures, with a difference in energy between them of 0.8 kJ mol^{-1}. In terms of overall conformation, the major difference between the crystallographic geometries and the geometry optimised structures relates to the relative orientations of the N-bound cyclohexyl rings. It was noted above that in the solid state the cyclohexyl portions of the molecules could be related to each other by a pseudo-mirror plane. It is interesting in this context that the starting geometries did not converge to a single structure but to two distinct structures in which the pseudo-mirror relationship has been maintained and, indeed, tightened; this is reflected in the equivalence of the C-N-C-C torsion angle data (Table 3.3) and is emphasised in Figure 3.4. The small (negligible) energy difference between the two optimised structures indicates that the structures are effectively isomers. Accordingly, there are no significant differences between the parameters describing the tin atom geometries in the optimised structures. Comparing the

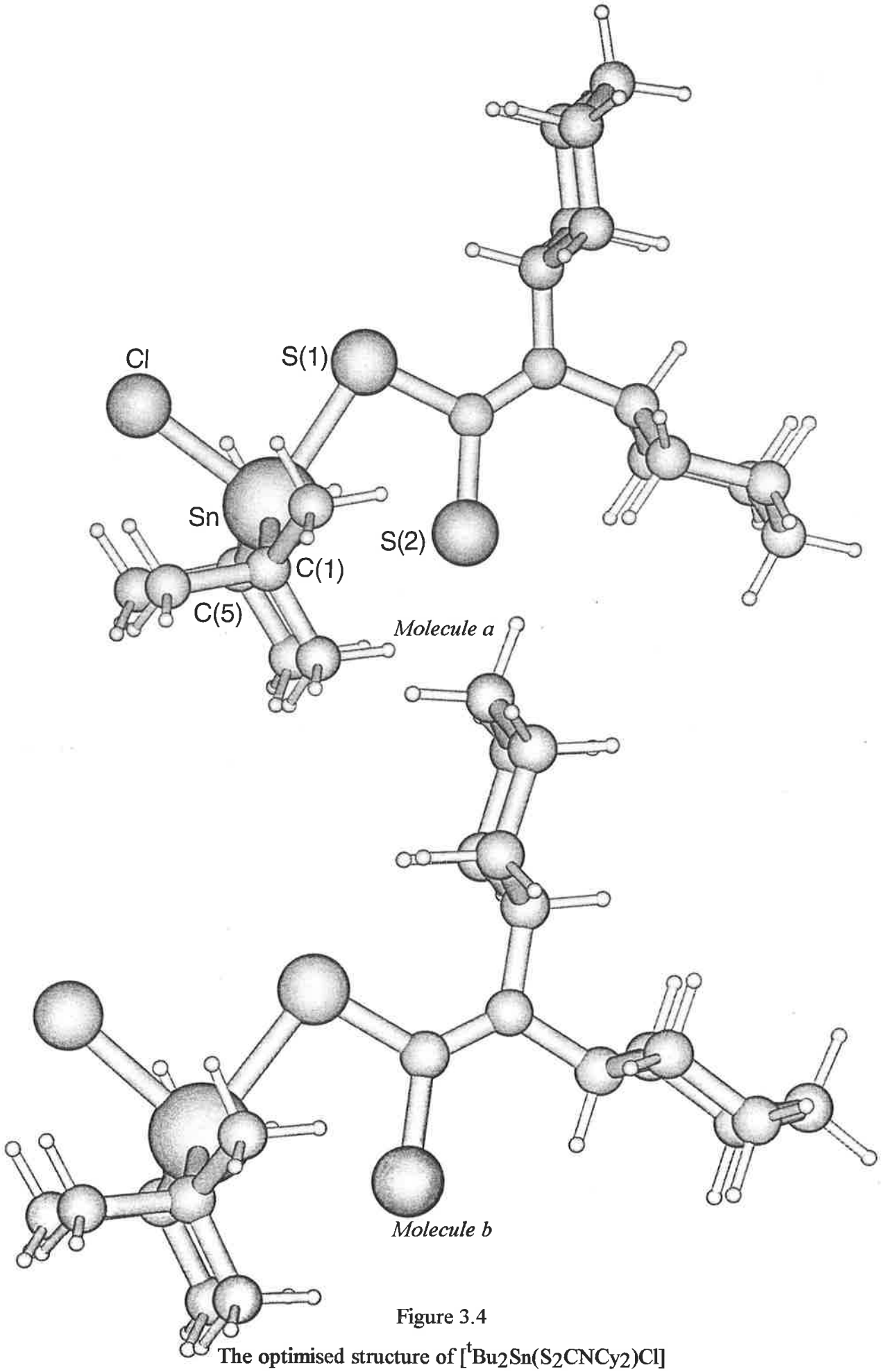


Figure 3.4

The optimised structure of [^{t}Bu$_2$Sn(S$_2$CNCy$_2$)Cl]

parameters for the gas phase and solid state structures, however, reveals a number of interesting trends.

There is a considerable expansion in the Sn-S separations but not so for the Sn-Cl distances suggesting that the Sn-Cl interaction is stronger in the gas phase structure compared with the solid state structure; differences in the Sn-C separations are marginal. This result could suggest that the dithiocarbamate ligand has more ionic character in the gas phase. Generally, there are few significant differences in bond angles between the solid state and gas phase structures. In terms of energy considerations, it has already been mentioned that the difference in energy between the optimised structures was found to be only 0.8 kJ mol^{-1}. Comparing the gas phase to the solid state structures shows that the optimised structure for molecule *a* was 1240.6 kJ mol^{-1} more stable than the molecular structure in the solid state and the comparable value for molecule *b* was calculated to be 1257.1 kJ mol^{-1}. These values indicate that there is a chemically significant difference of 15.8 kJ mol^{-1} between the two molecules comprising the crystallographic asymmetric unit.

3.3.1c $[Vin_2SnCl_2(2,2'\text{-bipyridyl})]\cdot 0.5C_6H_6$

An analysis of $[Vin_2SnCl_2(2,2'\text{-bipyridyl})]\cdot 0.5C_6H_6$ was performed as the molecule crystallises with occluded solvent molecules in the lattice and it was thought of interest to ascertain what extent non-coordinating solvent can influence molecular geometry.

The molecular structure of $[Vin_2SnCl_2(2,2'\text{-bipyridyl})]$, determined as its hemi-benzene solvate (situated about a crystallographic center of inversion), is shown in Figure 3.5 and selected geometric parameters are collected in Table 3.4. The tin atom exists in a distorted octahedral geometry with the tin atom 0.0114(7) Å above the N_2Cl_2 plane in the direction of the C(1) atom. The vinyl groups occupy *trans* positions and the dihedral angle between the SnC_2 planes is 152.0°, indicating that the vinyl groups are not coplanar; the C(2)-C(1)-C(3)-C(4) torsion angle is -29.7(9)°.

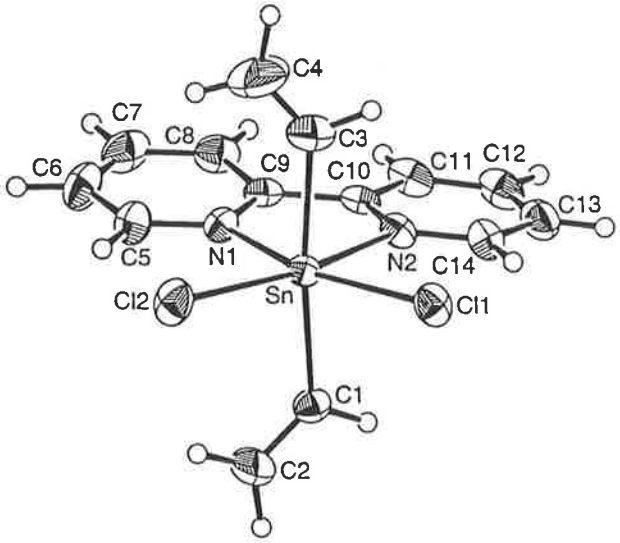


Figure 3.5

The molecular structure of [Vin$_2$SnCl$_2$(2,2'-bipyridyl)]·0.5C$_6$H$_6$

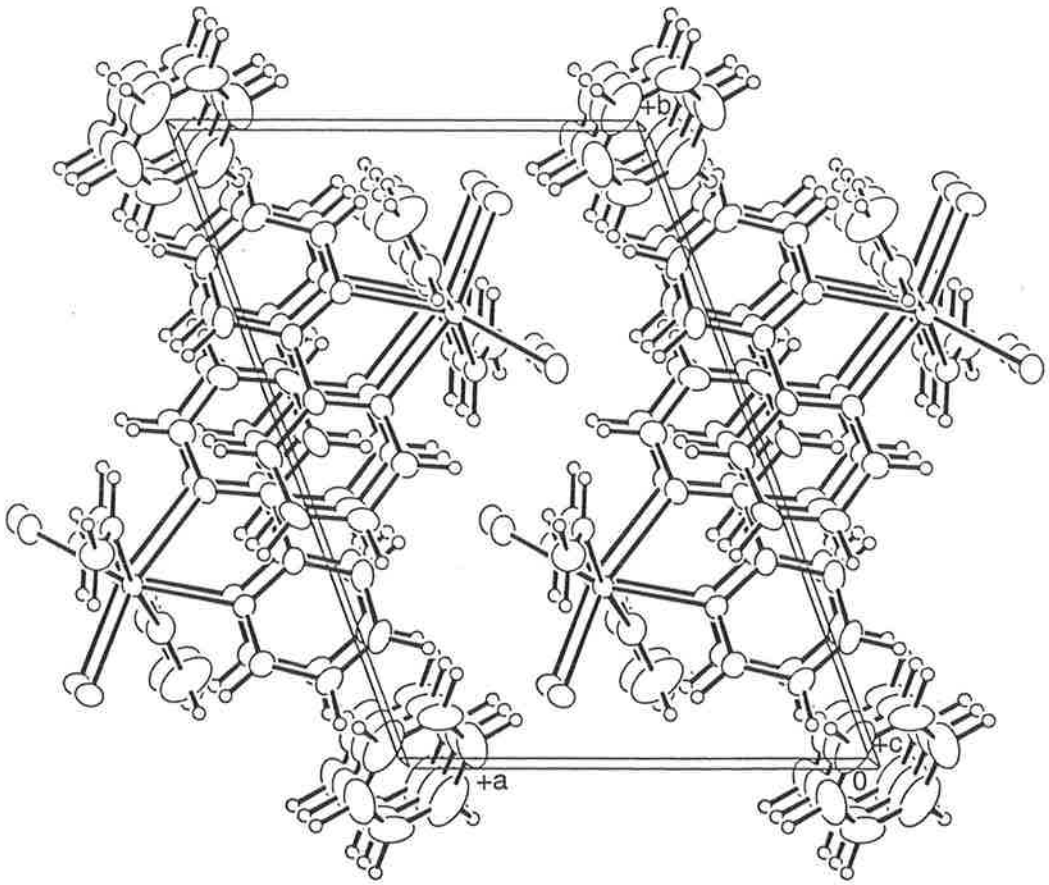


Figure 3.6

The unit cell contents for [Vin$_2$SnCl$_2$(2,2'-bipyridyl)]·0.5C$_6$H$_6$

TABLE 3.4: Geometric parameters (Å, deg.) and calculated energies (Hartrees) for $[Vin_2SnCl_2(2,2'\text{-bipyridyl})]\cdot 0.5C_6H_6$

	$[Vin_2SnCl_2(2,2'\text{-bipyridyl})]\cdot 0.5C_6H_6$	
Parameter	Solid State Structure	Optimised Structure
Sn-Cl(1)	2.529(1)	2.525
Sn-Cl(2)	2.463(1)	2.525
Sn-N(1)	2.360(3)	2.404
Sn-N(2)	2.396(3)	2.404
Sn-C(1)	2.119(3)	2.111
Sn-C(3)	2.119(4)	2.111
Cl(1)-Sn-Cl(2)	104.74(3)	109.7
Cl(1)-Sn-N(1)	161.50(7)	159.5
Cl(1)-Sn-N(2)	92.47(7)	90.8
Cl(1)-Sn-C(1)	89.71(9)	91.3
Cl(1)-Sn-C(3)	89.2(1)	94.4
Cl(2)-Sn-N(1)	93.72(7)	90.8
Cl(2)-Sn-N(2)	162.79(7)	159.5
Cl(2)-Sn-C(1)	94.2(1)	94.4
Cl(2)-Sn-C(3)	94.3(1)	91.3
N(1)-Sn-N(2)	69.1(1)	68.7
N(1)-Sn-C(1)	90.2(1)	86.9
N(1)-Sn-C(3)	88.1(1)	84.9
N(2)-Sn-C(1)	85.4(1)	84.9
N(2)-Sn-C(3)	86.1(1)	86.9
C(1)-Sn-C(3)	171.4(2)	170.1
C(1)/Sn/C(3)/C(4)	-54(6)	121.4
C(3)/Sn/C(1)/C(2)	125(6)	121.5
Calculated Energies	-679.5857	-679.7460

In the lattice, (Figure 3.6) the benzene molecules occupy columns that run parallel to the crystallographic *c*-axis; a view of the unit cell contents, projected down the *c*-direction, is shown in Figure 3.6. The closest non-hydrogen contact in the lattice of 3.473(6) Å occurs between the C(11) and C(13)^{i} atoms (symmetry operation *i*: - *x*, 1 - *y*, 1 - *z*).

This contact is one of several (the next closest is 3.560(6) Å) that arise as a result of the interlocking of centrosymmetrically related 2,2'-bipyridyl residues, also along the crystallographic *c*-direction, and is indicative of some π-stacking in the lattice. There are no non-hydrogen contacts less than the 3.6 Å involving [Vin_2SnCl_2(2,2'-bipyridyl)] and the benzene molecules. The chloride atoms form a number of contacts with hydrogen atoms of adjacent columns with the closest involving the Cl(1) atom of 2.78 Å with $H(8a)^{ii}$ (symmetry operation *ii*: $1 + x, y, z$); the closest involving the Cl(2) atom is 2.94 Å with $H(7a)^{ii}$. Both chloride atoms form contacts with the solvent molecule with the closest of 2.90 Å involving Cl(1) and H(101); Cl(2) forms a contact of 3.40 Å with $H(102)^{iii}$ (symmetry operation *iii*: $x, y, -1 + z$). It is of interest that Cl(1) forms the two shortest Cl...H interactions and that it forms the longer of the Sn-Cl bonds, i.e. 2.529(1) Å *cf.* 2.463(1) Å. In this context it is noteworthy that there are some close *intra*molecular Cl...H interactions as well. Thus, Cl(1) is separated by 2.81 Å from H(14a) and 3.11 Å from H(3a). By contrast, the Cl(2) atom forms two close contacts, one of 2.78 Å to H(5a) and 2.77 Å to H(2a). In the absence of other structural features, the disparity in the Sn-Cl distances and consequently, through the *trans* influence, the Sn-N distances (Table 3.4), may be ascribed to the intermolecular associations described above. To examine this hypothesis further, the geometry of [Vin_2SnCl_2(2,2'-bipyridyl)] was subjected to a geometry optimisation.

The optimised structure of [Vin_2SnCl_2(2,2'-bipyridyl)] is shown in Figure 3.7 and derived geometric parameters are listed in Table 3.4. The most notable difference in the structure is the symmetrisation that has occurred in the optimised geometry. There is a two-fold axis of symmetry in the optimised structure of [Vin_2SnCl_2(2,2'-bipyridyl)] with the axis bisecting the $SnCl_2N_2$ basal plane, passing through the Cl-Sn-Cl angle. Whereas in the solid state the terminal end of the vinyl substituents were found to lie on the same side of the molecule, in the optimised structure, the orientation of the vinyl groups is such that they each lie over a different Sn-Cl bond. In this arrangement, the Cl...H-C(5, 14) separations are both 2.60 Å and Cl...H-C(2, 4) 2.79 Å. Thus, the major structural difference between the experimental and calculated structures is a rotation about a Sn-C

bond. The symmetry in the molecule is reflected in the equivalence in the three pairs of Sn-donor atom distances (Table 3.4). For the optimised geometry there is an expansion in the Sn-Cl and Sn-N atom parameters but a small contraction in Sn-C bond lengths. It is noteworthy that the inequivalence in the Sn-Cl and Sn-N parameters found in the crystal structure no longer pertain in the gas phase structure. This observation further supports the conclusion that the differences that do exist in the solid state are due to intermolecular forces rather than any intrinsic chemistry associated with the molecule. In terms of bond angles, differences between equivalent angles in the solid state and calculated structures are in the order of 0 to 3° with the exception of the Cl(1)-Sn-Cl(2) and Cl(1)-Sn-C(3) angles which have expanded by approximately 5° in the calculated structure.

The crystallographically determined structure (single-point calculation) was found to be 420.9 kJ mol^{-1} higher in energy than the optimised structure.

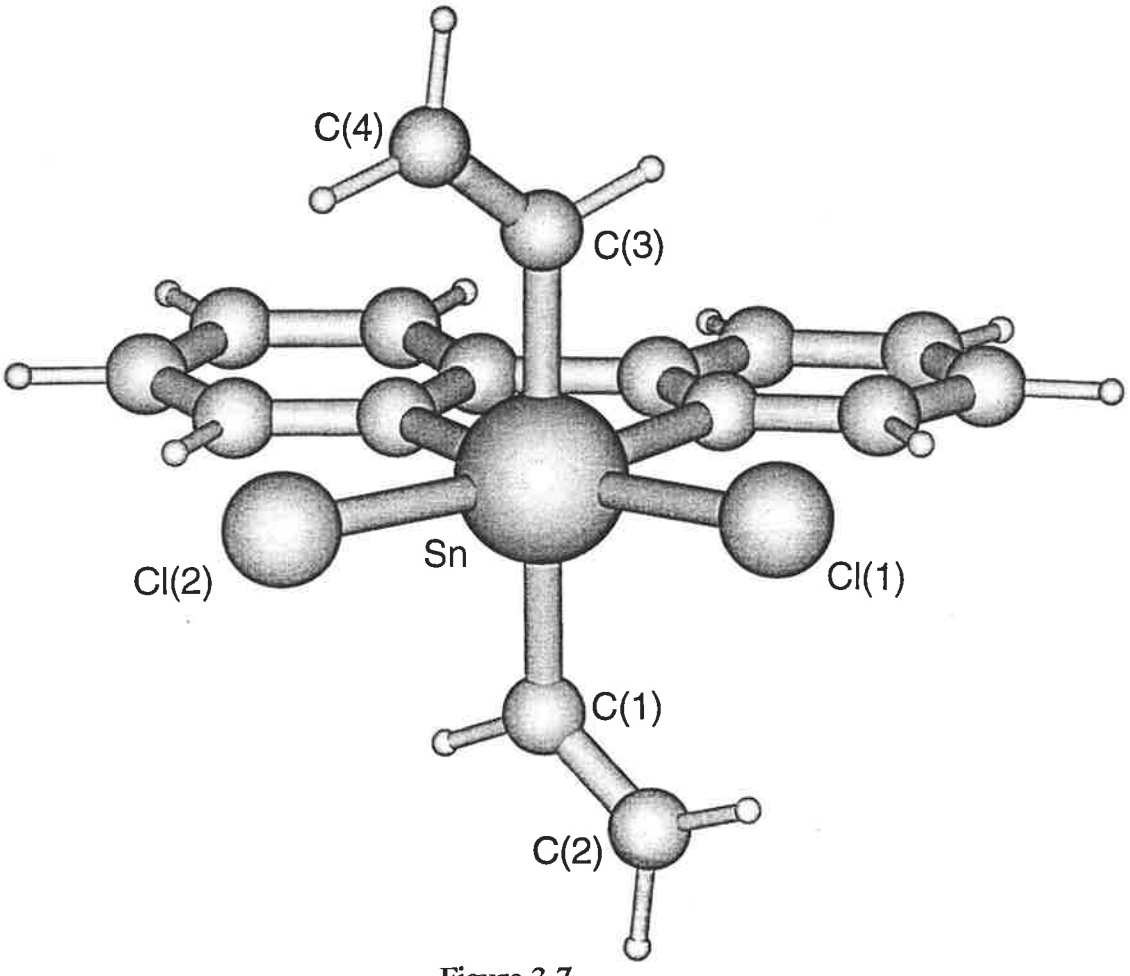


Figure 3.7

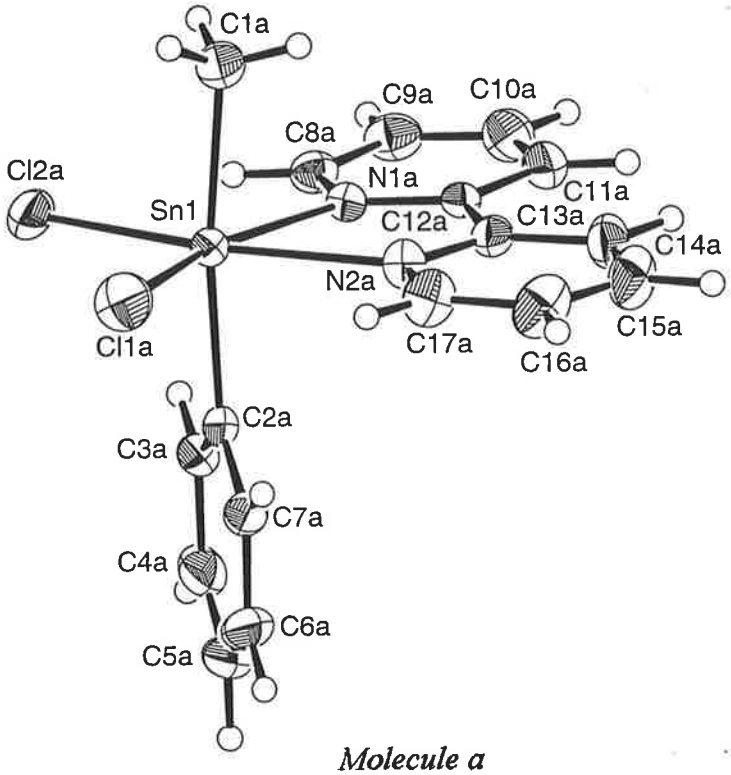
The optimised structure of [Vin_2SnCl_2(2,2'-bipyridyl)]

3.3.1d [Ph(Me)$SnCl_2$(2,2'-bipyridyl)]·0.25$CHCl_3$

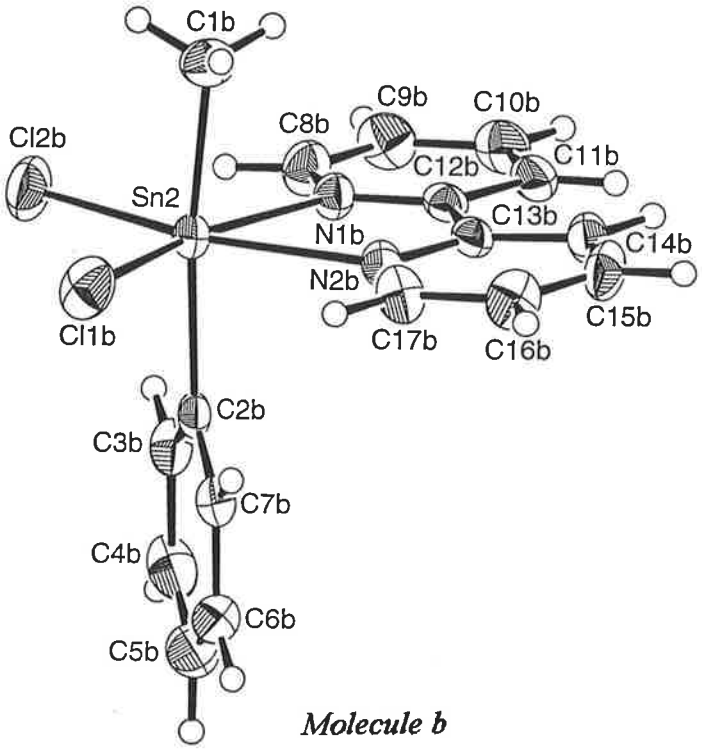
The [Ph(Me)$SnCl_2$(2,2'-bipyridyl)]·0.25$CHCl_3$ structure is an example where two independent molecules comprise the asymmetric unit in addition to occluded solvent. In this analysis the two effects examined earlier in $^tBu_2Sn(S_2CNCy_2)Cl$ (two independent molecules) and [Vin_2SnCl_2(2,2'-bipyridyl)]·0.5C_6H_6 (occluded solvent) are combined in the one lattice.

Two molecules (labeled *a* and *b*) of [Ph(Me)$SnCl_2$(2,2'-bipyridyl)] and half a chloroform molecule comprise the crystallographic asymmetric unit of [Ph(Me)$SnCl_2$(2,2'-bipyridyl)]·0.25$CHCl_3$. The overall geometry for [Ph(Me)$SnCl_2$(2,2'-bipyridyl)]·0.25$CHCl_3$ is, allowing for the necessary changes, essentially as described above for [Vin_2SnCl_2(2,2'-bipyridyl)]·0.5C_6H_6. From an inspection of the molecular structures illustrated in Figure 3.8 and the selected interatomic parameters collected in Table 3.5, it is clear that there are no major differences between the two independent molecules. There is a slight disparity in the Sn-Cl bond distances for molecule *b* that is not found for molecule *a*, and the greatest difference in bond angles between *a* and *b*, i.e. 4.2°, is found for the Cl(2)-Sn-N(1) angles. The tin atom lies 0.0091(4) Å [0.0166(5) Å for molecule *b*] above the N_2Cl_2 plane in the direction of the *ipso* carbon atom of the phenyl group. The orientation of the phenyl group with respect to the N_2Cl_2 plane is the same for the two molecules, i.e. the dihedral angle between the respective planes is 91.4° for both molecules, a result that emphasises the similarity between their structures. There are differences, however, in the nature of their intermolecular associations.

The most significant contact in the lattice involving the tin-bound chloride atoms is 2.72 Å which occurs between Cl(1b) and H(100), i.e. the chloroform hydrogen; Cl(1b)...C(100) is 3.51(1) Å. The next closest contact of 2.87 Å also involves Cl(1b) [Cl(1b)...H(9a)^i; symmetry operation *i*: 0.5 - *x*, -0.5 + *y*, 0.5 - *z*] and all other contacts



Molecule a



Molecule b

Figure 3.8

The molecular structure of [Ph(Me)$SnCl_2$(2,2'-bipyridyl)]·0.25$CHCl_3$

TABLE 3.5: Geometric parameters (Å, deg.) and calculated energies (Hartrees) for [Ph(Me)$SnCl_2$(2,2'-bipyridyl)]·0.25$CHCl_3$

	[Ph(Me)$SnCl_2$(2,2'-bipyridyl)]·0.25$CHCl_3$		
Parameter	Solid State Structure (molecule *a*)	Solid State Structure (molecule *b*)	Optimised Structure
Sn-Cl(1)	2.488(2)	2.500(2)	2.536
Sn-Cl(2)	2.492(2)	2.481(2)	2.536
Sn-N(1)	2.389(5)	2.388(5)	2.404
Sn-N(2)	2.401(5)	2.391(5)	2.404
Sn-C(1)	2.139(7)	2.110(8)	2.115
Sn-C(2)	2.154(7)	2.142(7)	2.140
Cl(1)-Sn-Cl(2)	101.89(7)	103.14(7)	110.0
Cl(1)-Sn-N(1)	161.7(1)	164.7(1)	159.3
Cl(1)-Sn-N(2)	93.1(1)	95.5(1)	90.7
Cl(1)-Sn-C(1)	93.7(2)	90.1(3)	90.4
Cl(1)-Sn-C(2)	93.2(2)	91.4(2)	93.5
Cl(2)-Sn-N(1)	96.4(1)	92.2(1)	90.7
Cl(2)-Sn-N(2)	165.0(1)	161.3(1)	159.3
Cl(2)-Sn-C(1)	91.7(2)	93.1(3)	90.4
Cl(2)-Sn-C(2)	91.4(2)	92.9(2)	93.5
N(1)-Sn-N(2)	68.5(2)	69.2(2)	68.6
N(1)-Sn-C(1)	85.2(2)	88.5(3)	88.2
N(1)-Sn-C(2)	86.9(2)	88.4(2)	86.2
N(2)-Sn-C(1)	86.9(2)	85.6(3)	88.2
N(2)-Sn-C(2)	88.1(2)	87.7(2)	86.2
C(1)-Sn-C(2)	171.8(3)	173.3(3)	173.3
C(1)/Sn/C(2)/C(3)	-72(2)	-120(3)	-90
C(1)/Sn/C(2)/C(7)	111(2)	63(3)	90
Calculated Energies	-794.3827	-794.3760	-794.5436

involving Sn-Cl are all longer than these and hence, it can be surmised that the elongation of the Sn(2)-Cl(1b) bond with respect to the other Sn-Cl bonds is due to intermolecular Cl...H interactions, as found in the structure of [Vin$_2$$SnCl_2$(2,2'-bipyridyl)]·0.5$C_6H_6$. A number of further interactions between the solvent chloroform molecule exist with

Cl(30)...H(15b)^{ii} (symmetry operation *ii*: -0.5 + *x*, 0.5 - *y*, 0.5 + *z*) of 2.79 Å being the closest. The closest non-hydrogen contact in the lattice is 3.43(1) Å and occurs between the C(9a) and C(15a)^{iii} atoms (symmetry operation *iii*: 1 - *x*, 1 - *y*, - *z*). This separation is indicative of some π-π interactions between centrosymmetrically pairs of molecule *a*; similar interactions of 3.44 Å are present for isolated pairs of molecule *b*. For [Ph(Me)$SnCl_2$(2,2'-bipyridyl)]·0.25$CHCl_3$, there are two essentially identical molecules which differ only in their (weak) intermolecular contacts. Not surprisingly, geometry optimisation calculations showed that both molecules converged to the same geometry and a comparison between the experimentally determined structures and the energy minimised molecule (Figure 3.9) reveal a number of notable trends.

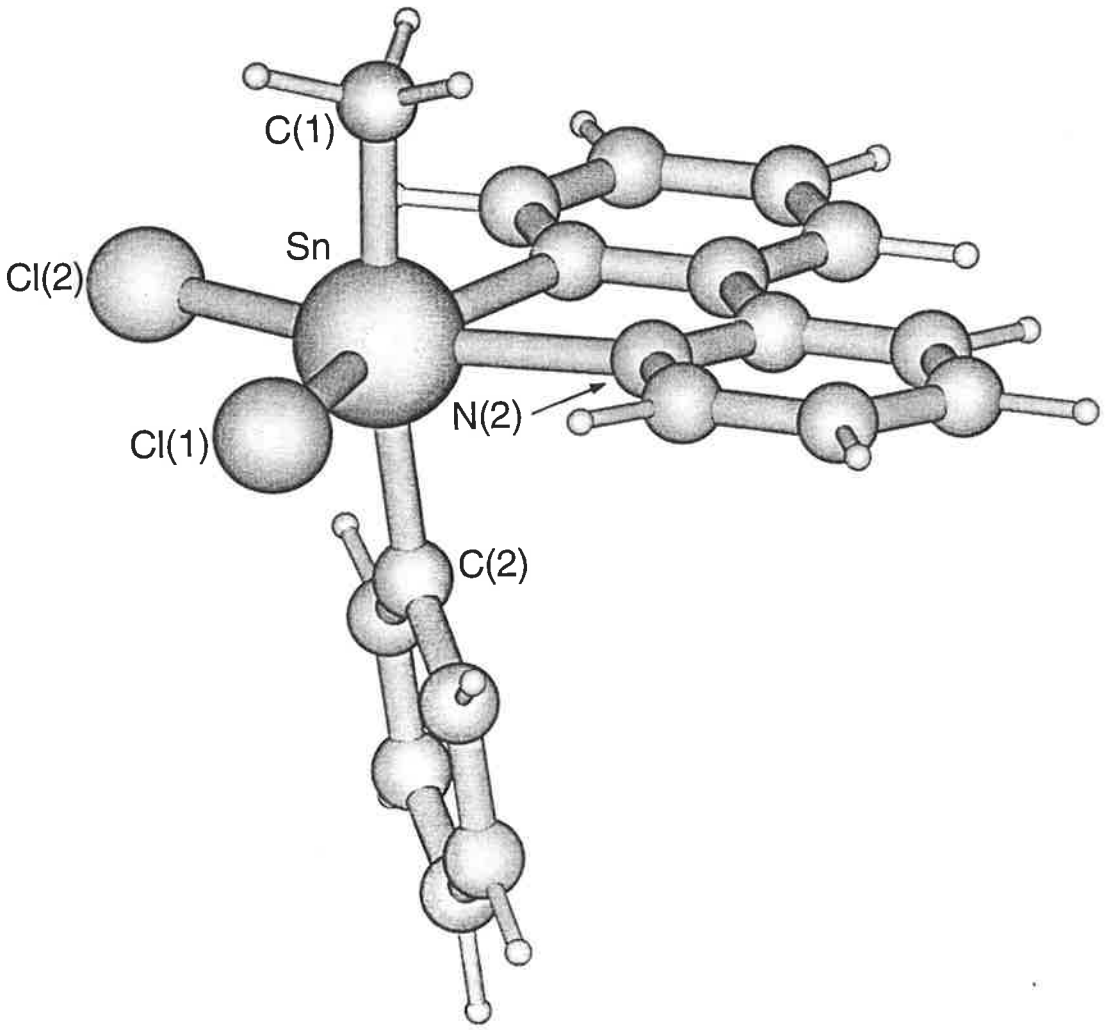


Figure 3.9

The optimised structure of [Ph(Me)$SnCl_2$(2,2'-bipyridyl)]·0.25$CHCl_3$

As can be seen from Table 3.5, the Sn-Cl and Sn-N distances in the optimised structure are longer than those found in the solid state. Comparison of Sn-C distances is problematic owing to the relatively high errors associated with these parameters, however, it is noteworthy that the Sn-C(methyl) distance in the optimised geometry is shorter than the Sn-C(phenyl) separation. In terms of angles, the greatest difference is found in the Cl-Sn-Cl angle which has expanded by *ca* 8° and 7°, respectively compared to molecules *a* and *b* in the solid state; there are concomitant changes in the other angles about the tin atom. In terms of overall geometry, the optimised structure presented in Figure 3.9, is more symmetrical, having mirror symmetry, with equivalence between similar Sn-ligand bond distances and, allowing for chemistry, between comparable angles.

The single point calculations based on the crystallographically determined structures of molecules *a* and *b* showed that molecule *a* was 17.6 kJ mol^{-1} more stable than molecule *b*. Further, the optimised structure of molecule *a* was 422.4 kJ mol^{-1} more stable than the crystallographic structure and the comparable value for molecule *b* was 440.0 kJ mol^{-1}. It can be therefore concluded that the differences noted above between the two independent molecules comprising the crystallographic asymmetric unit of [Ph(Me)$SnCl_2$(2,2'-bipyridyl)]·0.25$CHCl_3$ can be attributed to crystal packing effects and in the absence of these effects, solid state [Ph(Me)$SnCl_2$(2,2'-bipyridyl)]·0.25$CHCl_3$ converges to a single gas phase structure.

3.3.1e [Me_2SnCl_2(1,10-phenanthroline)]

The final example for analysis is [Me_2SnCl_2(1,10-phenanthroline)], which has crystallographic symmetry. A general feature of the crystallographically determined structures described above, is a lack of symmetry in the molecule as found in the solid state and after geometry optimisation, the symmetrisation of the structure, often accompanied by a significant change in geometric parameters. Hence, differences between individual geometric parameters may reflect changes in geometry/conformation rather than crystal packing effects alone. The geometry optimization of

$[Me_2SnCl_2(1,10\text{-phenanthroline})]$ was conducted in order to examine what changes in geometric parameters are apparent when, presumably, only minor changes in geometry occur upon optimization as the starting geometry is already highly symmetric.

The molecular structure as determined by X-ray diffraction for $[Me_2SnCl_2(1,10\text{-phenanthroline})]$ is shown in Figure 3.10 and selected interatomic parameters are collected in Table 3.7. The tin atom lies on a crystallographic site of symmetry *m2m* with one mirror plane being defined by the chloride atoms and the phenanthroline ligand, another by the methyl carbons (and two of the hydrogen atoms) and tin atom; the two-fold axis passes through the tin atom and bisects the Cl...Cl and N...N vectors. The overall structure is similar to that described above for $[Vin_2SnCl_2(2,2'\text{-bipyridyl})]\cdot 0.5C_6H_6$ and $[Ph(Me)SnCl_2(2,2'\text{-bipyridyl})]\cdot 0.25CHCl_3$. The closest non-hydrogen atom contact in the lattice is 3.39(2) Å and this occurs between two C(1) atoms (symmetry operation *i*: $+x, +y, 1.5 - z$). The closest contact involving chloride is 2.81 Å with $H(4)^{ii}$ (symmetry operation *ii*: $0.5 - x, -0.5 - y, 0.5 + z$).

Optimized parameters for $[Me_2SnCl_2(1,10\text{-phenanthroline})]$ are listed in Table 3.6 and the geometry is illustrated in Figure 3.11. The key result of the calculation is that there has been a uniform elongation in the tin-ligand parameters with Sn-Cl, Sn-N and Sn-C distances each elongating by 0.029, 0.034 and 0.038 Å, respectively. The major difference amongst the angles is the expansion of the Cl-Sn-Cl angle from 106.1(1)° in the crystal structure to 111.9° in the optimized structure.

The difference in energy between the experimentally observed and optimised structures, was found to be 414.1 kJ mol^{-1}, the latter being more stable.

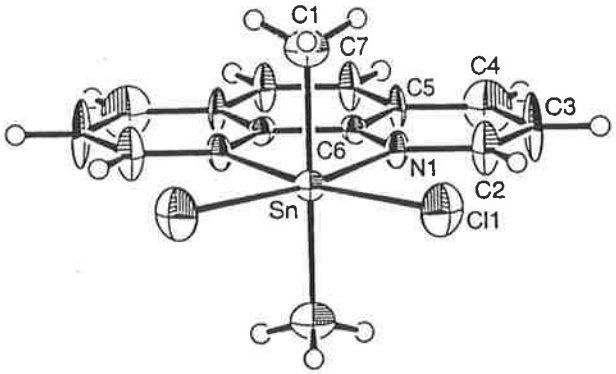


Figure 3.10
The molecular structure of [Me_2SnCl_2(1,10-phenanthroline)]

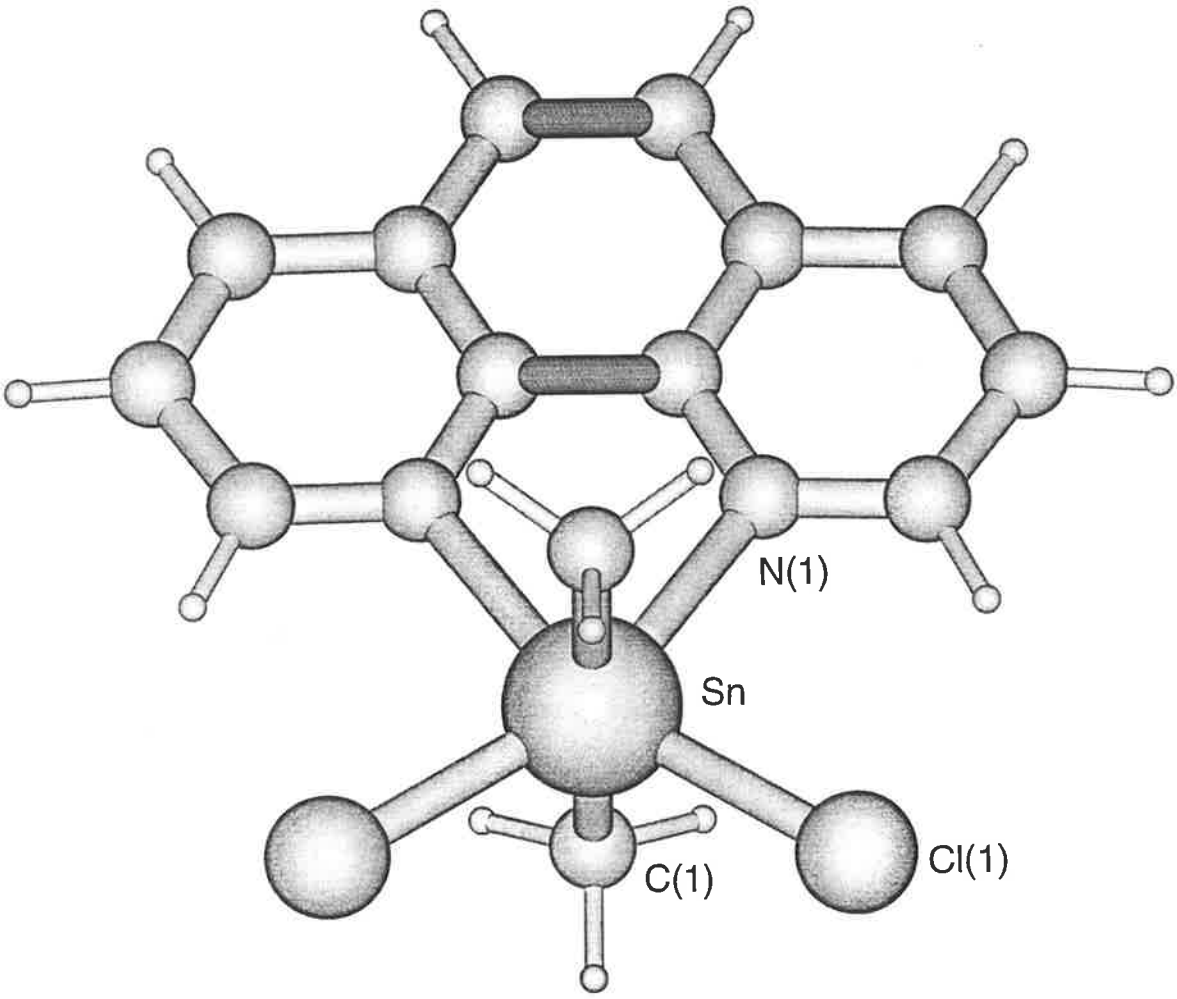


Figure 3.11
The optimised structure of [Me_2SnCl_2(1,10-phenanthroline)]

TABLE 3.6: Geometric parameters (Å, deg.) and calculated energies (Hartrees) for [Me_2SnCl_2(1,10-phenanthroline)]

	[Me_2SnCl_2(1,10-phenanthroline)]	
Parameter	Solid State Structure*	Optimised Structure*
Sn-Cl(1)	2.521(3)	2.550
Sn-Cl(2)	2.521(3)	2.550
Sn-N(1)	2.385(9)	2.419
Sn-N(2)	2.385(9)	2.419
Sn-C(1)	2.075(8)	2.113
Sn-C(2)	2.075(8)	2.113
Cl(1)-Sn-Cl(2)	106.1(1)	111.9
Cl(1)-Sn-N(1)	92.6(3)	89.5
Cl(1)-Sn-N(2)	161.3(3)	158.6
Cl(1)-Sn-C(1)	90.7(1)	91.1
Cl(1)-Sn-C(2)	90.7(1)	91.1
Cl(2)-Sn-N(1)	161.3(3)	158.6
Cl(2)-Sn-N(2)	92.6(3)	89.5
Cl(2)-Sn-C(1)	90.7(1)	91.1
Cl(2)-Sn-C(2)	90.7(1)	91.1
N(1)-Sn-N(2)	68.7(5)	69.2
N(1)-Sn-C(1)	89.1(1)	88.4
N(1)-Sn-C(2)	89.1(1)	88.4
N(2)-Sn-C(1)	89.1(1)	88.4
N(2)-Sn-C(2)	89.1(1)	88.4
C(1)-Sn-C(2)	177.8(4)	176.0
Calculated Energies	-679.6752	-679.8329

* molecule has *m2m* symmetry such that Cl(1) = Cl(2), N(1) = N(2) and C(1) = C(2)

3.3.2 Energy considerations

When considering energy differences calculated between single point and geometry optimised structures, one needs to be wary as errors in crystal structure determination can vary from system to system. Minor conformational differences and disorder (positional and thermal) can give rise to different energies. One obvious source of error concerns the treatment of hydrogen atoms which are normally included in their calculated positions in crystallographic refinements at 0.95 - 1.0 Å in order to model electron density maxima. In the optimised geometries the C-H distances were 1.07 - 1.08 Å. As a trial, three separate single point calculations were conducted for molecule *a* of [$^{t}Bu_2Sn(S_2CNCy_2)Cl$] in which the hydrogen atoms were included at C-H separations of 0.90 Å, 0.97 Å and 1.08 Å. The energy calculated for the structure with the longer C-H separations was found to be 608.8 kJ mol^{-1} more stable than the structure with C-H constrained to 0.97 Å and this was, in turn, 519.3 kJ mol^{-1} more stable than the structure with C-H constrained to 0.90 Å. Clearly, the treatment of hydrogen atoms in the X-ray experiment significantly influences the energy differences calculated for the molecules. The above calculations reveal that the treatment of hydrogen atoms in the X-ray experiment may account for approximately 30% of the energy difference between the experimental and calculated structures.

It should be noted that free energy differences calculated for polymorphs of organic compounds are estimated to be in the order of 4 - 8 kJ mol^{-1} [6]. Higher energies would be expected for the larger systems (in terms of both atoms sizes and numbers of atoms) described in the present study, however, it is certain that the energy differences calculated between the solid state and gas phase structures are overestimated.

It is not suggested that conclusions drawn from our energy analyses are seriously affected by possible over estimations bought about by the lack of electron correlation in our calculations. Incorporation of electron correlation will not significantly alter the semi-quantitative conclusion drawn here that, relative to the experimentally determined crystal structures, the more symmetric isolated molecular configurations are more stable

by chemically significant amounts of energy. Support for this conclusion is found by referring back to the energy differences calculated for the structures [Me_2SnCl_2] and [Me_3SnCl] [2]. Here both starting points converged to the same optimised geometry for each of the levels of theory. Additionally the energy difference between the optimised geometry and the experimental gas phase structure is an order of magnitude less than the energy difference between the solid state structure and optimised structure. Clearly indicating an influence of crystal packing effect. Also the magnitude of energy differences between the experimental structures (determined either in the solid state or in the gas phase) is smallest at the HF level of theory compared with the other levels of theories investigated.

3.4 Conclusions

This combined crystallographic and theoretical study of selected organotin systems has addressed the question whether crystal packing effects can significantly influence molecular geometry. It has been found that in the absence of crystal packing effects, the solid state geometries uniformly converged to more symmetric structures and hence, it is possible to conclude that crystal packing effects can influence molecular geometry about heavy metal centers such as tin. It was also found that Sn-ligand bond distances generally increased but that bond angles did not change greatly apart from those involved in the symmetrisation of the structure. In terms of energy differences, Table 3.7, it may be concluded that the energy difference between molecules in two distinct crystalline environments (i.e. polymorphs) as calculated for [$Ph_2Sn(S_2CNEt_2)_2$] are greater than energy differences between two molecules that crystallise in the one lattice, e.g. [$^tBu_2Sn(S_2CNCy_2)Cl$] and [Ph(Me)$SnCl_2$(2,2'-bipyridyl)]·0.25$CHCl_3$. Further, the presence of solvent in the lattice, as in [Vin_2SnCl_2(2,2'-bipyridyl)]·0.5C_6H_6 and [Ph(Me)$SnCl_2$(2,2'-bipyridyl)]·0.25$CHCl_3$, does not markedly alter the energy differences calculated between the condensed (solid state) and gas phases, allowing for different sizes of the molecules.

TABLE 3.7: Calculated Energies (Hartrees, kJ mol^{-1}) Employing the LanL2DZ Basis Set for Diorganotin compounds examined in this chapter.

	Calculated Energies		
diorganotin compounds	**Single point** (hartrees)	**Optimised geometry** (hartrees)	**Δ** (kJ mol^{-1})
$[Ph_2Sn(S_2CNEt_2)_2]$ *Tetragonal polymorph*[5]	-1001.6459	-1002.0139	966.2
$[Ph_2Sn(S_2CNEt_2)_2]$ *Monoclinic polymorph*[4b]	-1001.5889	-1002.0139	790.4
$[^tBu_2Sn(S_2CNCy_2)Cl]$ *molecule a*	-910.0397	-910.51223	1240.6
$[^tBu_2Sn(S_2CNCy_2)Cl]$ *molecule b*	-910.0337	-910.51253	1257.1
$[Ph(Me)SnCl_2$(2,2'-bipyridyl)] *molecule a*	-794.3827	-794.5436	422.4
$[Ph(Me)SnCl_2$(2,2'-bipyridyl)] *molecule b*	-794.3760	-794.5436	440.0
$[Me_2SnCl_2$(1,10-phenanthroline)]	-679.6752	-679.8329	414.1
$[Vin_2SnCl_2$(2,2'-bipyridyl)]	-679.5857	-679.7460	420.9

3.5 References

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Appendix-Chapter 3

Crystal data and refinement details for:

A. [$^{t}Bu_2Sn(S_2CNCy_2)Cl$]

B [Vin_2SnCl_2(2,2'-bipyridyl)]·$0.5C_6H_6$

C. [Ph(Me)$SnCl_2$(2,2'-bipyridyl)]·$0.25CHCl_3$

D. [Me_2SnCl_2(1,10-phenanthroline)].

A. $[^{t}Bu_2Sn(S_2CNCy_2)Cl]$

Crystallographic Data and Refinement details for [^{t}Bu$_2$Sn(S$_2$CNCy$_2$)Cl].

Formula	$C_{21}H_{40}ClNS_2Sn$
Formula weight	524.8
Crystal morphology	colourless needle
Crystal dimensions (mm)	0.06 x 0.11 x 0.44
Crystal system	triclinic
Space group	$P\bar{1}$, (C_i^1, No. 2)
Temperature (°C)	20.0
a (Å)	12.761(3)
b (Å)	18.329(6)
c (Å)	12.191(3)
α (°)	97.73(3)
β (°)	98.85(2)
γ (°)	107.90(2)
V (Å^3)	2630(1)
Z	4
D_{calc} (g cm^{-3})	1.325
F(000)	1088
Radiation	CuKα (λ = 1.5412Å)
μ (cm^{-1})	101.79
θ limits, data (°)	3.0 to 60.0
hkl range	0 to 14 , -21 to 21, -14 to 14
Range of transmission factors	0.798 to 1.000
Scan technique	ω:2θ
Scan width (°)	1.26
No. of data measured	8247
No. of unique data	7838
R_{amal}	0.20
Program for structure solution	Direct Methods (SHELXS86)
No. of unique data used	5293
No. of parameters	469
R	0.059
R_w	0.062
G.O.F.	2.73
Min./Max. residual electron density (e Å^{-3})	-1.57 to +1.12

Fractional atomic coordinates for the non-hydrogen atoms in [^{t}Bu$_2$Sn(S$_2$CNCy$_2$)Cl].

Atom	*x*	*y*	*z*
Sn(1)	0.24510(6)	-0.28747(4)	0.51033(6)
Sn(2)	-0.19430(6)	-0.21687(4)	0.00941(6)
Cl(1)	0.3044(3)	-0.3638(2)	0.6462(3)
Cl(2)	-0.2399(3)	-0.1073(2)	0.1121(3)
S(1a)	0.4495(2)	-0.2188(2)	0.5365(2)
S(1b)	-0.2956(3)	-0.2952(1)	0.1350(2)
S(2a)	0.2910(2)	-0.1748(2)	0.3832(3)
S(2b)	-0.2091(3)	-0.3708(2)	-0.0381(3)
N(1a)	0.5124(6)	-0.1242(4)	0.3930(6)
N(1b)	-0.2924(7)	-0.4417(4)	0.1215(6)
C(1a)	0.1726(9)	-0.3850(6)	0.3653(9)
C(1b)	-0.2835(8)	-0.2164(8)	-0.1594(6)
C(2a)	0.0888(8)	-0.4523(7)	0.4043(5)
C(2b)	-0.2579(9)	-0.1358(9)	-0.1825(8)
C(3b)	-0.2498(9)	-0.2656(9)	-0.2493(6)
C(3a)	0.1147(9)	-0.3612(8)	0.2685(8)
C(4a)	0.2669(9)	-0.4095(9)	0.3324(9)
C(4b)	-0.4119(5)	-0.2506(9)	-0.1593(6)
C(5a)	0.1476(6)	-0.2381(7)	0.6087(9)
C(5b)	-0.0106(8)	-0.1687(7)	0.0725(8)
C(6a)	0.0747(8)	-0.3006(9)	0.6624(7)
C(6b)	0.0318(9)	-0.0876(7)	0.0653(9)
C(7a)	0.0717(7)	-0.2084(7)	0.5344(7)
C(7b)	0.0437(9)	-0.2166(8)	0.0044(8)
C(8a)	0.2299(8)	-0.1736(9)	0.7044(7)
C(8b)	0.0115(8)	-0.1805(7)	0.1948(9)
C(9a)	0.4279(8)	-0.1665(5)	0.4312(8)
C(9b)	-0.2678(9)	-0.3777(6)	0.0796(8)
C(10a)	0.5044(8)	-0.0885(5)	0.2901(8)
C(10b)	-0.2776(10)	-0.5136(6)	0.0635(8)
C(11a)	0.4645(9)	-0.0188(6)	0.3056(9)
C(11b)	-0.3805(9)	-0.5855(6)	0.0464(9)

Fractional atomic coordinates for the non-hydrogen atoms in [$^{t}Bu_2Sn(S_2CNCy_2)Cl$] Cont'd.

Atom	*x*	*y*	*z*
C(12a)	0.4689(10)	0.0174(7)	0.2012(12)
C(12b)	-0.3619(7)	-0.6542(7)	-0.0242(9)
C(13a)	0.3985(8)	-0.0422(8)	0.0978(9)
C(13b)	-0.2575(9)	-0.6675(7)	0.0308(8)
C(14a)	0.4418(9)	-0.1109(7)	0.0806(9)
C(14b)	-0.1568(7)	-0.5966(8)	0.0536(11)
C(15a)	0.4391(10)	-0.1498(6)	0.1836(9)
C(15b)	-0.1724(9)	-0.5257(6)	0.1202(10)
C(16a)	0.6304(8)	-0.1152(5)	0.4493(8)
C(16b)	-0.3256(9)	-0.4478(6)	0.2326(8)
C(17a)	0.7109(9)	-0.0315(6)	0.4735(9)
C(17b)	-0.4441(12)	-0.4491(7)	0.2342(14)
C(18a)	0.8229(9)	-0.0273(7)	0.5410(10)
C(18b)	-0.4732(11)	-0.4651(9)	0.3471(9)
C(19a)	0.8717(9)	-0.0813(7)	0.4808(11)
C(19b)	-0.3892(9)	-0.4077(9)	0.4468(9)
C(20a)	0.7917(10)	-0.1656(7)	0.4497(9)
C(20b)	-0.2716(11)	-0.4067(7)	0.4437(10)
C(21a)	0.6758(9)	-0.1706(5)	0.3857(9)
C(21b)	-0.2395(7)	-0.3896(6)	0.3324(9)

Anisotropic Displacement Parameters ($Å^2$) for the non-hydrogen atoms in [$^tBu_2Sn(S_2CNCy_2)Cl$].

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Sn(1)	0.0410(4)	0.0510(4)	0.0509(5)	0.0127(4)	0.0142(4)	0.0171(3)
Sn(2)	0.0633(6)	0.0455(4)	0.0503(5)	0.0218(4)	0.0153(4)	0.0127(3)
Cl(1)	0.081(2)	0.084(2)	0.077(2)	0.034(2)	0.015(2)	0.040(2)
Cl(2)	0.112(3)	0.070(2)	0.098(2)	0.054(2)	0.047(2)	0.021(2)
S(1a)	0.044(2)	0.069(2)	0.061(2)	0.009(1)	0.012(1)	0.026(1)
S(1b)	0.089(2)	0.045(2)	0.068(2)	0.027(2)	0.035(2)	0.019(1)
S(2a)	0.042(2)	0.067(2)	0.082(2)	0.012(2)	0.014(2)	0.030(2)
S(2b)	0.141(3)	0.063(2)	0.068(2)	0.030(2)	0.060(2)	0.018(2)
N(1a)	0.042(5)	0.041(5)	0.040(5)	0.013(4)	0.015(4)	0.002(4)
N(1b)	0.057(6)	0.042(5)	0.047(5)	0.017(5)	0.020(4)	0.009(4)
C(1a)	0.081(9)	0.056(7)	0.053(7)	0.013(7)	0.005(7)	0.012(6)
C(1b)	0.13(1)	0.10(1)	0.049(8)	0.03(1)	-0.013(8)	0.037(7)
C(2a)	0.10(1)	0.068(9)	0.10(1)	-0.013(8)	0.011(9)	0.016(8)
C(2b)	0.17(2)	0.14(1)	0.09(1)	0.09(1)	0.00(1)	0.06(1)
C(3b)	0.34(3)	0.15(2)	0.05(1)	0.12(2)	0.04(1)	0.02(1)
C(3a)	0.14(1)	0.10(1)	0.06(1)	0.02(1)	-0.031(9)	0.000(8)
C(4a)	0.11(1)	0.13(1)	0.10(1)	0.05(1)	0.04(1)	-0.02(1)
C(4b)	0.08(1)	0.36(3)	0.13(2)	-0.05(2)	-0.04(1)	0.12(2)
C(5a)	0.081(9)	0.069(8)	0.10(1)	0.029(8)	0.059(8)	0.051(7)
C(5b)	0.063(9)	0.058(8)	0.12(1)	0.030(7)	0.008(8)	0.004(8)
C(6a)	0.11(1)	0.13(1)	0.12(1)	0.06(1)	0.09(1)	0.04(1)
C(6b)	0.06(1)	0.09(1)	0.42(4)	0.01(1)	0.00(2)	0.05(2)
C(7a)	0.13(1)	0.19(2)	0.15(2)	0.12(1)	0.08(1)	0.09(1)
C(7b)	0.09(1)	0.17(2)	0.30(3)	0.04(1)	0.03(2)	-0.11(2)
C(8a)	0.13(2)	0.14(2)	0.13(2)	0.02(1)	0.04(1)	-0.06(1)
C(8b)	0.08(1)	0.35(3)	0.14(2)	0.05(2)	-0.02(1)	0.06(2)
C(9a)	0.041(6)	0.040(6)	0.052(6)	0.005(5)	0.015(5)	0.009(5)
C(9b)	0.064(8)	0.050(7)	0.043(6)	0.010(6)	0.012(6)	0.006(5)
C(10a)	0.056(7)	0.032(5)	0.045(6)	0.005(5)	0.015(5)	0.007(4)
C(10b)	0.068(8)	0.043(6)	0.052(7)	0.015(6)	0.021(6)	0.003(5)
C(11a)	0.069(8)	0.051(7)	0.065(8)	0.022(6)	0.027(6)	0.009(5)
C(11b)	0.065(8)	0.051(7)	0.063(8)	0.019(7)	0.002(6)	-0.005(6)

Anisotropic Displacement Parameters ($Å^2$) for the non-hydrogen atoms in [$^tBu_2Sn(S_2CNCy_2)Cl$] Cont'd.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(12a)	0.08(1)	0.061(8)	0.09(1)	0.024(7)	0.012(8)	0.029(7)
C(12b)	0.11(1)	0.052(7)	0.070(9)	0.020(8)	0.020(8)	-0.007(6)
C(13a)	0.068(9)	0.11(1)	0.078(9)	0.033(9)	0.009(7)	0.050(8)
C(13b)	0.12(1)	0.063(8)	0.09(1)	0.051(9)	0.022(9)	-0.004(7)
C(14a)	0.09(1)	0.080(9)	0.049(7)	0.014(8)	0.013(7)	0.013(6)
C(14b)	0.09(1)	0.08(1)	0.10(1)	0.036(9)	0.017(9)	-0.019(8)
C(15a)	0.092(9)	0.047(6)	0.049(7)	0.020(7)	0.018(7)	0.006(5)
C(15b)	0.055(8)	0.060(7)	0.073(8)	0.017(7)	0.017(7)	-0.011(6)
C(16a)	0.041(6)	0.046(6)	0.046(6)	0.008(5)	0.015(5)	0.000(5)
C(16b)	0.058(7)	0.049(6)	0.041(6)	0.020(6)	0.028(5)	0.017(5)
C(17a)	0.054(7)	0.049(7)	0.063(7)	0.017(6)	0.021(6)	-0.011(5)
C(17b)	0.066(9)	0.083(9)	0.086(9)	0.036(7)	0.035(7)	0.036(7)
C(18a)	0.045(7)	0.073(8)	0.070(8)	0.002(7)	0.015(6)	0.001(6)
C(18b)	0.11(1)	0.10(1)	0.13(1)	0.06(1)	0.09(1)	0.07(1)
C(19a)	0.040(7)	0.069(8)	0.11(1)	0.013(7)	0.021(7)	0.015(7)
C(19b)	0.20(2)	0.09(1)	0.09(1)	0.06(1)	0.10(1)	0.036(8)
C(20a)	0.053(8)	0.062(8)	0.11(1)	0.028(7)	0.020(7)	0.011(7)
C(20b)	0.14(1)	0.076(9)	0.048(8)	0.04(1)	0.036(9)	0.014(6)
C(21a)	0.060(8)	0.036(6)	0.073(8)	0.019(6)	0.021(6)	-0.001(5)
C(21b)	0.088(9)	0.058(7)	0.051(7)	0.026(7)	0.022(7)	0.004(6)

Fractional atomic coordinates and B_{eq} values ($Å^2$) for the hydrogen atoms in [$^tBu_2Sn(S_2CNCy_2)Cl$].

Atom	x	y	z	B_{eq}
H(2a)	0.0258	-0.4362	0.4220	9.6368
H(2b)	0.1256	-0.4648	0.4703	9.6368
H(2c)	0.0591	-0.4980	0.3434	9.6368
H(2d)	-0.1756	-0.1117	-0.1708	11.7260
H(2e)	-0.2850	-0.1053	-0.1301	11.7260
H(2f)	-0.2914	-0.1376	-0.2591	11.7260
H(3a)	0.1654	-0.3157	0.2494	10.7798
H(3b)	0.0497	-0.3486	0.2880	10.7798
H(3c)	0.0877	-0.4038	0.2030	10.7798
H(3d)	-0.2831	-0.2609	-0.3237	16.5152
H(3e)	-0.2734	-0.3193	-0.2411	16.5152
H(3f)	-0.1674	-0.2460	-0.2399	16.5152
H(4a)	0.2364	-0.4502	0.2646	11.1703
H(4b)	0.2993	-0.4293	0.3932	11.1703
H(4c)	0.3221	-0.3650	0.3168	11.1703
H(4d)	-0.4541	-0.2439	-0.2278	20.9704
H(4e)	-0.4268	-0.2216	-0.0939	20.9704
H(4f)	-0.4310	-0.3047	-0.1548	20.9704
H(6a)	0.0206	-0.3421	0.6039	10.1616
H(6b)	0.0342	-0.2772	0.7100	10.1616
H(6c)	0.1224	-0.3219	0.7081	10.1616
H(6d)	0.1105	-0.0649	0.0985	18.7996
H(6e)	-0.0098	-0.0589	0.1043	18.7996
H(6f)	0.0194	-0.0821	-0.0143	18.7996
H(7a)	0.1147	-0.1716	0.4949	12.4930
H(7b)	0.0323	-0.1825	0.5808	12.4930
H(7c)	0.0156	-0.2518	0.4797	12.4930
H(7d)	0.0231	-0.2138	-0.0752	19.1248
H(7e)	0.0164	-0.2696	0.0140	19.1248
H(7f)	0.1242	-0.1945	0.0295	19.1248

Fractional atomic coordinates and B_{eq} values ($Å^2$) for the hydrogen atoms in [$^tBu_2Sn(S_2CNCy_2)Cl$] Cont'd.

Atom	*x*	*y*	*z*	B_{eq}
H(8a)	0.2804	-0.1344	0.6716	13.7969
H(8b)	0.2720	-0.1949	0.7539	13.7969
H(8c)	0.1873	-0.1473	0.7461	13.7969
H(8d)	-0.0072	-0.2348	0.1955	18.9473
H(8e)	-0.0347	-0.1581	0.2356	18.9473
H(8f)	0.0903	-0.1526	0.22841	8.9473
H(10a)	0.5808	-0.0683	0.2787	4.3470
H(10b)	-0.2671	-0.5051	-0.0115	5.1880
H(11a)	0.5134	0.0196	0.3706	5.6728
H(11b)	0.3881	-0.0356	0.3179	5.6728
H(11c)	-0.4455	-0.5760	0.0067	5.9560
H(11d)	-0.3934	-0.5975	0.1193	5.9560
H(12a)	0.5449	0.0373	0.1916	7.2419
H(12b)	0.4377	0.0600	0.2093	7.2419
H(12c)	-0.3534	-0.6432	-0.0983	7.5218
H(12d)	-0.4249	-0.7011	-0.0307	7.5218
H(13a)	0.4031	-0.0178	0.0307	7.8814
H(13b)	0.3206	-0.0609	0.1044	7.8814
H(13c)	-0.2447	-0.7086	-0.0197	8.0100
H(13d)	-0.2678	-0.6838	0.1014	8.0100
H(14a)	0.5174	-0.0925	0.0693	7.1146
H(14b)	0.3931	-0.1489	0.0146	7.1146
H(14c)	-0.1386	-0.5845	-0.0187	8.5385
H(14d)	-0.0931	-0.6070	0.0958	8.5385
H(15a)	0.3612	-0.1730	0.1908	5.9665
H(15b)	0.4727	-0.1901	0.1744	5.9665
H(15c)	-0.1789	-0.5343	0.1960	6.1422
H(15d)	-0.1080	-0.4796	0.1244	6.1422
H(16a)	0.6258	-0.1301	0.5223	4.3736
H(16b)	-0.3253	-0.4989	0.2453	4.3534

Fractional atomic coordinates and B_{eq} values ($Å^2$) for the hydrogen atoms in [$^tBu_2Sn(S_2CNCy_2)Cl$] Cont'd.

Atom	x	y	z	B_{eq}
H(17a)	0.6799	0.0023	0.5163	5.3509
H(17b)	0.7213	-0.0147	0.4026	5.3509
H(17c)	-0.4963	-0.4899	0.1732	6.7820
H(17d)	-0.4504	-0.3989	0.2230	6.7820
H(18a)	0.8124	-0.0420	0.6131	6.4292
H(18b)	0.8747	0.0258	0.5539	6.4292
H(18c)	-0.4735	-0.5174	0.3540	9.1997
H(18d)	-0.5468	-0.4617	0.3496	9.1997
H(19a)	0.9409	-0.0796	0.5275	6.8500
H(19b)	0.8880	-0.0637	0.4105	6.8500
H(19c)	-0.4082	-0.4224	0.5160	10.4735
H(19d)	-0.3924	-0.3559	0.4432	10.4735
H(20a)	0.7837	-0.1859	0.5177	6.9173
H(20b)	0.8227	-0.1967	0.4012	6.9173
H(20c)	-0.2654	-0.4573	0.4531	8.3098
H(20d)	-0.2186	-0.3667	0.5052	8.3098
H(21a)	0.6820	-0.1576	0.3119	5.2762
H(21b)	0.6243	-0.2236	0.3764	5.2762
H(21c)	-0.2366	-0.3370	0.3261	6.1376
H(21d)	-0.1653	-0.3940	0.3306	6.1376

Bond Distances (Å) for [$^{t}Bu_2Sn(S_2CNCy_2)Cl$].

Atom - Atom	Distance	Atom - Atom	Distance
Sn(1) - Cl(1)	2.482(3)	C(5a) - C(8a)	1.55(2)
Sn(1) - S(1a)	2.471(3)	C(5b) - C(6b)	1.45(2)
Sn(1) - S(2a)	2.722(3)	C(5b) - C(7b)	1.50(2)
Sn(1) - C(1a)	2.19(1)	C(5b) - C(8b)	1.52(2)
Sn(1) - C(5a)	2.16(1)	C(10a) - C(11a)	1.51(1)
Sn(2) - Cl(2)	2.492(3)	C(10a) - C(15a)	1.53(1)
Sn(2) - S(1b)	2.477(3)	C(10b) - C(11b)	1.51(1)
Sn(2) - S(2b)	2.743(3)	C(10b) - C(15b)	1.51(1)
Sn(2) - C(1b)	2.19(1)	C(11a) - C(12a)	1.52(1)
Sn(2) - C(5b)	2.21(1)	C(11b) - C(12b)	1.53(1)
S(1a) - C(9a)	1.740(9)	C(12a) - C(13a)	1.51(2)
S(1b) - C(9b)	1.73(1)	C(12b) - C(13b)	1.49(2)
S(2a) - C(9a)	1.71(1)	C(13a) - C(14a)	1.52(2)
S(2b) - C(9b)	1.72(1)	C(13b) - C(14b)	1.48(2)
N(1a) - C(9a)	1.31(1)	C(14a) - C(15a)	1.53(1)
N(1a) - C(10a)	1.49(1)	C(14b) - C(15b)	1.53(1)
N(1a) - C(16a)	1.51(1)	C(16a) - C(17a)	1.52(1)
N(1b) - C(9b)	1.31(1)	C(16a) - C(21a)	1.50(1)
N(1b) - C(10b)	1.49(1)	C(16b) - C(17b)	1.51(1)
N(1b) - C(16b)	1.49(1)	C(16b) - C(21b)	1.53(1)
C(1a) - C(2a)	1.55(2)	C(17a) - C(18a)	1.51(1)
C(1a) - C(3a)	1.49(2)	C(17b) - C(18b)	1.53(2)
C(1a) - C(4a)	1.49(2)	C(18a) - C(19a)	1.50(2)
C(1b) - C(2b)	1.48(2)	C(18b) - C(19b)	1.51(2)
C(1b) - C(3b)	1.52(2)	C(19a) - C(20a)	1.52(1)
C(1b) - C(4b)	1.55(2)	C(19b) - C(20b)	1.51(2)
C(5a) - C(6a)	1.53(2)	C(20a) - C(21a)	1.53(1)
C(5a) - C(7a)	1.49(2)	C(20b) - C(21b)	1.52(2)

Bond Angles (°) for [$^{t}Bu_2Sn(S_2CNCy_2)Cl$].

Atom - Atom - Atom	Angle	Atom - Atom - Atom	Angle
Cl(1) - Sn(1) - S(1a)	83.9(1)	S(1b) - C(9b) - S(2b)	114.9(6)
Cl(1) - Sn(1) - S(2a)	152.0(1)	S(1b) - C(9b) - N(1b)	123.0(8)
Cl(1) - Sn(1) - C(1a)	96.4(3)	S(2b) - C(9b) - N(1b)	122.1(8)
Cl(1) - Sn(1) - C(5a)	98.6(3)	N(1a) - C(10a) - C(11a)	113.3(8)
S(1a) - Sn(1) - S(2a)	68.04(8)	N(1a) - C(10a) - C(15a)	112.0(7)
S(1a) - Sn(1) - C(1a)	115.3(4)	C(11a) C(10a) - C(15a)	113.5(8)
S(1a) - Sn(1) - C(5a)	119.8(4)	N(1b) - C(10b) - C(11b)	113.0(9)
S(2a) - Sn(1) - C(1a)	95.1(3)	N(1b) - C(10b) - C(15b)	112.1(8)
S(2a) - Sn(1) - C(5a)	96.0(3)	C(11b) - C(10b) - C(15b)	112.2(9)
C(1a) - Sn(1) - C(5a)	123.9(5)	C(10a) - C(11a) - C(12a)	109.7(9)
Cl(2) - Sn(2) - S(1b)	85.0(1)	C(10b) - C(11b) - C(12b)	109(1)
Cl(2) - Sn(2) - S(2b)	152.3(1)	C(11a) - C(12a) - C(13a)	111(1)
Cl(2) - Sn(2) - C(1b)	96.3(4)	C(11b) - C(12b) - C(13b)	112(1)
Cl(2) - Sn(2) - C(5b)	96.9(3)	C(12a) - C(13a) - C(14a)	110.9(9)
S(1b) - Sn(2) - S(2b)	67.50(9)	C(12b) - C(13b) - C(14b)	113(1)
S(1b) - Sn(2) - C(1b)	120.1(4)	C(13a) - C(14a) - C(15a)	111(1)
S(1b) - Sn(2) - C(5b)	113.5(4)	C(13b) - C(14b) - C(15b)	112(1)
S(2b) - Sn(2) - C(1b)	95.2(4)	C(10a) - C(15a) - C(14a)	109.4(9)
S(2b) - Sn(2) - C(5b)	96.6(3)	C(10b) - C(15b) - C(14b)	110.3(9)
C(1b) - Sn(2) - C(5b)	125.6(6)	N(1a) - C(16a) - C(17a)	113.5(8)
Sn(1) - S(1a) - C(9a)	91.6(3)	N(1a) - C(16a) - C(21a)	111.9(8)
Sn(2) - S(1b) - C(9b)	92.6(4)	C(10a) - N(1a) - C(16a)	114.6(7)
Sn(1) - S(2a) - C(9a)	84.1(3)	C(9b) - N(1b) - C(10b)	120.7(8)
Sn(2) - S(2b) - C(9b)	84.2(4)	C(9b) - N(1b) - C(16b)	124.7(8)
C(9a) - N(1a) - C(10a)	126.3(8)	C(10b) N(1b) - C(16b)	114.3(7)
C(9a) - N(1a) - C(16a)	118.8(8)	Sn(1) - C(1a) - C(2a)	107.6(8)
C(6b) - C(5b) - C(8b)	111(2)	Sn(1) - C(1a) - C(3a)	111.1(8)
C(7b) - C(5b) - C(8b)	109(2)	Sn(1) - C(1a) - C(4a)	107.7(8)
S(1a) - C(9a) - S(2a)	115.3(5)	C(2a) - C(1a) - C(3a)	110(1)
S(1a) - C(9a) - N(1a)	121.1(8)	C(2a) - C(1a) - C(4a)	111(1)
S(2a) - C(9a) - N(1a)	123.6(7)	C(3a) - C(1a) - C(4a)	110(1)

Bond Angles (°) for [$^{t}Bu_2Sn(S_2CNCy_2)Cl$] Cont'd.

Atom - Atom - Atom	Angle	Atom - Atom - Atom	Angle
Sn(2) - C(1b) - C(2b)	111.1(9)	C(6b) - C(5b) - C(7b)	112(2)
Sn(2) - C(1b) - C(3b)	110(1)	C(17a) - C(16a) - C(21a)	111.8(8)
Sn(2) - C(1b) - C(4b)	106.1(9)	N(1b) - C(16b) - C(17b)	114.4(8)
C(2b) - C(1b) - C(3b)	108(1)	N(1b) - C(16b) - C(21b)	113.5(8)
C(2b) - C(1b) - C(4b)	109(1)	C(17b) - C(16b) - C(21b)	112.8(9)
C(3b) - C(1b) - C(4b)	112(2)	C(16a) - C(17a) - C(18a)	109.4(9)
Sn(1) - C(5a) - C(6a)	109.9(8)	C(16b) - C(17b) - C(18b)	109(1)
Sn(1) - C(5a) - C(7a)	111.0(9)	C(17a) - C(18a) - C(19a)	111.2(9)
Sn(1) - C(5a) - C(8a)	107.8(9)	C(17b) - C(18b) - C(19b)	112(1)
C(6a) - C(5a) - C(7a)	109(1)	C(18a) - C(19a) - C(20a)	112(1)
C(6a) - C(5a) - C(8a)	108(1)	C(18b) - C(19b) - C(20b)	111(1)
C(7a) - C(5a) - C(8a)	112(1)	C(19a) - C(20a) - C(21a)	111.1(9)
Sn(2) - C(5b) - C(6b)	110.0(9)	C(19b) - C(20b) - C(21b)	111(1)
Sn(2) - C(5b) - C(7b)	108(1)	C(16a) - C(21a) - C(20a)	111.3(9)
Sn(2) - C(5b) - C(8b)	107(1)	C(16b) - C(21b) - C(20b)	110(1)

Observed and calculated structure factors for [^{t}Bu$_2$Sn(S$_2$CNCy$_2$)Cl].

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	265	139	7	0	3	-8	647	656	11	0	5	0	728	663	9	0	8	1	384	374	8	0	11	1	524	474	12
0	0	2	2698	2732	19	0	3	-7	493	482	10	0	5	1	518	538	7	0	8	2	416	389	8	0	11	2	132	90	18
0	0	4	999	939	10	0	3	-6	1250	1279	12	0	5	2	459	462	7	0	8	3	492	458	11	0	11	3	299	284	12
0	0	6	1152	1079	13	0	3	-5	1423	1397	12	0	5	3	1290	1275	11	0	8	4	442	379	9	0	11	5	562	508	13
0	0	8	834	824	16	0	3	-4	908	886	9	0	5	4	720	708	9	0	8	5	314	305	9	0	11	7	326	326	15
0	0	10	273	298	21	0	3	-3	804	758	10	0	5	5	1104	1079	12	0	8	6	146	175	17	0	11	9	188	187	28
0	1	-13	145	168	12	0	3	-2	596	669	10	0	5	6	238	246	9	0	8	7	216	204	15	0	12	-10	93	122	11
0	1	-12	239	260	10	0	3	-1	1771	1849	14	0	5	7	543	543	11	0	8	8	187	224	22	0	12	-8	501	534	10
0	1	-11	156	164	15	0	3	0	519	482	6	0	5	9	422	450	13	0	8	11	200	108	28	0	12	-7	323	343	8
0	1	-10	159	148	13	0	3	1	600	599	6	0	5	11	217	308	30	0	9	-13	84	139	7	0	12	-6	573	539	13
0	1	-9	238	232	9	0	3	2	607	592	6	0	6	-13	302	326	7	0	9	-12	112	150	8	0	12	-5	165	168	15
0	1	-8	534	536	12	0	3	3	136	122	7	0	6	-11	251	269	9	0	9	-11	268	324	7	0	12	-4	628	548	16
0	1	-7	797	805	10	0	3	4	190	177	6	0	6	-9	206	222	9	0	9	-10	210	248	8	0	12	-2	717	849	14
0	1	-6	359	385	7	0	3	5	757	713	10	0	6	-8	177	185	10	0	9	-9	702	751	11	0	12	-1	171	153	21
0	1	-5	390	377	8	0	3	6	447	431	9	0	6	-7	484	500	12	0	9	-8	275	265	7	0	12	0	943	920	17
0	1	-4	222	231	6	0	3	7	646	604	14	0	6	-6	180	176	11	0	9	-7	751	729	11	0	12	2	605	541	13
0	1	-3	1150	1101	9	0	3	8	488	485	11	0	6	-4	748	692	12	0	9	-6	267	242	9	0	12	3	288	247	13
0	1	-2	205	206	8	0	3	9	339	312	14	0	6	-3	626	562	12	0	9	-5	563	523	13	0	12	4	474	405	11
0	1	-1	709	708	9	0	3	10	353	396	17	0	6	-2	243	245	10	0	9	-4	356	348	9	0	12	6	505	496	12
0	1	1	464	448	5	0	3	11	224	227	29	0	6	-1	145	138	13	0	9	-3	901	916	15	0	12	8	269	333	21
0	1	2	394	397	6	0	4	-13	288	310	7	0	6	0	182	176	10	0	9	-2	204	235	14	0	13	-10	309	359	6
0	1	4	229	219	6	0	4	-12	239	240	9	0	6	1	656	626	8	0	9	-1	1379	1381	15	0	13	-8	391	401	8
0	1	5	99	90	13	0	4	-11	165	149	13	0	6	2	663	654	8	0	9	1	845	778	12	0	13	-6	403	384	10
0	1	6	199	187	10	0	4	-10	336	350	8	0	6	3	120	113	9	0	9	3	457	436	9	0	13	-5	181	140	14
0	1	7	126	122	20	0	4	-9	293	303	8	0	6	4	109	149	12	0	9	4	143	121	14	0	13	-4	328	264	11
0	1	8	366	341	12	0	4	-8	447	475	9	0	6	5	430	414	9	0	9	5	705	707	15	0	13	-2	428	512	12
0	1	10	553	576	14	0	4	-7	402	409	8	0	6	7	167	161	16	0	9	7	553	551	13	0	13	0	199	238	23
0	1	12	253	218	26	0	4	-6	1299	1365	12	0	7	-13	164	222	8	0	9	9	298	312	17	0	13	1	216	193	20
0	2	-13	128	144	14	0	4	-5	117	148	12	0	7	-11	463	519	12	0	10	-11	193	227	6	0	13	2	326	302	15
0	2	-12	258	285	10	0	4	-4	853	866	10	0	7	-10	124	128	13	0	10	-9	246	261	7	0	13	3	232	238	20
0	2	-11	271	278	9	0	4	-3	609	595	10	0	7	-9	610	651	11	0	10	-8	305	308	8	0	13	5	184	148	25
0	2	-10	278	276	9	0	4	-2	347	333	9	0	7	-8	124	143	13	0	10	-7	162	156	11	0	14	-10	94	126	9
0	2	-8	897	889	12	0	4	-1	273	284	6	0	7	-7	581	561	11	0	10	-6	479	464	9	0	14	-8	287	320	7
0	2	-7	323	310	8	0	4	0	121	112	10	0	7	-6	493	457	11	0	10	-5	674	636	13	0	14	-7	160	175	11
0	2	-6	1641	1653	13	0	4	1	620	622	6	0	7	-5	927	897	12	0	10	-4	143	134	18	0	14	-6	849	806	13
0	2	-5	560	564	8	0	4	2	1553	1561	12	0	7	-3	1872	1771	16	0	10	-3	319	358	11	0	14	-4	794	722	17
0	2	-4	1755	1732	13	0	4	3	778	760	8	0	7	-2	233	233	11	0	10	-2	545	601	13	0	14	-2	414	488	14
0	2	-3	1086	1053	9	0	4	4	1332	1321	11	0	7	-1	1584	1602	14	0	10	0	866	779	14	0	14	0	507	563	14
0	2	-2	1965	1813	15	0	4	5	187	170	8	0	7	1	1220	1178	11	0	10	2	834	795	13	0	14	1	265	244	20
0	2	-1	216	231	7	0	4	6	197	195	10	0	7	2	500	517	9	0	10	3	150	133	14	0	14	2	662	649	14
0	2	0	1968	1933	14	0	4	8	521	500	13	0	7	3	1403	1359	13	0	10	4	559	495	11	0	14	4	586	570	15
0	2	1	543	522	6	0	4	10	190	237	30	0	7	4	382	376	8	0	10	6	356	341	11	0	14	6	326	357	19
0	2	2	1533	1476	11	0	5	-13	234	262	7	0	7	5	750	752	12	0	10	7	180	169	22	0	15	-10	246	290	6
0	2	3	1120	1100	9	0	5	-12	224	224	9	0	7	6	134	102	17	0	11	-12	168	228	5	0	15	-8	520	563	10
0	2	4	804	779	9	0	5	-11	453	470	10	0	7	7	508	510	12	0	11	-11	154	205	7	0	15	-6	254	219	9
0	2	6	721	678	11	0	5	-10	443	482	10	0	7	9	266	263	18	0	11	-10	298	341	7	0	15	-5	199	168	14
0	2	8	675	634	17	0	5	-9	363	394	8	0	7	11	237	281	26	0	11	-9	276	291	6	0	15	-3	252	274	17
0	2	9	190	208	24	0	5	-8	342	345	8	0	8	-13	179	225	6	0	11	-7	363	345	8	0	15	-2	270	312	18
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11	-9	-2	170	174	20	11	-3	-7	315	311	17	11	4	-8	146	166	21	12	-8	-3	197	296	22	12	-1	1	194	208	16
11	-9	3	173	165	14	11	-3	-6	495	490	13	11	4	-7	367	343	11	12	-8	-1	152	183	21	12	-1	3	184	170	14
11	-9	5	191	193	13	11	-3	-5	286	288	19	11	4	-6	142	53	23	12	-8	0	135	31	21	12	0	-7	348	305	12
11	-8	-9	195	199	22	11	-3	-4	415	453	13	11	4	-5	260	258	15	12	-8	2	152	108	17	12	0	-5	441	415	12
11	-8	-7	293	278	18	11	-3	-2	461	548	12	11	4	-3	361	350	13	12	-8	4	245	259	11	12	0	-3	205	253	21
11	-8	-6	230	225	24	11	-3	0	647	612	15	11	4	-1	381	372	12	12	-7	-8	240	215	18	12	0	1	201	236	17
11	-8	-5	439	445	15	11	-3	2	448	448	12	11	4	1	238	243	15	12	-7	-6	309	306	18	12	0	3	200	204	14
11	-8	-3	511	551	12	11	-3	4	261	292	11	11	4	3	198	217	15	12	-7	-4	325	339	15	12	1	-8	201	205	16
11	-8	-2	266	276	13	11	-3	6	182	192	13	11	6	-7	272	244	10	12	-7	-3	150	148	25	12	1	-6	321	324	13
11	-8	-1	394	400	10	11	-2	-10	244	235	16	11	6	-5	311	313	12	12	-7	-2	461	476	11	12	1	-4	328	376	15
11	-8	1	400	385	9	11	-2	-3	146	151	24	11	6	-3	287	277	13	12	-7	-1	307	312	12	12	1	-2	249	253	16
11	-8	3	465	466	12	11	-2	2	300	292	11	11	6	-1	293	278	13	12	-7	0	356	360	11	12	1	0	209	237	17
11	-8	4	140	150	18	11	-2	4	172	149	15	11	6	0	164	165	20	12	-7	1	163	143	17	12	1	2	197	224	16
11	-8	5	406	412	10	11	-2	6	141	149	16	11	6	1	216	246	16	12	-7	2	241	247	12	12	2	-7	232	205	14
11	-8	6	214	219	12	11	-1	-10	199	172	17	11	7	-6	162	127	14	12	-7	3	151	145	17	12	2	-5	213	220	19
11	-8	7	217	244	11	11	-1	-8	333	300	14	11	7	-5	168	168	16	12	-7	4	274	290	10	12	2	-3	228	177	17
11	-7	-8	254	236	18	11	-1	-6	671	617	15	11	7	-4	205	192	14	12	-7	5	221	270	12	12	2	-2	154	157	24
11	-7	-4	176	223	27	11	-1	-5	260	280	18	11	7	-3	141	121	22	12	-6	-7	400	386	14	12	3	-6	255	219	13
11	-7	-2	386	424	11	11	-1	-4	635	718	15	11	7	-2	221	228	16	12	-6	-5	243	257	21	12	3	-4	285	254	14
11	-7	0	242	231	13	11	-1	-2	489	573	12	12	-16	-1	206	232	12	12	-6	-3	269	340	17	12	3	-2	296	334	14
11	-7	2	160	157	17	11	-1	-1	154	97	20	12	-15	0	137	202	18	12	-6	-1	409	458	11	12	3	0	273	302	14
11	-7	5	156	162	16	11	-1	0	444	475	11	12	-15	1	138	152	16	12	-6	1	307	320	11	12	5	-4	249	250	13
11	-6	-9	215	181	20	11	-1	1	196	218	15	12	-14	-3	163	194	22	12	-6	2	156	152	17	12	5	-2	292	273	12
11	-6	-5	186	212	29	11	-1	2	425	429	10	12	-14	-1	285	300	12	12	-6	3	165	163	15	13	-14	-1	159	182	18
11	-6	-4	198	274	23	11	-1	3	216	221	13	12	-14	1	219	249	12	12	-6	4	140	137	16	13	-13	0	162	141	16
11	-6	-3	313	336	13	11	-1	4	261	306	11	12	-13	-4	225	193	19	12	-5	-4	188	220	24	13	-13	1	192	203	13
11	-6	-1	509	541	12	11	0	-10	232	209	15	12	-13	-2	158	187	22	12	-5	-2	247	295	16	13	-12	-3	285	303	13
11	-6	0	172	162	16	11	0	-9	256	223	15	12	-13	0	301	312	11	12	-5	-1	192	191	17	13	-12	-1	267	285	13
11	-6	1	375	375	10	11	0	-8	199	201	21	12	-13	2	269	306	10	12	-5	0	282	270	12	13	-12	1	283	317	11
11	-6	3	273	268	11	11	0	-7	196	183	22	12	-13	4	153	141	13	12	-5	1	288	280	11	13	-11	-1	162	163	20
11	-6	4	159	145	16	11	0	-5	285	278	17	12	-12	2	247	260	11	12	-5	3	207	193	13	13	-11	1	207	208	14
11	-6	5	341	339	9	11	0	2	185	170	16	12	-12	3	132	116	17	12	-5	5	154	185	15	13	-11	3	255	268	9
11	-6	6	258	279	11	11	0	4	133	120	20	12	-12	4	160	182	14	12	-4	-9	348	321	13	13	-10	-5	324	347	16
13	-10	-3	398	439	11	14	-10	-1	132	109	20																		
13	-10	-1	197	243	18	14	-9	-3	147	184	24																		
13	-10	1	211	242	14	14	-9	-2	223	234	15																		
13	-10	2	147	141	16	14	-9	-1	185	192	17																		
13	-10	3	243	290	11	14	-8	-3	157	197	22																		
13	-9	-1	176	162	19	14	-7	-4	234	218	15																		
13	-9	1	186	198	16	14	-7	-3	228	243	16																		
13	-9	3	223	266	11	14	-7	-2	167	177	21																		
13	-8	-7	227	226	19	14	-7	-1	202	260	16																		
13	-8	-5	304	316	16	14	-6	-1	175	199	18																		
13	-8	-3	281	319	15	14	-5	-1	170	213	20																		
13	-8	-2	249	325	16	14	-4	-3	165	161	21																		
13	-8	-1	253	255	14	14	-4	-1	186	204	18																		
13	-8	0	156	182	21																								
13	-8	1	152	167	18																								
13	-8	3	173	215	14																								
13	-7	-6	266	269	18																								
13	-7	-4	306	347	16																								
13	-7	-2	215	297	18																								
13	-7	0	214	226	15																								
13	-7	3	180	146	12																								
13	-6	-5	184	169	23																								
13	-6	-3	301	312	14																								
13	-6	-2	194	205	19																								
13	-6	-1	287	317	14																								
13	-6	0	219	270	16																								
13	-5	-6	356	362	14																								
13	-5	-4	206	195	19																								
13	-5	-2	277	302	14																								
13	-5	0	254	284	14																								
13	-5	2	164	191	17																								
13	-4	-2	155	192	23																								
13	-4	0	241	281	14																								
13	-4	2	206	232	14																								
13	-3	-6	363	345	13																								
13	-3	-4	253	232	15																								
13	-3	-2	188	182	18																								
13	-3	0	212	251	16																								
13	-3	2	179	206	15																								
13	-2	-3	210	213	17																								
13	-2	0	144	168	23																								
13	-1	-6	354	356	12																								
13	-1	-5	178	167	21																								
13	-1	-4	316	322	14																								
13	-1	0	170	173	18																								
13	-1	2	176	229	16																								
13	0	-5	183	195	20																								
13	0	-4	175	120	19																								
13	0	-3	221	232	17																								
13	0	-1	226	249	16																								
13	0	1	150	179	20																								
13	1	-4	159	155	22																								
13	1	-3	173	160	19																								
13	2	-3	281	281	13																								
13	2	-1	291	300	12																								

B. $[Vin_2SnCl_2(2,2'\text{-bipyridyl})]\cdot 0.5C_6H_6$

Crystallographic Data and Refinement details for $[Vin_2SnCl_2(2,2'\text{-bipyridyl})].^1/_2C_6H_6$.

Formula	$C_{17}H_{17}Cl_2N_2Sn$
Formula weight	438.9
Crystal morphology	colourless needle
Crystal dimensions (mm)	0.08 x 0.13 x 0.44
Crystal system	triclinic
Space group	$P\bar{1}$, (C_i^1, No. 2)
Temperature (°C)	20.0
a (Å)	9.260(1)
b (Å)	13.253(3)
c (Å)	7.8702(8)
α (°)	95.21(1)
β (°)	90.792(9)
γ (°)	69.76(1)
V (Å^3)	902.3(3)
Z	2
D_{calc} (g cm^{-3})	1.615
F(000)	434
Radiation	MoKα (λ = 0.7107Å)
μ (cm^{-1})	17.09
θ limits, data (°)	3.0 to 27.5
hkl range	0 to 12 , -17 to 17, -10 to 10
Range of transmission factors	0.974 to 1
Scan technique	ω:2θ
Scan width (°)	1.31
No. of data measured	4413
No. of unique data	4157
R_{amal}	0.033
Program for structure solution	Direct Methods (SHELXS86)
No. of unique data used	3261
No. of parameters	199
R	0.029
R_w	0.030
G.O.F.	1.35
Min./Max. residual electron density (e Å^{-3})	-0.42 to +0.41

Fractional atomic coordinates for the non-hydrogen atoms in $[Vin_2SnCl_2(2,2'\text{-bipyridyl})].{}^1/_2C_6H_6$.

Atom	*x*	*y*	*z*
Sn	0.44354(2)	0.28377(2)	0.14967(3)
Cl(1)	0.6149(1)	0.3683(1)	0.3163(1)
Cl(2)	0.6219(1)	0.1137(1)	0.0082(2)
N(1)	0.2223(3)	0.2537(2)	0.0391(4)
N(2)	0.2148(3)	0.4306(2)	0.2423(3)
C(1)	0.4471(4)	0.3755(3)	-0.0561(4)
C(2)	0.5008(6)	0.3376(4)	-0.2081(5)
C(3)	0.4132(5)	0.2131(4)	0.3713(5)
C(4)	0.3984(11)	0.1321(7)	0.3934(8)
C(5)	0.2316(4)	0.1642(3)	-0.0604(5)
C(6)	0.1036(5)	0.1387(4)	-0.1098(6)
C(7)	-0.0374(5)	0.2076(4)	-0.0547(6)
C(8)	-0.0496(4)	0.3013(4)	0.0468(5)
C(9)	0.0827(4)	0.3235(3)	0.0912(4)
C(10)	0.0785(3)	0.4234(3)	0.1957(4)
C(11)	-0.0585(4)	0.5068(4)	0.2415(5)
C(12)	-0.0522(4)	0.5986(3)	0.3347(5)
C(13)	0.0865(5)	0.6052(2)	0.3835(5)
C(14)	0.2181(4)	0.5191(3)	0.3356(5)
C(100)	1.0489(20)	0.0441(14)	0.3807(9)
C(101)	0.9057(16)	0.0897(5)	0.4416(18)
C(102)	0.8586(8)	0.0438(12)	0.5621(15)

Anisotropic displacement parameters (Å) for the non-hydrogen atoms in $[Vin_2SnCl_2(2,2'\text{-bipyridyl})].{}^1/_2C_6H_6$.

Atom	$U11$	$U22$	$U33$	$U12$	$U13$	$U23$
Sn	0.0339(1)	0.0380(1)	0.0346(1)	-0.0115(8)	-0.0007(8)	0.0049(9)
Cl(1)	0.048(2)	0.067(2)	0.048(2)	-0.024(4)	-0.007(4)	-0.002(1)
Cl(2)	0.054(2)	0.041(2)	0.085(2)	-0.008(4)	0.010(2)	-0.004(2)
N(1)	0.040(1)	0.040(2)	0.045(2)	-0.017(1)	-0.003(1)	0.005(1)
N(2)	0.037(1)	0.049(2)	0.037(2)	-0.010(1)	0.003(1)	0.001(1)
C(1)	0.04(2)	0.05(2)	0.05(2)	-0.02(2)	-0.01(1)	0.01(2)
C(2)	0.09(3)	0.07(3)	0.04(2)	-0.03(3)	0.01(1)	0.02(2)
C(3)	0.07(3)	0.08(3)	0.06(3)	-0.03(2)	-0.01(2)	0.02(2)
C(4)	0.26(1)	0.154(7)	0.09(5)	-0.138(7)	-0.01(5)	0.05(5)
C(5)	0.05(2)	0.05(2)	0.06(2)	-0.02(2)	-0.01(2)	0.01(2)
C(6)	0.07(3)	0.06(3)	0.08(3)	-0.04(2)	-0.02(2)	0.01(2)
C(7)	0.06(3)	0.09(4)	0.08(3)	-0.05(3)	-0.02(2)	0.02(3)
C(8)	0.04(2)	0.08(3)	0.06(2)	-0.03(2)	-0.01(2)	0.01(2)
C(9)	0.04(2)	0.05(2)	0.04(2)	-0.02(2)	-0.01(1)	0.02(2)
C(10)	0.04(2)	0.05(2)	0.03(2)	-0.01(1)	0.01(1)	0.01(2)
C(11)	0.04(2)	0.07(3)	0.05(2)	-0.01(2)	0.01(2)	0.01(2)
C(12)	0.05(2)	0.06(3)	0.05(2)	0.01(2)	0.01(2)	0.01(2)
C(13)	0.07(3)	0.05(2)	0.05(2)	-0.01(2)	0.01(2)	0.01(2)
C(14)	0.05(2)	0.05(2)	0.05(2)	-0.02(2)	0.01(2)	-0.01(2)
C(100)	0.196(9)	0.21(1)	0.08(4)	-0.153(9)	-0.03(6)	0.04(6)
C(101)	0.157(8)	0.05(3)	0.161(8)	-0.03(4)	-0.10(6)	0.02(4)
C(102)	0.065(4)	0.162(8)	0.115(6)	-0.03(5)	0.01(4)	-0.06(6)

Fractional Atomic coordinates and B_{eq} values ($Å^2$) for the hydrogen atoms in $[Vin_2SnCl_2(2,2'\text{-bipyridyl})].{}^1/_2C_6H_6$.

Atom	x	y	z	B_{eq}
H(1a)	0.4033	0.4550	-0.0337	4.0
H(2a)	0.5464	0.2598	-0.2375	6.4
H(2b)	0.4990	0.3857	-0.2968	6.1
H(3a)	0.4114	0.2577	0.4806	5.0
H(4a)	0.3853	0.1090	0.5029	11.8
H(4b)	0.3986	0.0806	0.2900	6.6
H(5a)	0.3343	0.1145	-0.1003	5.1
H(6a)	0.1162	0.0720	-0.1850	6.0
H(7a)	-0.1302	0.1906	-0.0851	6.4
H(8a)	-0.1519	0.3529	0.0867	5.3
H(11a)	-0.1583	0.5003	0.2070	5.0
H(12a)	-0.1482	0.6589	0.3661	5.6
H(13a)	0.0923	0.6701	0.4513	5.5
H(14a)	0.3194	0.5232	0.3706	5.0
H(100)	1.0882	0.0746	0.2888	12.8
H(101)	0.8390	0.1584	0.3991	11.2
H(102)	0.7465	0.0825	0.5957	4.0

Bond distances (Å) for $[Vin_2SnCl_2(2,2'\text{-bipyridyl})].{}^1/_2C_6H_6$.

Atom - Atom	Distance	Atom - Atom	Distance
Sn - Cl(1)	2.529(9)	C(5) - C(6)	1.382(5)
Sn - Cl(2)	2.463(1)	C(6) - C(7)	1.359(6)
Sn - N(1)	2.360(3)	C(7) - C(8)	1.384(6)
Sn - N(2)	2.396(3)	C(8) - C(9)	1.389(5)
Sn - C(1)	2.119(3)	C(9) - C(10)	1.482(5)
Sn - C(3)	2.119(4)	C(10) - C(11)	1.390(5)
N(1) - C(5)	1.337(5)	C(11) - C(12)	1.381(6)
N(1) - C(9)	1.347(4)	C(12) - C(13)	1.365(6)
N(2) - C(10)	1.342(4)	C(13) - C(14)	1.379(5)
N(2) - C(14)	1.335(4)	C(100) - C(101)	1.33(1)
C(1) - C(2)	1.290(5)	C(100) - C(102)'	1.30(1)
C(3) - C(4)	1.157(7)	C(101) - C(102)	1.33(1)

' atom related by a crystallographic centre of symmetry

Bond angles (°) for $[Vin_2SnCl_2(2,2'\text{-bipyridyl})].{}^1/_2C_6H_6$.

Atom - Atom - Atom	Angle	Atom - Atom - Atom	Angle
Cl(1) - Sn - Cl(2)	104.74(3)	C(10) - N(2) - C(14)	119.2(3)
Cl(1) - Sn - N(1)	161.50(7)	Sn - C(1) - C(2)	126.2(3)
Cl(1) - Sn - N(2)	92.47(7)	Sn - C(3) - C(4)	133.4(5)
Cl(1) - Sn - C(1)	89.71(9)	N(1) - C(5) - C(6)	122.8(4)
Cl(1) - Sn - C(3)	89.2(1)	C(5) - C(6) - C(7)	118.4(4)
Cl(2) - Sn - N(1)	93.72(7)	C(6) - C(7) - C(8)	119.7(3)
Cl(2) - Sn - N(2)	162.79(7)	C(7) - C(8) - C(9)	119.5(4)
Cl(2) - Sn - C(1)	94.2(1)	N(1) - C(9) - C(8)	120.4(3)
Cl(2) - Sn - C(3)	94.3(1)	N(1) - C(9) - C(10)	116.9(3)
N(1) - Sn - N(2)	69.1(1)	C(8) - C(9) - C(10)	122.6(3)
N(1) - Sn - C(1)	90.2(1)	N(2) - C(10) - C(9)	116.6(3)
N(1) - Sn - C(3)	88.1(1)	N(2) - C(10) - C(11)	121.0(3)
N(2) - Sn - C(1)	85.4(1)	C(9) - C(10) - C(11)	122.3(3)
N(2) - Sn - C(3)	86.1(1)	C(10) - C(11) - C(12)	118.7(3)
C(1) - Sn - C(3)	171.4(2)	C(11) - C(12) - C(13)	120.1(3)
Sn - N(1) - C(5)	121.8(2)	C(12) - C(13) - C(14)	118.3(4)
Sn - N(1) - C(9)	118.7(2)	N(2) - C(14) - C(13)	122.6(4)
C(5) - N(1) - C(9)	119.1(3)	C(101) - C(100) - C(102)'	120.8(7)
Sn - N(2) - C(10)	118.1(2)	C(100) - C(101) - C(102)	118.7(7)
Sn - N(2) - C(14)	122.7(2)	C(100) - C(102)' - C(101)'	120.5(7)

' atom related by a crystallographic centre of symmetry

Observed and calculated structure factors for [Vin$_2$SnCl$_2$(2,2'-bipyridyl)].$^1/_2$C$_6$H$_6$.

h	k	l	Fo	Fc	sigF
0	0	2	59	45	5
0	0	3	0	39	18*
0	0	4	450	448	6
0	0	5	71	72	7
0	0	6	376	366	7
0	0	7	221	218	5
0	0	8	48	34	28*
0	0	9	56	77	31*
0	0	10	148	133	8
0	1	-10	75	53	13*
0	1	-9	140	139	7
0	1	-8	297	291	6
0	1	-7	170	161	5
0	1	-6	342	333	7
0	1	-5	385	385	6
0	1	-4	151	152	4
0	1	-3	329	318	4
0	1	-2	1356	1330	13
0	1	1	999	964	9
0	1	2	277	258	4
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6	1	-5	0	27	22*	6	4	-1	157	160	4	6	7	3	387	389	7	6	11	-6	165	166	7	6	15	0	131	129	9				
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6	1	-2	339	327	6	6	4	2	461	472	6	6	7	6	134	138	7	6	11	-3	36	73	24*	6	15	3	95	111	11				
6	16	-4	127	130	12	7	-5	6	178	190	5	7	-1	4	252	247	5	7	3	-7	174	170	5	7	6	-3	212	211	6				
6	16	-3	0	36	38*	7	-4	-6	162	162	5	7	-1	5	318	318	8	7	3	-6	133	136	5	7	6	-2	268	262	6				
6	16	-2	0	110	37*	7	-4	-5	48	49	12*	7	-1	6	0	30	26*	7	3	-5	0	23	22*	7	6	-1	92	96	6				
6	16	-1	106	109	13	7	-4	-4	126	121	5	7	-1	7	108	115	8	7	3	-4	142	142	5	7	6	0	77	70	6				
6	16	0	49	6	34*	7	-4	-3	121	118	5	7	0	-7	176	203	6	7	3	-3	534	532	7	7	6	1	422	423	7				
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6	17	-1	80	87	17*	7	-4	0	340	344	7	7	0	-4	302	295	7	7	3	0	217	219	5	7	6	4	157	153	5				
7	-9	-2	19	40	26*	7	-4	1	272	263	7	7	0	-3	292	282	6	7	3	1	305	309	6	7	6	5	107	91	6				
7	-9	-1	147	148	6	7	-4	2	0	19	22*	7	0	-2	129	124	4	7	3	2	81	76	6	7	6	6	43	94	29*				
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7	-8	-1	31	73	24*	7	-3	-5	170	172	5	7	0	5	155	162	5	7	4	-8	140	144	7	7	7	-3	106	104	6				
7	-8	0	0	39	25*	7	-3	-4	94	96	6	7	0	6	249	257	6	7	4	-7	70	42	9	7	7	-2	194	190	5				
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7	-7	0	56	41	10*	7	-3	5	259	258	6	7	1	-2	238	235	6	7	4	2	464	463	7	7	7	7	118	128	8				
7	-7	1	37	53	20*	7	-3	6	155	152	5	7	1	-1	39	36	20*	7	4	3	70	53	8	7	8	-8	0	37	25*				
7	-7	2	228	222	5	7	-3	7	42	56	19*	7	1	0	234	234	6	7	4	4	288	286	7	7	8	-7	76	77	10				
7	-7	3	226	221	6	7	-2	-7	123	112	6	7	1	1	360	366	6	7	4	5	245	226	6	7	8	-6	291	294	7				
7	-7	4	18	24	26*	7	-2	-6	110	119	6	7	1	2	242	243	6	7	4	6	112	104	7	7	8	-5	210	206	5				
7	-7	5	76	89	10	7	-2	-5	71	91	9	7	1	3	64	54	8	7	4	7	0	21	29*	7	8	-4	153	147	5				
7	-6	-5	126	109	6	7	-2	-4	280	263	7	7	1	4	327	341	7	7	4	8	130	129	8	7	8	-3	226	222	6				
7	-6	-4	47	49	25*	7	-2	-3	230	238	5	7	1	5	165	165	5	7	5	-8	78	83	10	7	8	-2	263	261	6				
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7	-6	-1	38	19	23*	7	-2	0	404	396	6	7	1	8	106	103	9	7	5	-5	33	26	19*	7	8	1	314	319	7				
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7	-6	4	147	146	5	7	-2	5	47	26	24*	7	2	-4	234	237	5	7	5	0	239	238	5	7	8	6	25	9	28*				
7	-6	5	114	106	7	7	-2	6	209	196	5	7	2	-3	130	122	4	7	5	1	147	133	4	7	8	7	157	157	7				
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7	-5	3	148	147	5	7	-1	1	207	199	5	7	2	7	39	48	27*	7	6	-6	247	246	6	7	9	2	211	218	5				
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7	-5	5	190	192	5	7	-1	3	33	45	17*	7	3	-8	38	24	20*	7	6	-4	167	172	5	7	9	4	44	14	22*				
7	9	5	178	176	6	7	14	-5	53	47	23*	8	-4	1	240	237	5	8	0	3	287	293	7	8	4	-2	258	259	7				
7	9	6	194	191	6	7	14	-4	122	135	10	8	-4	2	31	31	23*	8	0	4	201	198	5	8	4	-1	341	350	6				
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7	10	-7	96	109	10	7	14	-2	115	125	10	8	-4	4	167	170	5	8	0	6	99	104	8	8	4	1	79	83	7				
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7	10	-5	24	33	23*	7	14	0	152	160	7	8	-4	6	81	72	9	8	1	-7	40	44	28*	8	4	3	185	188	5				
7	10	-4	194	190	5	7	14	1	84	68	11	8	-3	-5	136	135	5	8	1	-6	157	143	5	8	4	4	114	113	6				
7	10	-3	258	250	6	7	14	2	49	64	18*	8	-3	-4	0	46	23*	8	1	-5	197	196	5	8	4	5	161	143	5				
7	10	-2	247	242	6	7	14	3	135	138	8	8	-3	-3	42	32	22*	8	1	-4	164	161	4	8	4	6	166	162	5				
7	10	-1	30	36	18*	7	14	4	38	62	23*	8	-3	-2	195	209	5	8	1	-3	183	178	5	8	4	7	49	46	27*				
7	10	0	331	338	8	7	15	-4	98	55	13	8	-3	-1	332	333	7	8	1	-2	267	273	7	8	5	-7	101	112	8				
7	10	1	264	271	6	7	15	-3	194	182	8	8	-3	0	107	102	5	8	1	-1	165	170	4	8	5	-6	140	152	6				
7	10	2	55	57	12*	7	15	-2	179	193	8	8	-3	1	131	129	5	8	1	0	341	355	7	8	5	-5	75	66	8				
7	10	3	150	161	6	7	15	-1	59	55	19*	8	-3	2	173	177	4	8	1	1	364	357	6	8	5	-4	149	145	5				
7	10	4	216	218	6	7	15	0	53	46	32*	8	-3	3	184	190	5	8	1	2	363	375	7	8	5	-3	279	276	7				
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7	11	-5	221	225	6	7	16	-2	85	92	16*	8	-2	-5	48	7	10*	8	1	7	52	43	27*	8	5	2	191	197	5				
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7	11	-2	147	139	6	7	16	1	44	25	26*	8	-2	-2	129	138	5	8	2	-5	90	85	6	8	5	5	100	90	7				
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7	11	0	0	10	27*	8	-8	1	108	109	7	8	-2	0	283	280	7	8	2	-3	107	99	5	8	5	7	170	179	6				
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7	12	-5	49	20	30*	8	-6	-2	140	150	5	8	-1	-5	117	112	5	8	2	5	104	105	7	8	6	0	0	9	22*				
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7	12	-2	0	73	30*	8	-6	1	187	185	5	8	-1	-2	307	306	7	8	3	-7	67	77	11	8	6	3	0	51	24*				
7	12	-1	285	293	7	8	-6	2	68	68	9	8	-1	-1	272	270	7	8	3	-6	190	186	5	8	6	4	55	41	11*				
7	12	0	322	332	6	8	-6	3	64	50	9	8	-1	0	17	39	19*	8	3	-5	145	153	5	8	6	5	137	146	6				
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7	12	3	146	144	6	8	-5	-3	0	62	24*	8	-1	3	104	104	6	8	3	-2	30	23	16*	8	7	-7	172	178	6				
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7	13	-4	50	93	33*	8	-5	2	208	208	5	8	0	-7	102	108	7	8	3	3	195	193	5	8	7	-2	81	77	7				
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7	13	-1	61	74	15*	8	-5	5	0	47	28*	8	0	-4	224	220	5	8	3	6	39	17	22*	8	7	1	0	15	23*				
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8	8	-3	133	127	5	8	12	-1	0	42	29*	9	-3	0	71	73	8	9	2	-6	86	84	8	9	6	-3	0	16	24*				
8	8	-2	234	226	6	8	12	0	166	166	6	9	-3	1	0	46	22*	9	2	-5	64	68	10	9	6	-2	155	153	5				

8	8	-1	143	141	5	8	12	1	137	144	6	9	-3	2	133	134	5	9	2	-4	242	237	6	9	6	-1	316	327	7
8	8	0	248	255	5	8	12	2	31	29	23*	9	-3	3	175	175	5	9	2	-3	236	239	5	9	6	0	123	126	5
8	8	1	327	347	7	8	12	3	125	124	7	9	-3	4	25	27	25*	9	2	-2	29	26	18*	9	6	1	150	148	4
8	8	2	133	139	5	8	12	4	163	162	7	9	-3	5	131	134	6	9	2	-1	204	209	5	9	6	2	196	202	5
8	8	3	63	54	10	8	12	5	59	5	15*	9	-2	-5	70	73	9	9	2	0	241	246	5	9	6	3	124	131	5
8	8	4	105	107	7	8	13	-5	139	133	8	9	-2	-4	38	37	24*	9	2	1	110	112	5	9	6	4	37	30	20*
8	8	5	174	181	5	8	13	-4	160	160	7	9	-2	-3	158	163	5	9	2	2	232	240	5	9	6	5	179	185	5
8	8	6	26	7	21*	8	13	-3	0	13	31*	9	-2	-2	104	106	6	9	2	3	237	238	6	9	6	6	139	138	7
8	9	-7	195	188	6	8	13	-2	167	163	7	9	-2	-1	66	72	8	9	2	4	46	46	12*	9	7	-6	52	74	27*
8	9	-6	101	93	8	8	13	-1	111	112	9	9	-2	0	203	200	5	9	2	5	34	39	24*	9	7	-5	42	49	26*
8	9	-5	120	105	6	8	13	0	0	35	29*	9	-2	1	188	186	5	9	2	6	105	108	7	9	7	-4	165	167	5
8	9	-4	137	141	6	8	13	1	142	139	6	9	-2	2	108	100	6	9	3	-6	158	147	6	9	7	-3	259	251	6
8	9	-3	92	82	7	8	13	2	202	204	5	9	-2	3	97	96	6	9	3	-5	221	211	5	9	7	-2	218	214	6
8	9	-2	89	89	7	8	13	3	72	87	12*	9	-2	4	174	183	5	9	3	-4	25	14	22*	9	7	-1	113	95	5
8	9	-1	373	368	7	8	13	4	48	91	31*	9	-2	5	48	37	26*	9	3	-3	260	259	6	9	7	0	316	320	7
8	9	0	272	268	7	8	14	-4	88	112	14	9	-1	-5	109	106	6	9	3	-2	237	229	5	9	7	1	117	127	6
8	9	1	40	30	24*	8	14	-3	167	188	8	9	-1	-4	133	123	5	9	3	-1	84	76	6	9	7	2	68	66	8
8	9	2	75	87	9	8	14	-2	0	1	32*	9	-1	-3	49	17	10*	9	3	0	135	126	4	9	7	3	152	155	5
8	9	3	152	150	5	8	14	-1	123	132	9	9	-1	-2	251	253	5	9	3	1	354	363	7	9	7	4	205	207	5
8	9	4	93	102	8	8	14	0	133	147	9	9	-1	-1	206	209	5	9	3	2	202	210	5	9	7	5	0	36	27*
8	9	5	134	141	7	8	14	1	123	135	8	9	-1	0	109	104	5	9	3	3	40	64	24*	9	7	6	119	118	8
8	9	6	156	162	7	8	14	2	55	19	28*	9	-1	1	38	16	22*	9	3	4	24	50	24*	9	8	-6	124	123	7
8	10	-7	53	63	30*	8	14	3	121	117	8	9	-1	2	171	170	4	9	3	5	98	94	7	9	8	-5	184	182	5
8	10	-6	165	163	6	8	15	-3	154	142	9	9	-1	3	85	82	7	9	3	6	50	27	26*	9	8	-4	120	117	6
8	10	-5	86	78	9	8	15	-2	148	157	9	9	-1	4	109	119	7	9	4	-6	90	84	8	9	8	-3	0	9	23*
8	10	-4	69	63	10	8	15	-1	44	67	35*	9	-1	5	173	170	5	9	4	-5	159	169	5	9	8	-2	251	248	6
8	10	-3	183	180	5	8	15	0	0	15	32*	9	-1	6	81	90	10	9	4	-4	222	215	5	9	8	-1	221	223	6
8	10	-2	259	248	6	8	15	1	127	120	8	9	0	-6	45	50	15*	9	4	-3	0	25	23*	9	8	0	115	93	5
8	10	-1	42	10	25*	8	15	2	103	98	10	9	0	-5	0	4	24*	9	4	-2	163	160	4	9	8	1	191	200	5
8	10	0	196	211	5	8	16	-1	81	93	16*	9	0	-4	187	186	5	9	4	-1	265	275	7	9	8	2	158	155	5
8	10	1	119	132	6	8	16	0	113	109	11	9	0	-3	271	264	6	9	4	0	284	281	6	9	8	3	97	95	7
8	10	2	85	80	8	9	-6	-1	129	136	6	9	0	-2	84	71	6	9	4	1	37	55	14*	9	8	4	85	92	8
8	10	3	77	60	9	9	-6	0	24	21	25*	9	0	-1	81	85	6	9	4	2	233	222	5	9	8	5	185	198	5
8	10	4	224	214	6	9	-6	1	139	135	5	9	0	0	165	170	4	9	4	3	103	110	6	9	8	6	75	51	11
8	10	5	87	107	10	9	-6	2	74	74	9	9	0	1	213	209	5	9	4	4	0	25	24*	9	9	-6	70	68	12*
8	10	6	73	61	13*	9	-5	-2	0	33	25*	9	0	2	0	27	23*	9	4	5	101	90	7	9	9	-5	43	39	22*
8	11	-6	79	56	11	9	-5	-1	129	123	5	9	0	3	253	255	6	9	4	6	211	211	5	9	9	-4	152	140	5
8	11	-5	142	147	7	9	-5	0	115	121	6	9	0	4	165	159	5	9	5	-6	207	203	5	9	9	-3	178	171	5
8	11	-4	184	182	6	9	-5	1	68	75	9	9	0	5	0	9	25*	9	5	-5	0	16	23*	9	9	-2	0	33	25*
8	11	-3	72	74	11	9	-5	2	130	133	6	9	0	6	74	82	10	9	5	-4	239	242	6	9	9	-1	340	342	8
8	11	-2	121	125	7	9	-5	3	150	147	5	9	1	-6	79	86	9	9	5	-3	253	249	6	9	9	0	257	268	6
8	11	-1	212	210	6	9	-4	-3	82	81	7	9	1	-5	189	192	5	9	5	-2	280	278	7	9	9	1	89	90	7
8	11	0	46	83	27*	9	-4	-2	164	168	5	9	1	-4	151	147	5	9	5	-1	71	88	8	9	9	2	0	9	24*
8	11	1	76	55	9	9	-4	-1	0	14	23*	9	1	-3	92	97	6	9	5	0	203	209	5	9	9	3	166	170	5
8	11	2	138	151	6	9	-4	0	158	156	5	9	1	-2	198	200	5	9	5	1	242	235	5	9	9	4	118	121	7
8	11	3	170	172	6	9	-4	1	138	137	5	9	1	-1	170	180	4	9	5	2	37	46	14*	9	9	5	111	99	8
8	11	4	33	17	24*	9	-4	2	82	78	7	9	1	0	0	39	22*	9	5	3	86	75	7	9	10	-6	114	113	8
8	11	5	188	176	6	9	-4	3	0	3	25*	9	1	1	226	226	5	9	5	4	147	155	5	9	10	-5	147	150	6
8	12	-6	48	86	34*	9	-4	4	150	151	6	9	1	2	270	264	7	9	5	5	120	122	6	9	10	-4	37	35	27*
9	10	-3	201	184	5	10	-2	-2	95	98	7	10	3	4	78	87	8	10	8	4	85	81	8	11	1	2	147	148	5
9	10	-2	265	249	6	10	-2	-1	35	65	23*	10	3	5	156	149	5	10	8	5	127	123	6	11	1	3	44	60	25*
9	10	-1	82	75	8	10	-2	0	130	123	5	10	4	-5	65	51	10	10	9	-5	50	47	28*	11	2	-3	153	152	5
9	10	0	124	113	6	10	-2	1	191	186	5	10	4	-4	124	128	6	10	9	-4	111	97	7	11	2	-2	159	154	5
9	10	1	111	118	6	10	-2	2	148	139	5	10	4	-3	146	154	5	10	9	-3	184	180	5	11	2	-1	30	15	22*
9	10	2	120	128	6	10	-2	3	36	51	25*	10	4	-2	0	17	23*	10	9	-2	74	78	9	11	2	0	152	167	5
9	10	3	30	18	26*	10	-1	-4	151	140	5	10	4	-1	217	214	5	10	9	-1	97	86	7	11	2	1	97	87	6
9	10	4	220	223	6	10	-1	-3	0	27	24*	10	4	0	233	245	5	10	9	0	157	158	5	11	2	2	76	64	8
9	10	5	126	126	8	10	-1	-2	160	162	5	10	4	1	31	14	22*	10	9	1	113	110	6	11	2	3	117	113	6
9	11	-5	83	88	10	10	-1	-1	158	164	4	10	4	2	136	143	5	10	9	2	44	29	24*	11	3	-3	32	26	17*
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9	11	-3	57	66	14*	10	-1	1	0	25	23*	10	4	4	101	97	6	10	9	4	139	137	6	11	3	-1	147	154	5
9	11	-2	157	156	6	10	-1	2	173	173	5	10	4	5	22	64	26*	10	10	-5	154	152	7	11	3	0	19	42	22*
9	11	-1	210	214	5	10	-1	3	97	105	7	10	5	-5	122	132	7	10	10	-4	126	122	7	11	3	1	164	166	5
9	11	0	147	154	6	10	-1	4	62	69	11*	10	5	-4	35	8	23*	10	10	-3	77	66	10	11	3	2	128	133	5
9	11	1	39	64	27*	10	0	-4	105	105	7	10	5	-3	126	135	6	10	10	-2	164	169	6	11	3	3	89	86	7
9	11	2	95	95	8	10	0	-3	159	155	5	10	5	-2	229	234	6	10	10	-1	82	81	8	11	4	-4	104	108	7
9	11	3	150	148	6	10	0	-2	43	52	23*	10	5	-1	95	86	6	10	10	0	36	31	24*	11	4	-3	182	170	5
9	11	4	44	27	28*	10	0	-1	32	19	21*	10	5	0	177	187	4	10	10	1	154	152	5	11	4	-2	99	88	6
9	12	-5	31	64	30*	10	0	0	151	159	5	10	5	1	170	173	4	10	10	2	160	176	5	11	4	-1	129	130	5
9	12	-4	82	71	11	10	0	1	223	220	6	10	5	2	68	55	8	10	10	3	39	30	21*	11	4	0	108	118	6
9	12	-3	242	232	6	10	0	2	0	3	23*	10	5	3	0	20	23*	10	10	4	106	100	8	11	4	1	44	9	24*
9	12	-2	158	146	6	10	0	3	151	152	5	10	5	4	133	144	6	10	11	-4	172	168	6	11	4	2	67	61	9
9	12	-1	0	11	28*	10	0	4	87	96	8	10	5	5	145	138	6	10	11	-3	134	135	7	11	4	3	149	147	5
9	12	0	0	58	27*	10	1	-5	125	130	7	10	6	-5	114	131	7	10	11	-2	54	35	13*	11	4	4	129	129	6
9	12	1	125	144	7	10	1	-4	80	94	8	10	6	-4	129	133	6	10	11	-1	144	127	6	11	5	-4	51	65	14*
9	12	2	0	36	28*	10	1	-3	66	49	9	10	6	-3	81	80	8	10	11	0	153	152	5	11	5	-3	40	58	25*
9	12	3	161	152	6	10	1	-2	147	151	5	10	6	-2	130	131	5	10	11	1	89	98	8	11	5	-2	164	168	5
9	12	4	163	159	6	10	1	-1	176	169	4	10	6	-1	302	304	7	10	11	2	100	85	7	11	5	-1	30	61	24*
9	13	-4	118	140	10	10	1	0	102	107	6	10	6	0	126	121	5	10	11	3	149	153	6	11	5	0	93	107	7
9	13	-3	0	2	31*	10	1	1	143	145	5	10	6	1	0	49	23*	10	12	-4	25	7	30*	11	5	1	143	141	5
9	13	-2	73	92	13*	10	1	2	180	184	5	10	6	2	97	91	6	10	12	-3	150	151	7	11	5	2	158	159	5
9	13	-1	97	89	9	10	1	3	0	4	23*	10	6	3	165	168	5	10	12	-2	122	124	8	11	5	3	70	69	9
9	13	0	0	66	30*	10	1	4	70	75	9	10	6	4	36	39	17*	10	12	-1	66	58	12*	11	5	4	124	118	6
9	13	1	66	67	12*	10	1	5	136	135	6	10	6	5	160	154	5	10	12	0	56	47	12*	11	6	-4	111	106	7
9	13	2	178	172	6	10	2	-5	0	25	26*	10	7	-5	12	39	27*	10	12	1	155	166	6	11	6	-3	119	113	6
9	13	3	86	85	11	10	2	-4	162	171	5	10	7	-4	74	68	9	10	12	2	107	102	8	11	6	-2	39	49	25*
9	14	-3	129	125	9	10	2	-3	163	158	5	10	7	-3	223	212	5	10	12	3	50	66	29*	11	6	-1	170	177	5
9	14	-2	0	68	33*	10	2	-2	104	99	5	10	7	-2	214	218	5	10	13	-3	76	62	12	11	6	0	128	119	5
9	14	-1	37	20	21*	10	2	-1	60	50	8	10	7	-1	0	28	23*	10	13	-2	53	29	16*	11	6	1	0	31	24*
9	14	0	108	115	10	10	2	0	189	195	5	10	7	0	97	102	6	10	13	-1	37	76	30*	11	6	2	81	77	8
9	14	1	111	116	8	10	2	1	98	105	6	10	7	1	72	52	8	10	13	0	89	105	10	11	6	3	167	176	5
9	14	2	0	34	31*	10	2	2	110	109	6	10	7	2	0	25	23*	10	13	1	59	46	14*	11	6	4	40	52	26*
9	15	-2	109	107	11	10	2	3	149	150	5	10	7	3	138	140	5	10	13	2	163	164	6	11	7	-4	35	4	21*
9	15	-1	86	96	13	10	2	4	97	98	7	10	7	4	219	227	5	11	-1	0	144	141	5	11	7	-3	157	153	5
9	15	0	24	20	33*	10	2	5	50	43	26*	10	7	5	54	53	27*	11	-1	1	34	10	18*	11	7	-2	183	180	5
10	-4	0	56	58	11*	10	3	-5	158	149	6	10	8	-5	142	148	6	11	0	-2	98	98	7	11	7	-1	40	17	23*
10	-4	1	123	134	6	10	3	-4	45	60	14*	10	8	-4	141	151	6	11	0	-1	17	22	23*	11	7	0	82	90	8
10	-3	-2	25	44	24*	10	3	-3	0	31	23*	10	8	-3	42	20	15*	11	0	0	100	93	6	11	7	1	118	117	6
10	-3	-1	152	152	5	10	3	-2	137	132	5	10	8	-2	174	159	5	11	0	1	178	171	5	11	7	2	94	96	7
10	-3	0	108	99	6	10	3	-1	146	142	4	10	8	-1	167	168	5	11	0	2	76	52	8	11	7	3	96	94	7
10	-3	1	42	6	24*	10	3	0	78	83	7	10	8	0	0	22	23*	11	1	-2	96	83	6	11	8	-4	155	158	6
10	-3	2	95	98	7	10	3	1	256	260	5	10	8	1	24	72	25*	11	1	-1	175	173	4	11	8	-3	0	50	27*
10	-3	3	165	161	5	10	3	2	162	174	5	10	8	2	192	191	5	11	1	0	132	133	5	11	8	-2	120	115	6
10	-2	-3	143	132	5	10	3	3	31	23	19*	10	8	3	154	153	5	11	1	1	60	60	10	11	8	-1	121	132	6
11	8	0	93	81	6																								
11	8	1	0	5	24*																								
11	8	2	142	147	5																								
11	8	3	127	123	6																								
11	9	-3	157	153	6																								
11	9	-2	55	55	12*																								
11	9	-1	0	32	26*																								
11	9	0	101	100	6																								
11	9	1	144	142	5																								
11	9	2	0	12	26*																								
11	9	3	170	170	5																								
11	10	-3	0	18	25*																								
11	10	-2	54	67	27*																								
11	10	-1	96	90	7																								
11	10	0	37	49	25*																								
11	10	1	106	107	7																								
11	10	2	156	161	5																								
11	11	-2	0	10	28*																								

11	11	-1	82	67	9
11	11	0	176	176	5
11	11	1	87	99	8
11	12	-1	102	96	8
11	12	0	0	17	26*
12	5	0	0	30	24*
12	6	-1	126	131	6
12	6	0	119	127	6
12	7	0	44	23	13*

C. [Ph(Me)$SnCl_2$(2,2'-bipyridyl)]·0.25$CHCl_3$

Crystallographic Data and Refinement details for $[Ph(Me)SnCl_2(2,2'\text{-bipyridyl})].^1/_4CHCl_3$.

Formula	$C_{17.25}H_{16.25}Cl_{2.75}N_2Sn$
Formula weight	467.7
Crystal morphology	colourless block
Crystal dimensions (mm)	0.08 x 0.32 x 0.37
Crystal system	monoclinic
Space group	$P2_1/n$ (C_{2h}^5, No. 14)
Temperature (°C)	20.0
a (Å)	14.039(3)
b (Å)	16.525(2)
c (Å)	17.174(1)
β (°)	91.34(1)
V (Å^3)	3983(1)
Z	8
D_{calc} (g cm^{-3})	1.560
$F(000)$	1844
Radiation	MoKα (λ = 0.7107Å)
μ (cm^{-1})	16.51
θ limits, data (°)	3.0 to 27.5
hkl range	0 to 18, 0 to 22, -22 to 22
Range of transmission factors	0.978 to 1.000
Scan technique	ω:2θ
Scan width (°)	1.00
No. of data measured	9889
No. of unique data	9516
R_{amal}	0.046
Program for structure solution	Direct Methods (SHELXS86)
No. of unique data used	5888
No. of parameters	413
R	0.048
R_w	0.051
G.O.F.	2.37
Min./Max. residual electron density (e Å^{-3})	-1.00 to +1.84

Fractional atomic coordinates ($Å^2$) for the non-hydrogen atoms in [Ph(Me)$SnCl_2$(2,2'-bipyridyl)].$^1/_4CHCl_3$. *

Atom	*x*	*y*	*z*
Sn(1)	0.68823(3)	0.63231(3)	0.15806(2)
Sn(2)	0.30270(4)	0.10677(3)	0.16004(3)
Cl(1a)	0.8637(1)	0.6244(1)	0.1807(1)
Cl(1b)	0.3602(2)	0.1694(1)	0.2851(1)
Cl(2a)	0.6327(2)	0.6780(1)	0.2877(1)
Cl(2b)	0.1351(1)	0.0710(2)	0.1870(1)
N(1a)	0.5344(4)	0.6274(3)	0.0958(3)
N(1b)	0.2896(4)	0.0561(3)	0.0300(3)
N(2a)	0.6981(4)	0.5905(3)	0.0246(3)
N(2b)	0.4487(4)	0.1251(3)	0.0933(3)
C(1a)	0.6929(6)	0.7549(5)	0.1161(4)
C(1b)	0.2655(7)	0.2223(5)	0.1166(5)
C(2a)	0.6667(5)	0.5073(4)	0.1885(3)
C(2b)	0.3548(5)	-0.0096(4)	0.1958(3)
C(3a)	0.5885(5)	0.4846(4)	0.2296(4)
C(3b)	0.3019(6)	-0.0792(5)	0.1829(4)
C(4a)	0.5758(7)	0.4042(6)	0.2511(4)
C(4b)	0.3386(8)	-0.1551(5)	0.2090(5)
C(5a)	0.6428(9)	0.3472(5)	0.2321(5)
C(5b)	0.4228(8)	-0.1607(6)	0.2474(5)
C(6a)	0.7209(8)	0.3703(5)	0.1922(6)
C(6b)	0.4758(6)	-0.0917(6)	0.2605(5)
C(7a)	0.7330(6)	0.4497(5)	0.1696(4)
C(7b)	0.4418(5)	-0.0155(5)	0.2353(4)
C(8a)	0.4549(5)	0.6460(4)	0.1332(4)
C(8b)	0.2107(5)	0.0192(5)	0.0018(4)
C(9a)	0.3655(5)	0.6491(5)	0.0961(5)
C(9b)	0.2008(6)	-0.0078(5)	-0.0728(5)

Fractional atomic coordinates ($Å^2$) for the non-hydrogen atoms in [Ph(Me)$SnCl_2$(2,2'-bipyridyl)].$^1/_4CHCl_3$. Cont'd.*

Atom	*x*	*y*	*z*
C(10a)	0.3607(6)	0.6317(5)	0.0189(5)
C(10b)	0.2762(6)	0.0013(5)	-0.1208(4)
C(11a)	0.4403(6)	0.6129(4)	-0.0210(4)
C(11b)	0.3589(6)	0.0372(5)	-0.0935(4)
C(12a)	0.5278(5)	0.6101(4)	0.0192(3)
C(12b)	0.3629(5)	0.0644(4)	-0.0165(4)
C(13a)	0.6178(5)	0.5886(4)	-0.0191(4)
C(13b)	0.4410(5)	0.1038(4)	0.0175(4)
C(14a)	0.6213(6)	0.5672(5)	-0.0973(4)
C(14b)	0.5298(6)	0.1218(4)	-0.0275(4)
C(15a)	0.7058(7)	0.5462(5)	-0.1293(4)
C(15b)	0.6066(6)	0.1577(5)	0.0077(5)
C(16a)	0.7875(6)	0.5482(5)	-0.0840(5)
C(16b)	0.6047(6)	0.1769(5)	0.0842(5)
C(17a)	0.7818(6)	0.5709(5)	-0.0078(4)
C(17b)	0.5236(6)	0.1602(5)	0.1262(4)
Cl(30)*	0.3521(4)	0.2809(4)	0.4752(3)
Cl(40)*	0.5567(8)	0.2710(7)	0.5004(7)
Cl(50)*	0.4462(7)	0.1443(6)	0.5151(6)
C(100)*	0.4589(11)	0.2287(9)	0.4661(8)

*atom has site occupancy of 0.5

Anisotropic displacement parameters (Å) for the non-hydrogen atoms in [Ph(Me)$SnCl_2$(2,2'-bipyridyl)].$^1/_4CHCl_3$.*

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Sn(1)	0.0389(3)	0.0298(2)	0.0340(2)	0.0006(2)	-0.0060(2)	0.0001(2)
Sn(2)	0.0412(3)	0.0422(3)	0.0326(2)	0.0047(2)	0.0080(2)	-0.0008(2)
Cl(1a)	0.043(1)	0.067(1)	0.082(1)	0.001(1)	-0.018(1)	-0.006(1)
Cl(1b)	0.070(2)	0.077(2)	0.051(1)	0.008(1)	-0.001(1)	-0.027(1)
Cl(2a)	0.083(2)	0.044(1)	0.042(1)	-0.002(1)	0.006(1)	-0.008(1)
Cl(2b)	0.041(1)	0.109(2)	0.064(1)	0.006(1)	0.017(9)	0.002(1)
N(1a)	0.038(3)	0.031(3)	0.033(3)	0.002(3)	-0.001(2)	0.001(2)
N(1b)	0.035(3)	0.049(4)	0.034(3)	0.001(3)	0.002(2)	-0.003(3)
N(2a)	0.038(3)	0.048(4)	0.038(3)	-0.002(3)	0.001(3)	-0.002(3)
N(2b)	0.044(3)	0.038(3)	0.038(3)	-0.001(3)	0.009(3)	-0.001(3)
C(1a)	0.068(6)	0.041(4)	0.051(4)	-0.011(4)	-0.004(4)	0.002(4)
C(1b)	0.090(7)	0.059(6)	0.061(5)	0.029(5)	0.007(5)	0.006(4)
C(2a)	0.044(4)	0.032(4)	0.032(3)	0.001(3)	-0.010(3)	-0.003(3)
C(2b)	0.042(4)	0.040(4)	0.031(3)	0.003(3)	0.015(3)	-0.001(3)
C(3a)	0.058(5)	0.038(4)	0.041(4)	-0.002(4)	-0.013(3)	0.004(3)
C(3b)	0.052(5)	0.050(5)	0.046(4)	-0.006(4)	0.014(4)	-0.008(4)
C(4a)	0.083(7)	0.054(6)	0.050(4)	-0.019(5)	-0.014(4)	0.013(4)
C(4b)	0.105(8)	0.039(5)	0.057(5)	-0.011(5)	0.028(5)	-0.007(4)
C(5a)	0.122(9)	0.036(5)	0.066(6)	-0.008(6)	-0.040(6)	0.011(4)
C(5b)	0.104(9)	0.052(6)	0.065(6)	0.022(6)	0.024(6)	0.005(5)
C(6a)	0.096(8)	0.035(5)	0.080(6)	0.013(5)	-0.038(6)	-0.008(5)
C(6b)	0.067(6)	0.076(7)	0.053(5)	0.025(4)	0.010(4)	0.009(5)
C(7a)	0.062(5)	0.042(5)	0.054(4)	0.020(4)	-0.023(4)	-0.010(4)
C(7b)	0.045(4)	0.051(5)	0.043(4)	-0.002(4)	0.011(3)	0.004(3)
C(8a)	0.042(4)	0.036(4)	0.044(4)	0.006(3)	0.005(3)	-0.001(3)
C(8b)	0.040(4)	0.076(6)	0.048(4)	0.002(4)	-0.001(3)	-0.004(4)
C(9a)	0.038(4)	0.046(5)	0.070(5)	0.008(4)	0.001(4)	0.006(4)
C(9b)	0.055(5)	0.072(6)	0.052(5)	-0.008(5)	-0.014(4)	-0.003(4)
C(10a)	0.046(5)	0.059(5)	0.064(5)	0.007(4)	-0.016(4)	-0.002(4)
C(10b)	0.075(6)	0.061(5)	0.038(4)	0.006(5)	-0.007(4)	-0.009(4)
C(11a)	0.054(5)	0.045(5)	0.044(4)	-0.003(4)	-0.011(3)	0.002(3)
C(11b)	0.063(5)	0.051(5)	0.032(4)	0.009(4)	0.002(3)	0.002(3)

Anisotropic displacement parameters (Å) for the non-hydrogen atoms in $[Me(Ph)SnCl_2(2,2'\text{-bipyridyl})].^1/_4CHCl_3$.* Continued

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(12a)	0.040(4)	0.025(3)	0.033(3)	-0.002(3)	-0.004(3)	0.003(3)
C(12b)	0.051(5)	0.028(4)	0.034(3)	0.003(3)	0.001(3)	0.003(3)
C(13a)	0.050(4)	0.032(4)	0.034(3)	-0.005(3)	0.001(3)	0.001(3)
C(13b)	0.053(5)	0.031(4)	0.033(3)	0.007(3)	0.008(3)	0.004(3)
C(14a)	0.069(6)	0.055(5)	0.034(4)	-0.013(4)	0.001(4)	-0.001(3)
C(14b)	0.056(5)	0.041(5)	0.048(4)	0.001(4)	0.020(4)	0.003(3)
C(15a)	0.081(7)	0.073(6)	0.036(4)	-0.016(5)	0.023(4)	-0.008(4)
C(15b)	0.050(5)	0.048(5)	0.073(5)	-0.007(4)	0.030(4)	-0.002(4)
C(16a)	0.060(6)	0.070(6)	0.060(5)	-0.012(5)	0.028(4)	-0.014(4)
C(16b)	0.047(5)	0.047(5)	0.075(6)	-0.018(4)	0.007(4)	-0.007(4)
C(17a)	0.046(5)	0.064(6)	0.055(5)	-0.001(4)	0.008(4)	-0.007(4)
C(17b)	0.058(5)	0.045(4)	0.047(4)	-0.017(4)	0.007(4)	-0.007(3)
Cl(30)	0.099(5)*					
Cl(40)	0.215(5)*					
Cl(50)	0.183(4)*					
C(100)	0.049(4)*					

* atom refined isotropically

Fractional Atomic coordinates and B_{eq} values ($Å^2$) for the hydrogen atoms in [Ph(Me)$SnCl_2$(2,2'-bipyridyl)].$^1/_4CHCl_3$.*

Atom	*x*	*y*	*z*	*B*eq
H(1a1)	0.7526	0.7791	0.1328	5.1
H(1a2)	0.6884	0.7540	0.0596	5.1
H(1a3)	0.6401	0.7845	0.1367	5.7
H(1b1)	0.3116	0.2617	0.1351	6.1
H(1b2)	0.2645	0.2210	0.0601	6.1
H(1b3)	0.2026	0.2368	0.1345	7.5
H(3a1)	0.5416	0.5249	0.2437	4.7
H(3b1)	0.2402	-0.0764	0.1561	4.9
H(4a1)	0.5202	0.3882	0.2796	6.7
H(4b1)	0.3020	-0.2039	0.1988	6.1
H(5a1)	0.6349	0.2911	0.2470	6.9
H(5b1)	0.4457	-0.2127	0.2658	7.0
H(6a1)	0.7689	0.3305	0.1792	6.6
H(6b1)	0.5372	-0.0956	0.2873	6.6
H(7a1)	0.7886	0.4651	0.1402	5.0
H(7b1)	0.4794	0.0328	0.2456	4.6
H(8a1)	0.4595	0.6578	0.1886	3.7
H(8b1)	0.1580	0.0113	0.0366	5.8
H(9a1)	0.3086	0.6631	0.1244	5.5
H(9b1)	0.1419	-0.0328	-0.0911	5.5
H(10a1)	0.2995	0.6330	-0.0085	4.7
H(10b1)	0.2714	-0.0174	-0.1743	5.7
H(11a1)	0.4363	0.6015	-0.0765	4.8
H(11b1)	0.4131	0.0434	-0.1269	4.6
H(14a1)	0.5633	0.5674	-0.1293	4.8
H(14b1)	0.5302	0.1088	-0.0824	4.6

Fractional atomic coordinates and B_{eq} values ($Å^2$) for the hydrogen atoms in [Ph(Me)$SnCl_2$(2,2'-bipyridyl)].$^1/_4CHCl_3$.* Continued

Atom	*x*	*y*	*z*	*B*eq
H(15a1)	0.7083	0.5298	-0.1834	5.9
H(15b1)	0.6626	0.1693	-0.0221	5.7
H(16a1)	0.8484	0.5340	-0.1057	5.8
H(16b1)	0.6594	0.2021	0.1094	5.5
H(17a1)	0.8404	0.5731	0.0242	4.7
H(17b1)	0.5220	0.1749	0.1808	5.2
H(100)	0.4672	0.2154	0.4115	5.0

* For molecule *a*, H atoms were labeled with a1, a2 or a3
For molecule *b*, H atoms were labeled with b1, b2 or b3.

Bond distances (Å) for [Ph(Me)$SnCl_2$(2,2'-bipyridyl)J.$^1/_4CHCl_3$.

Atom - Atom	Distance	Atom - Atom	Distance
Sn(1) - Cl(1a)	2.488(2)	C(4b) - C(5b)	1.34(1)
Sn(1) - Cl(2a)	2.492(2)	C(5b) - C(6b)	1.38(1)
Sn(1) - N(1a)	2.389(5)	C(5a) - C(6a)	1.36(1)
Sn(1) - N(2a)	2.401(5)	C(6a) - C(7a)	1.38(1)
Sn(1) - C(1a)	2.139(7)	C(6b) - C(7b)	1.41(1)
Sn(1) - C(2a)	2.154(7)	C(8b) - C(9b)	1.36(1)
Sn(2) - Cl(1b)	2.500(2)	C(8a) - C(9a)	1.395(9)
Sn(2) - Cl(2b)	2.481(2)	C(9b) - C(10b)	1.37(1)
Sn(2) - N(1b)	2.388(5)	C(9a) - C(10a)	1.36(1)
Sn(2) - N(2b)	2.391(5)	C(10b) - C(11b)	1.38(1)
Sn(2) - C(1b)	2.110(8)	C(10a) - C(11a)	1.36(1)
Sn(2) - C(2b)	2.142(7)	C(11a) - C(12a)	1.396(9)
N(1a) - C(8a)	1.338(8)	C(11b) - C(12b)	1.396(9)
N(1a) - C(12a)	1.346(7)	C(12a) - C(13a)	1.482(9)
N(1b) - C(8b)	1.345(9)	C(12b) - C(13b)	1.492(9)
N(1b) - C(12b)	1.325(8)	C(13a) - C(14a)	1.389(9)
N(2b) - C(13b)	1.349(8)	C(13b) - C(14b)	1.408(9)
N(2b) - C(17b)	1.316(8)	C(14a) - C(15a)	1.37(1)
N(2a) - C(13a)	1.340(8)	C(14b) - C(15b)	1.36(1)
N(2a) - C(17a)	1.352(9)	C(15b) - C(16b)	1.35(1)
C(2b) - C(3b)	1.385(9)	C(15a) - C(16a)	1.37(1)
C(2b) - C(7b)	1.386(9)	C(16b) - C(17b)	1.39(1)
C(2a) - C(3a)	1.372(9)	C(16a) - C(17a)	1.37(1)
C(2a) - C(7a)	1.376(9)	Cl(30) - C(100)	1.74(2)
C(3b) - C(4b)	1.42(1)	Cl(40) - C(100)	1.64(2)
C(3a) - C(4a)	1.39(1)	Cl(50) - C(100)	1.64(2)
C(4a) - C(5a)	1.38(1)		

Bond angles (°) for [Ph(Me)$SnCl_2$(2,2'-bipyridyl)].$^1/_4CHCl_3$.

Atom - Atom - Atom	Angle	Atom - Atom - Atom	Angle
Cl(1a) - Sn(1) - Cl(2a)	101.89(7)	Sn(2) - N(1b) - C(12b)	118.9(4)
Cl(1a) - Sn(1) - N(1a)	161.7(1)	C(8b) - N(1b) - C(12b)	118.3(6)
Cl(1a) - Sn(1) - N(2a)	93.1(1)	Sn(2) - N(2b) - C(13b)	117.4(4)
Cl(1a) - Sn(1) - C(1a)	93.7(2)	Sn(2) - N(2b) - C(17b)	122.4(4)
Cl(1a) - Sn(1) - C(2a)	93.2(2)	C(13b) - N(2b) - C(17b)	120.0(6)
Cl(2a) - Sn(1) - N(1a)	96.4(1)	Sn(1) - N(2a) - C(13a)	118.4(4)
Cl(2a) - Sn(1) - N(2a)	165.0(1)	Sn(1) - N(2a) - C(17a)	122.1(5)
Cl(2a) - Sn1) - C(1a)	91.7(2)	C(13a) - N(2a) - C(17a)	119.5(6)
Cl(2a) - Sn(1) - C(2a)	91.4(2)	Sn(2) - C(2b) - C(3b)	121.4(5)
N(1a) - Sn(1) - N(2a)	68.5(2)	Sn(2) - C(2b) - C(7b)	119.6(5)
N(1a) - Sn(1) - C(1a)	85.2(2)	C(3b) - C(2b) - C(7b)	118.9(7)
N(1a) - Sn(1) - C(2a)	86.9(2)	Sn(1) - C(2a) - C(3a)	120.4(5)
N(2a) - Sn(1) - C(1a)	86.9(2)	Sn(1) - C(2a) - C(7a)	120.4(5)
N(2a) - Sn(1) - C(2a)	88.1(2)	C(3a) - C(2a) - C(7a)	119.2(7)
C(1a) - Sn(1) - C(2a)	171.8(3)	C(2b) - C(3b) - C(4b)	119.5(7)
Cl(1b) - Sn(2) - Cl(2b)	103.14(7)	C(2a) - C(3a) - C(4a)	120.4(7)
Cl(1b) - Sn(2) - N(1b)	164.7(1)	C(3a) - C(4a) - C(5a)	120.0(8)
Cl(1b) - Sn(2) - N(2b)	95.5(1)	C(3b) - C(4b) - C(5b)	121.6(8)
Cl(1b) - Sn(2) - C(1b)	90.1(3)	C(4b) - C(5b) - C(6b)	119.3(8)
Cl(1b) - Sn(2) - C(2b)	91.4(2)	C(4a) - C(5a) - C(6a)	119.3(8)
Cl(2b) - Sn(2) - N(1b)	92.2(1)	C(5a) - C(6a) - C(7a)	121.0(9)
Cl(2b) - Sn(2) - N(2b)	161.3(1)	C(5b) - C(6b) - C(7b)	120.7(8)
Cl(2b) - Sn(2) - C(1b)	93.1(3)	C(2b) - C(7b) - C(6b)	120.0(7)
Cl(2b) - Sn(2) - C(2b)	92.9(2)	C(2a) - C(7a) - C(6a)	120.2(8)
N(1b) - Sn(2) - N(2b)	69.2(2)	N(1b) - C(8b) - C(9b)	123.6(7)
N(1b) - Sn(2) - C(1b)	88.5(3)	N(1a) - C(8a) - C(9a)	122.7(6)
N(1b) - Sn(2) - C(2b)	88.4(2)	C(8b) - C(9b) - C(10b)	117.9(7)
N(2b) - Sn(2) - C(1b)	85.6(3)	C(8a) - C(9a) - C(10a)	117.6(7)
N(2b) - Sn(2) - C(2b)	87.7(2)	C(9b) - C(10b) - C(11b)	120.1(7)
C(1b) - Sn(2) - C(2b)	173.3(3)	C(9a) - C(10a) - C(11a)	121.2(7)
Sn(1) - N(1a) - C(8a)	122.2(4)	C(10a) - C(11a) - C(12a)	118.8(6)
Sn(1) - N(1a) - C(12a)	119.1(4)	C(10b) - C(11b) - C(12b)	118.5(7)
C(8a) - N(1a) - C(12a)	118.6(5)	N(1a) - C(12a) - C(11a)	121.1(6)
Sn(2) - N(1b) - C(8b)	122.8(4)	N(1a) - C(12a) - C(13a)	116.4(5)

Bond angles (°) for [Ph(Me)$SnCl_2$(2,2'-bipyridyl)].$^1/_4CHCl_3$. Continued

Atom - Atom - Atom	Angle	Atom - Atom - Atom	Angle
C(11a) - C(12a) - C(13a)	122.5(6)	C(13b) - C(14b) - C(15b)	118.8(6)
N(1b) - C(12b) - C(11b)	121.5(7)	C(14b) - C(15b) - C(16b)	120.0(7)
N(1b) - C(12b) - C(13b)	116.7(5)	C(14a) - C(15a) - C(16a)	119.3(7)
C(11b) - C(12b) - C(13b)	121.8(6)	C(15b) - C(16b) - C(17b)	119.5(7)
N(2a) - C(13a) - C(12a)	117.4(5)	C(15a) - C(16a) - C(17a)	118.9(7)
N(2a) - C(13a) - C(14a)	119.9(7)	N(2a) - C(17a) - C(16a)	122.1(7)
C(12a) - C(13a) - C(14a)	122.7(6)	N(2b) - C(17b) - C(16b)	121.4(7)
N(2b) - C(13b) - C(12b)	117.6(6)	Cl(30) - C(100) - Cl(40)	118(1)
N(2b) - C(13b) - C(14b)	120.2(6)	Cl(30) - C(100) - Cl(50)	105.7(9)
C(12b) - C(13b) - C(14b)	122.2(6)	Cl(40) - C(100) - Cl(50)	106(1)
C(13a) - C(14a) - C(15a)	120.3(7)		

Observed and calculated structure factors for [Ph(Me)$SnCl_2$(2,2'-bipyridyl)].$^1/_4CHCl_3$.

h	k	l	Fo	Fc	sigF
0	0	6	3647	3760	20
0	0	8	144	217	11
0	0	10	413	367	9
0	0	12	1382	1466	14
0	0	14	0	35	47*
0	0	16	1200	1265	16
0	0	18	421	390	10
0	0	20	150	131	21
0	0	22	593	596	14
0	1	3	105	85	7
0	1	4	11	98	29*
0	1	5	55	64	21*
0	1	6	119	74	12
0	1	7	242	196	7
0	1	8	422	472	8
0	1	9	248	218	8
0	1	10	37	82	32*
0	1	11	207	188	10
0	1	12	87	20	47*
0	1	13	82	111	48*
0	1	14	0	109	50*
0	1	15	112	49	23*
0	1	16	0	15	55*
0	1	17	81	47	55*
0	1	18	13	98	53*
0	1	19	18	69	54*
0	1	20	85	13	53*
0	1	21	96	68	56*
0	1	22	0	46	61*
0	2	6	518	525	10
0	2	8	261	325	8
0	2	9	143	195	13
0	2	10	0	38	43*
0	2	11	1294	1361	13
0	2	12	614	592	14
0	2	13	503	464	11
0	2	14	293	312	11
0	2	15	1001	1038	15
0	2	16	0	175	60*
0	2	17	1047	1099	17
0	2	18	156	148	22
0	2	19	85	151	57*
0	2	20	75	6	57*
0	2	21	492	488	11
0	2	22	0	26	64*
0	3	3	678	685	8
0	3	4	158	160	8
0	3	5	610	570	9
0	3	6	96	138	16*
0	3	7	491	407	11
0	3	8	376	424	10
0	3	9	341	386	9
0	3	10	178	136	12
0	3	11	126	96	17
0	3	12	0	25	49*
0	3	13	236	266	12
0	3	14	249	286	12
0	3	15	220	208	14
0	3	16	186	148	17
0	3	17	87	52	56*
0	3	18	0	9	56*
0	3	19	50	70	56*
0	3	20	0	90	58*
0	3	21	80	31	59*
0	3	22	109	44	60*
0	4	-6	3005	3006	18
0	4	0	4975	5061	27
0	4	2	1360	1344	10
0	4	3	67	284	19*
0	4	4	980	974	10
0	4	8	354	414	9
0	4	9	395	332	10
0	4	10	1218	1229	13
0	4	11	510	470	11
0	4	12	1437	1468	15
0	4	13	336	380	10
0	4	14	128	115	23*
0	4	15	319	280	12
0	4	16	1214	1212	17
0	4	17	0	34	58*
0	4	18	407	391	11
0	4	19	61	52	57*
0	4	20	277	276	15
0	4	21	0	57	61*
0	5	1	1292	1252	11
0	5	2	1830	1796	13
0	5	3	1067	1074	10
0	5	4	1118	1189	11
0	5	5	0	40	40*
0	5	6	137	185	14
0	5	7	186	130	10
0	5	8	761	743	12
0	5	9	845	899	13
0	5	10	471	464	11
0	5	11	76	16	31*
0	5	12	207	218	13
0	5	13	246	257	13
0	5	14	426	394	10
0	5	15	318	306	12
0	5	16	67	63	57*
0	5	17	16	67	56*
0	5	18	207	232	18
0	5	19	0	139	62*
0	5	20	163	142	23
0	5	21	98	53	51*
0	6	-5	2579	2695	16
0	6	0	145	87	12
0	6	1	2617	2606	16
0	6	2	1285	1283	12
0	6	3	1395	1276	12
0	6	4	314	337	7
0	6	6	1298	1219	13
0	6	7	1210	1192	13
0	6	8	120	34	18
0	6	9	576	617	14
0	6	10	419	490	10
0	6	11	1473	1458	15
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0	6	14	556	580	13
0	6	15	713	752	13
0	6	16	34	59	58*
0	6	17	737	710	19
0	6	18	0	44	57*
0	6	19	43	55	49*
0	6	20	0	36	60*
0	6	21	461	428	12
0	7	-3	1873	1804	14
0	7	1	1051	1081	12
0	7	2	0	46	45*
0	7	4	477	522	10
0	7	5	1002	1036	12
0	7	6	169	236	13
0	7	7	683	716	13
0	7	8	344	346	9
0	7	9	1001	924	14
0	7	10	278	287	11
0	7	11	100	136	54*
0	7	12	250	267	14
0	7	13	342	341	11
0	7	14	407	398	11
0	7	15	406	391	11
0	7	16	88	142	59*
0	7	17	0	124	59*
0	7	18	164	131	21
0	7	19	284	249	14
0	7	20	140	163	29*
0	7	21	34	93	64*
0	8	0	2238	2299	16
0	8	1	248	230	10
0	8	2	415	362	11
0	8	3	95	49	22*
0	8	4	1433	1414	14
0	8	5	474	478	11
0	8	6	1700	1687	15
0	8	7	308	293	10
0	8	8	0	66	50*
0	8	9	157	119	16
0	8	10	1032	1101	15
0	8	11	472	463	11
0	8	12	1101	1057	17
0	8	13	349	310	12
0	8	14	123	118	26*
0	8	15	0	4	56*
0	8	16	514	512	12
0	9	17	99	180	64*
0	8	18	270	243	15
0	8	19	98	75	60*
0	8	20	226	243	20
0	9	-2	1728	1764	15
0	9	1	247	332	10
0	9	3	623	562	15
0	9	4	1203	1208	14
0	9	5	459	415	12
0	9	6	242	209	12
0	9	7	431	443	10
0	9	8	813	836	15
0	9	9	306	284	11
0	9	10	467	484	11
0	9	11	127	112	24*
0	9	12	104	194	62*
0	9	13	425	426	11
0	9	14	561	584	12
0	9	15	242	226	15
0	9	16	79	57	57*
0	9	17	88	44	37*
0	9	18	421	400	12
0	9	19	264	255	18
0	9	20	296	304	17
0	10	0	190	165	13
0	10	1	847	822	14
0	10	2	61	180	52*
0	10	3	766	704	15
0	10	4	253	234	12
0	10	5	1460	1466	15
0	10	6	379	386	10
0	10	7	689	642	16
0	10	8	65	122	54*
0	10	9	535	507	13
0	10	10	352	318	12
0	10	11	1102	1119	17
0	10	12	330	315	13
0	10	13	693	697	14
0	10	14	89	83	57*
0	10	15	241	250	18
0	10	16	15	106	59*
0	10	17	371	358	13
0	10	18	99	107	62*
0	10	19	119	2	61*
0	11	1	890	883	15
0	11	2	292	287	11
0	11	3	1867	1903	17
0	11	4	242	259	14
0	11	5	356	382	11
0	11	6	256	225	13
0	11	7	688	670	17
0	11	8	262	253	14
0	11	9	941	961	17
0	11	10	0	98	57*
0	11	11	137	112	26*
0	11	12	289	319	15
0	11	13	668	651	14
0	11	14	270	259	17
0	11	15	310	294	14
0	11	16	0	63	61*
0	11	17	57	131	64*
0	11	18	114	143	38*
0	11	19	456	434	13
0	12	0	560	584	12
0	12	1	339	348	11
0	12	2	64	124	45*
0	12	3	107	85	55*
0	12	4	974	972	17
0	12	5	153	106	21
0	12	6	849	871	18
0	12	7	282	290	13
0	12	8	119	149	60*
0	12	9	109	30	61*
0	12	10	674	678	14
0	12	11	80	103	62*
0	12	12	697	683	15
0	12	13	0	110	64*
0	12	14	118	100	64*
0	12	15	240	251	19
0	12	16	434	457	13
0	12	17	195	180	23
0	12	18	120	129	38*
0	13	1	0	92	56*
0	13	2	1154	1140	17
0	13	3	193	186	18
0	13	4	814	828	18
0	13	5	0	19	55*
0	13	6	277	245	14
0	13	7	0	72	62*
0	13	8	1055	1053	19
0	13	9	184	148	21
0	13	10	416	404	12
0	13	11	0	88	65*
0	13	12	426	423	13
0	13	13	276	276	18
0	13	14	673	710	16
0	13	15	196	230	24
0	13	16	126	48	33*
0	13	17	158	152	28*
0	14	0	216	151	17
0	14	1	651	651	13
0	14	2	63	168	59*
0	14	3	114	123	58*
0	14	4	102	67	62*
0	14	5	359	354	13
0	14	6	0	8	62*
0	14	7	186	168	21
0	14	8	92	24	61*
0	14	9	218	235	21
0	14	10	0	85	63*
1	1	-14	943	944	15
1	1	-13	755	840	15
1	1	-12	372	365	9
1	1	-11	226	332	12
1	1	-10	1132	1136	13
1	1	-9	1846	1797	14
1	1	-8	2356	2380	15
1	1	-7	2096	2164	14
1	1	-6	580	585	10
1	1	-5	320	289	7
1	1	-4	3531	3439	19
1	1	-3	1817	1844	11
1	1	3	2239	2209	13
1	1	6	492	436	10
1	1	7	1991	2081	13
1	1	8	2519	2436	16
1	1	9	1635	1695	13
1	1	10	1168	1196	12
1	1	11	346	304	8
1	1	12	220	221	12
1	1	13	707	681	15
1	1	14	861	887	15
1	1	15	634	639	12
1	1	16	402	403	11
1	1	17	37	65	56*
1	1	18	342	329	12
1	1	19	302	326	13
1	1	20	277	279	14
1	1	21	88	72	39*
1	1	22	116	63	59*
1	2	-22	0	55	64*
1	2	-21	127	131	30*
1	2	-20	0	99	60*
1	2	-19	107	71	33*
1	2	-18	158	91	21
1	2	-17	89	17	57*
1	2	-16	143	110	23
1	2	-15	269	233	13
1	2	-14	504	535	12
1	2	-13	0	7	51*
1	2	-12	257	268	11
1	2	-11	77	39	40*
1	2	-10	284	316	8
1	2	-8	1149	1044	11
1	2	-7	622	556	10
1	2	-5	1575	1472	11
1	2	2	1270	1276	8
1	2	5	396	314	10
1	2	7	219	255	9
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1	2	13	123	141	21*
1	2	14	776	807	15
1	2	15	0	55	56*
1	2	16	141	121	22
1	2	17	245	225	14
1	2	18	274	275	14
1	2	19	65	16	57*
1	2	20	219	227	17
1	2	21	61	37	49*
1	2	22	0	55	61*
1	3	-22	0	27	62*
1	3	-21	204	195	19
1	3	-20	375	378	13
1	3	-19	554	530	14
1	3	-18	251	269	15
1	3	-17	380	418	12
1	3	-16	395	434	11
1	3	-15	683	754	17
1	3	-14	920	922	15
1	3	-13	975	961	14
1	3	-12	440	407	11
1	3	-11	176	122	14
1	3	-10	1105	1064	12
1	3	-9	1307	1367	12
1	3	-8	1792	1869	13
1	3	-7	1345	1260	11
1	3	-6	1167	1086	10
1	3	-5	1096	1011	10
1	3	-4	801	852	9
1	3	-2	2064	2048	12
1	3	-1	2338	2331	13
1	3	1	2417	2496	14
1	3	5	1534	1581	11
1	3	6	1097	1196	11
1	3	7	1539	1565	12
1	3	8	1545	1546	13
1	3	9	1302	1340	13
1	3	10	745	725	13
1	3	11	381	419	9
1	3	12	439	427	10
1	3	13	963	980	15
1	3	14	706	757	16
1	3	15	769	781	16
1	3	16	70	58	56*
1	3	17	206	234	17
1	3	18	265	256	14
1	3	19	392	403	12
1	3	20	201	211	19
1	3	21	239	270	18
1	3	22	111	131	61*
1	4	-21	105	127	59*
1	4	-20	296	272	13
1	4	-19	0	93	58*
1	4	-18	109	13	28*
1	4	-17	189	231	19
1	4	-16	296	333	13
1	4	-15	344	363	11
1	4	-14	111	67	26*
1	4	-13	530	528	12
1	4	-12	73	52	49*
1	4	-11	96	89	23*
1	4	-10	234	194	10
1	4	-9	174	171	12
1	4	-8	772	691	11
1	4	-7	1702	1656	13
1	4	-5	173	197	9
1	4	-3	181	134	7
1	4	-1	2209	2164	13
1	4	0	1044	1014	9
1	4	1	1985	2011	13
1	4	3	694	673	9
1	4	5	0	73	38*
1	4	7	804	795	11
1	4	8	104	129	17*
1	4	9	620	653	13
1	4	10	677	726	13
1	4	11	236	210	11
1	4	12	790	808	15
1	4	13	493	489	12
1	4	14	152	80	19
1	4	15	482	470	11
1	4	16	351	331	12
1	4	17	275	306	15
1	4	18	305	306	13
1	4	19	328	313	13
1	4	20	0	52	60*
1	4	21	185	209	21
1	5	-21	180	165	21
1	5	-20	444	507	12
1	5	-19	367	396	12
1	5	-18	546	595	12
1	5	-17	139	162	24*
1	5	-16	70	136	57*
1	5	-15	704	760	17
1	5	-14	853	854	16
1	5	-13	752	727	15
1	5	-12	606	636	15
1	5	-11	140	166	18
1	5	-10	735	765	14
1	5	-9	2261	2290	16
1	5	-8	1613	1563	13
1	5	-7	1144	1076	12
1	5	-6	499	538	11
1	5	-5	53	95	40*
1	5	-4	2049	2031	13
1	5	-3	1694	1786	12
1	5	-2	2896	2927	17
1	5	-1	817	813	10
1	5	0	0	22	38*
1	5	1	907	864	10
1	5	2	2665	2686	16
1	5	3	1173	1183	11
1	5	4	1818	1855	13
1	5	5	187	161	10
1	5	6	184	218	11
1	6	15	205	209	17
1	6	16	152	153	22
1	6	17	511	500	12
1	6	18	108	192	62*
1	8	-15	328	316	13
1	8	-14	258	257	15
1	8	-13	447	475	11
1	8	-12	428	432	10
1	9	-1	0	57	46*
1	9	0	0	16	48*
1	9	1	575	574	14
1	9	2	1251	1229	14
1	10	14	268	273	16
1	10	15	266	290	15
1	10	16	0	78	43*
1	10	17	526	518	12

1	5	7	1185	1191	12	1	6	19	232	255	18	1	8	-11	371	325	10	1	9	3	583	582	14	1	10	18	166	193	25
1	5	8	1137	1119	13	1	6	20	252	215	16	1	8	-10	577	607	12	1	9	4	1594	1625	15	1	10	19	0	108	66*
1	5	9	1275	1282	13	1	6	21	89	58	61*	1	8	-9	0	12	50*	1	9	5	451	415	11	1	11	-19	396	405	15
1	5	10	903	894	14	1	7	-21	250	263	18	1	8	-8	451	449	10	1	9	6	132	158	19	1	11	-18	98	81	51*
1	5	11	160	149	16	1	7	-20	226	204	18	1	8	-7	359	398	8	1	9	7	395	389	10	1	11	-17	114	122	67*
1	5	12	463	489	10	1	7	-19	572	567	12	1	8	-6	1316	1335	14	1	9	8	404	401	10	1	11	-16	99	172	65*
1	5	13	790	776	16	1	7	-18	137	153	25*	1	8	-5	18	71	48*	1	9	9	189	174	15	1	11	-15	287	307	17
1	5	14	1012	952	16	1	7	-17	194	206	19	1	8	-4	1518	1532	14	1	9	10	418	412	10	1	11	-14	274	316	17
1	5	15	358	350	11	1	7	-16	262	285	15	1	8	-3	671	699	13	1	9	11	403	379	10	1	11	-13	627	625	15
1	5	16	210	255	18	1	7	-15	548	552	13	1	8	-2	881	874	13	1	9	12	270	234	13	1	11	-12	0	32	65*
1	5	17	203	186	17	1	7	-14	715	721	17	1	8	-1	1763	1666	14	1	9	13	634	602	14	1	11	-11	119	92	62*
1	5	18	340	350	13	1	7	-13	972	1020	16	1	8	0	1123	1135	13	1	9	14	611	619	15	1	11	-10	357	345	13
1	5	19	265	289	17	1	7	-12	225	243	14	1	8	1	88	236	46*	1	9	15	0	17	56*	1	11	-9	596	623	14
1	5	20	460	470	12	1	7	-11	269	241	12	1	8	2	794	836	13	1	9	16	0	45	60*	1	11	-8	333	330	12
1	5	21	57	13	43*	1	7	-10	737	775	15	1	8	3	1002	1039	13	1	9	17	185	213	23	1	11	-7	680	680	17
1	6	-21	346	364	14	1	7	-9	1000	952	14	1	8	4	657	709	13	1	9	18	357	326	14	1	11	-6	354	366	11
1	6	-20	151	128	26*	1	7	-8	759	734	13	1	8	5	1018	1011	13	1	9	19	257	242	18	1	11	-5	180	187	18
1	6	-19	0	124	64*	1	7	-7	857	915	13	1	8	6	449	447	11	1	9	20	400	401	14	1	11	-4	1016	957	16
1	6	-18	212	263	18	1	7	-6	158	208	13	1	8	7	290	262	10	1	10	-19	70	99	68*	1	11	-3	1327	1354	15
1	6	-17	151	115	22	1	7	-5	840	894	12	1	8	8	66	32	36*	1	10	-18	283	292	18	1	11	-2	475	458	10
1	6	-16	107	34	53*	1	7	-4	1454	1456	13	1	8	9	113	70	23*	1	10	-17	445	441	12	1	11	-1	754	766	16
1	6	-15	285	288	13	1	7	-3	2673	2571	17	1	8	10	908	902	15	1	10	-16	198	202	21	1	11	0	361	355	10
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3	18	4	93	149	66*	4	0	-8	231	259	8	4	2	-21	196	205	21	4	3	-8	277	262	9	4	4	7	283	236	8						
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3	18	6	99	114	56*	4	0	-2	1092	1110	9	4	2	-19	66	83	41*	4	3	-6	1574	1595	13	4	4	9	552	619	11						
3	18	7	144	158	35*	4	0	0	1274	1310	10	4	2	-18	64	55	58*	4	3	-5	1781	1711	13	4	4	10	207	227	13						
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3	18	9	101	116	59*	4	0	4	1212	1209	11	4	2	-16	268	274	14	4	3	-3	1002	956	10	4	4	12	150	180	19						
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3	19	-9	112	85	58*	4	0	10	742	678	13	4	2	-13	212	232	15	4	3	3	297	329	7	4	4	15	224	184	16						
3	19	-8	0	97	74*	4	0	12	194	257	14	4	2	-12	277	283	11	4	3	4	1519	1453	12	4	4	16	0	30	49*						
3	19	-7	0	37	79*	4	0	14	8	22	54*	4	2	-11	568	591	11	4	3	5	1824	1793	13	4	4	17	354	338	13						
3	19	-6	570	619	14	4	0	16	0	127	60*	4	2	-10	206	213	12	4	3	7	527	623	12	4	4	18	229	214	18						
3	19	-5	111	59	70*	4	0	18	51	31	59*	4	2	-9	888	873	13	4	3	8	0	162	46*	4	4	19	308	297	15						
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3	19	-3	89	106	65*	4	1	-21	207	246	19	4	2	-7	567	535	12	4	3	10	1883	1838	15	4	4	21	0	30	59*						
3	19	-2	247	232	21	4	1	-20	0	78	61*	4	2	-6	117	193	16	4	3	11	1104	1072	14	4	5	-21	255	221	18						
3	19	-1	0	67	67*	4	1	-19	105	165	60*	4	2	-5	199	175	10	4	3	12	698	687	16	4	5	-20	246	198	17						
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3	19	3	0	57	68*	4	1	-15	388	380	10	4	2	-1	1400	1354	11	4	3	16	824	816	18	4	5	-16	314	309	13						
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3	20	-7	257	247	23	4	1	-8	67	57	44*	4	2	6	33	93	42*	4	4	-21	222	228	21	4	5	-9	521	520	11						
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4	6	-9	122	60	22*	4	7	5	1512	1585	14	4	8	19	441	453	13	4	10	-5	102	142	30*	4	11	12	576	592	13						
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4	6	17	0	80	60*	4	8	-10	159	140	19	4	9	5	1680	1715	16	4	11	-17	175	138	27	4	12	2	302	292	13						
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| | | |

5	9	-11	955	928	19	5	10	6	995	1006	17	5	12	-12	233	217	21	5	13	9	337	344	15	5	15	2	40	193	70*
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7	3	-15	580	618	15	7	4	-1	701	712	14	7	5	13	503	503	12	7	7	-10	338	346	13	7	8	6	309	294	12		
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7	3	9	567	576	11	7	5	-18	120	103	63*	7	6	-2	923	895	15	7	7	14	450	449	12	7	9	-7	754	707	19				
7	3	10	438	450	11	7	5	-17	113	135	63*	7	6	-1	799	838	15	7	7	15	200	189	21	7	9	-6	145	96	26*				
7	3	11	112	140	26*	7	5	-16	298	289	16	7	6	0	288	242	12	7	7	16	213	213	18	7	9	-5	452	472	11				
7	9	-4	925	953	17	7	10	14	0	43	62*	7	12	0	724	684	14	7	14	-7	399	377	15	7	16	-6	330	318	19				
7	9	-3	789	779	18	7	10	15	364	390	15	7	12	1	469	493	12	7	14	-6	290	295	19	7	16	-5	333	310	18				
7	9	-2	818	752	17	7	10	16	92	101	49*	7	12	2	0	74	64*	7	14	-5	288	307	19	7	16	-4	116	120	61*				
7	9	-1	1008	1046	16	7	10	17	362	333	15	7	12	3	272	282	16	7	14	-4	272	235	19	7	16	-3	185	236	30				
7	9	0	220	204	17	7	11	-17	141	105	75*	7	12	4	740	727	14	7	14	-3	0	84	67*	7	16	-2	415	434	16				
7	9	1	256	203	14	7	11	-16	82	98	62*	7	12	5	322	272	14	7	14	-2	188	195	23	7	16	-1	281	243	18				
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7	9	3	447	453	11	7	11	-14	91	160	72*	7	12	7	408	441	13	7	14	0	410	398	13	7	16	1	367	363	16				
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7	9	8	665	657	13	7	11	-9	568	557	14	7	12	12	265	267	18	7	14	5	739	728	16	7	16	6	488	500	15				
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7	9	13	269	283	16	7	11	-4	284	288	16	7	13	-15	0	63	80*	7	14	10	175	105	23	7	16	11	296	292	19				
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7	9	15	330	340	15	7	11	-2	705	682	13	7	13	-13	231	254	26	7	14	12	281	299	18	7	17	-10	146	35	42*				
7	9	16	113	120	64*	7	11	-1	53	96	62*	7	13	-12	167	93	31*	7	14	13	0	31	69*	7	17	-9	0	128	80*				
7	9	17	98	48	62*	7	11	0	583	580	14	7	13	-11	400	408	17	7	14	14	0	79	65*	7	17	-8	0	54	81*				
7	9	18	277	273	18	7	11	1	692	677	13	7	13	-10	199	212	28	7	15	-13	0	65	81*	7	17	-7	218	263	30				
7	10	-18	0	81	74*	7	11	2	207	174	17	7	13	-9	231	204	23	7	15	-12	375	353	19	7	17	-6	92	16	69*				
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7	10	-15	87	128	69*	7	11	5	110	11	59*	7	13	-6	70	6	67*	7	15	-9	260	276	24	7	17	-3	0	119	74*				
7	10	-14	263	254	20	7	11	6	454	414	11	7	13	-5	531	561	13	7	15	-8	81	206	77*	7	17	-2	82	141	76*				
7	10	-13	507	525	13	7	11	7	340	342	14	7	13	-4	312	258	15	7	15	-7	143	32	73*	7	17	-1	382	369	16				
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7	10	-11	543	521	14	7	11	9	154	185	26*	7	13	-2	348	365	15	7	15	-5	0	59	71*	7	17	1	105	195	73*				
7	10	-10	675	688	16	7	11	10	406	438	14	7	13	-1	540	531	14	7	15	-4	166	151	29*	7	17	2	124	185	44*				
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7	10	-6	383	405	13	7	11	14	340	349	15	7	13	3	318	266	14	7	15	0	398	415	15	7	17	6	111	36	66*				
7	10	-5	613	599	14	7	11	15	52	73	62*	7	13	4	138	78	30*	7	15	1	402	392	14	7	17	7	0	117	69*				
7	10	-4	376	415	13	7	11	16	253	222	18	7	13	5	441	440	13	7	15	2	0	63	71*	7	17	8	0	7	75*				
7	10	-3	101	122	51*	7	11	17	207	200	23	7	13	6	238	225	19	7	15	3	268	259	19	7	17	9	266	274	21				
7	10	-2	256	238	16	7	12	-16	254	248	25	7	13	7	55	9	67*	7	15	4	412	411	14	7	17	10	93	21	56*				
7	10	-1	955	929	17	7	12	-15	214	228	28	7	13	8	311	309	15	7	15	5	0	12	71*	7	18	-8	0	73	85*				
7	10	0	618	581	13	7	12	-14	53	105	73*	7	13	9	399	398	14	7	15	6	225	291	24	7	18	-7	282	289	25				
7	10	1	345	367	12	7	12	-13	27	103	75*	7	13	10	56	108	63*	7	15	7	277	275	19	7	18	-6	267	342	27				
7	10	2	480	492	12	7	12	-12	503	501	14	7	13	11	368	392	15	7	15	8	0	64	61*	7	18	-5	304	278	22				
7	10	3	178	187	19	7	12	-11	364	341	15	7	13	12	203	191	23	7	15	9	86	74	50*	7	18	-4	136	176	78*				
7	10	4	96	48	54*	7	12	-10	276	213	18	7	13	13	132	136	69*	7	15	10	394	407	15	7	18	-3	96	64	52*				
7	10	5	679	645	13	7	12	-9	436	431	14	7	13	14	140	93	32*	7	15	11	0	23	67*	7	18	-2	0	33	75*				
7	10	6	750	791	14	7	12	-8	292	331	19	7	13	15	229	265	23	7	15	12	91	130	54*	7	18	-1	401	392	16				
7	10	7	0	56	60*	7	12	-7	256	247	18	7	14	-14	106	187	61*	7	15	13	148	161	32*	7	18	0	288	287	20				
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7	10	13	110	110	61*	7	12	-1	103	83	38*	7	14	-8	183	126	27	7	16	-7	162	213	37*	7	18	6	306	298	19				
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7	18	8	0	7	70*	8	1	2	90	22	49*	8	2	17	577	589	13	8	4	-7	128	117	24*	8	5	9	245	226	14				
7	19	-6	348	352	21	8	1	3	183	179	15	8	2	18	10	2	60*	8	4	-6	1617	1603	16	8	5	10	196	215	18				
7	19	-5	0	31	62*	8	1	4	744	726	15	8	2	19	137	109	28*	8	4	-5	372	384	10	8	5	11	0	12	56*				
7	19	-4	103	108	64*	8	1	5	443	419	11	8	3	-20	129	189	70*	8	4	-4	780	782	16	8	5	12	299	294	13				
7	19	-3	88	67	64*	8	1	6	201	207	15	8	3	-19	84	100	68*	8	4	-3	177	121	16	8	5	13	0	36	58*				
7	19	-2	233	267	28	8	1	7	306	332	11	8	3	-18	108	77	38*	8	4	-2	649	615	15	8	5	14	318	295	14				
7	19	-1	51	21	75*	8	1	8	72	80	54*	8	3	-17	0	12	65*	8	4	-1	614	647	16	8	5	15	118	90	29*				
7	19	0	275	295	22	8	1	9	98	101	53*	8	3	-16	253	236	16	8	4	0	1351	1395	15	8	5	16	0	71	61*				
7	19	1	0	59	72*	8	1	10	349	322	11	8	3	-15	277	277	16	8	4	1	128	68	21*	8	5	17	0	63	51*				
7	19	2	117	76	59*	8	1	11	248	241	14	8	3	-14	204	171	19	8	4	2	338	290	10	8	5	18	193	196	22				
7	19	3	90	48	62*	8	1	12	150	118	22	8	3	-13	292	286	15	8	4	3	257	279	13	8	5	19	104	42	63*				
7	19	4	284	283	21	8	1	13	255	249	15	8	3	-12	0	49	63*	8	4	4	1560	1466	16	8	6	-19	271	234	19				
7	19	5	147	9	75*	8	1	14	0	49	58*	8	3	-11	490	473	12	8	4	5	0	15	52*	8	6	-18	236	208	21				
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8	0	-18	430	449	12	8	1	16	0	3	58*	8	3	-9	109	115	30*	8	4	7	57	79	52*	8	6	-16	251	250	19				
8	0	-16	526	539	12	8	1	17	110	31	56*	8	3	-8	59	30	55*	8	4	8	33	58	45*	8	6	-15	367	365	15				
8	0	-14	100	145	60*	8	1	18	74	98	54*	8	3	-7	534	525	12	8	4	9	290	307	12	8	6	-14	70	12	63*				
8	0	-12	1224	1228	16	8	1	19	113	16	59*	8	3	-6	463	425	11	8	4	10	1122	1118	17	8	6	-13	349	321	14				
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8	0	-8	130	155	21	8	2	-19	174	230	27	8	3	-4	39	87	49*	8	4	12	572	568	14	8	6	-11	989	962	19				
8	0	-6	1530	1515	15	8	2	-18	143	132	30*	8	3	-3	81	41	44*	8	4	13	0	77	59*	8	6	-10	151	69	25*				
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8	0	-2	587	584	13	8	2	-16	150	150	26*	8	3	-1	346	365	9	8	4	15	391	362	12	8	6	-8	284	286	15				
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8	0	18	189	197	20	8	2	-6	130	71	21	8	3	9	403	421	10	8	5	-14	234	217	18	8	6	2	338	246	11				
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8	1	-19	0	75	64*	8	2	-4	282	303	11	8	3	11	81	84	37*	8	5	-12	603	583	15	8	6	4	146	236	21				
8	1	-18	116	58	33*	8	2	-3	324	287	9	8	3	12	61	41	57*	8	5	-11	391	388	13	8	6	5	1204	1241	16				
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8	1	-15	323	339	13	8	2	0	295	302	10	8	3	15	137	130	26*	8	5	-8	378	426	12	8	6	8	311	271	12				
8	1	-14	109	14	56*	8	2	1	623	662	15	8	3	16	41	150	60*	8	5	-7	382	361	11	8	6	9	529	531	14				
8	1	-13	52	16	45*	8	2	2	94	33	52*	8	3	17	245	231	17	8	5	-6	584	554	12	8	6	10	0	24	59*				
8	1	-12	0	153	61*	8	2	3	1244	1222	15	8	3	18	0	14	64*	8	5	-5	726	741	16	8	6	11	928	960	18				
8	1	-11	484	481	11	8	2	4	114	143	24*	8	3	19	215	229	20	8	5	-4	116	58	26*	8	6	12	124	101	27*				
8	1	-10	470	430	11	8	2	5	1715	1784	16	8	4	-19	73	140	60*	8	5	-3	309	284	12	8	6	13	0	11	57*				
8	1	-9	188	203	17	8	2	6	189	123	16	8	4	-18	401	416	14	8	5	-2	0	197	55*	8	6	14	249	217	15				
8	1	-8	69	51	40*	8	2	7	664	644	16	8	4	-17	281	289	17	8	5	-1	482	430	10	8	6	15	523	522	13				
8	1	-7	537	522	11	8	2	8	78	146	44*	8	4	-16	616	611	15	8	5	0	186	74	16	8	6	16	192	197	21				
8	1	-6	514	543	11	8	2	9	1131	1140	15	8	4	-15	286	290	17	8	5	1	984	998	15	8	6	17	472	481	13				
8	1	-5	366	375	9	8	2	10	319	294	12	8	4	-14	0	99	62*	8	5	2	417	358	10	8	6	18	0	56	66*				
8	1	-4	287	286	10	8	2	11	1217	1271	16	8	4	-13	160	162	26*	8	5	3	746	717	16	8	7	-18	57	56	71*				
8	1	-3	0	97	49*	8	2	12	85	24	46*	8	4	-12	1133	1121	18	8	5	4	252	323	15	8	7	-17	63	131	54*				
8	1	-2	552	526	14	8	2	13	396	387	11	8	4	-11	264	273	17	8	5	5	445	407	11	8	7	-16	324	329	17				
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8	1	0	194	163	12	8	2	15	714	747	14	8	4	-9	72	161	59*	8	5	7	508	528	12	8	7	-14	367	373	15				
8	7	-13	295	255	17	8	8	5	103	113	28*	8	10	-11	544	532	13	8	11	11	286	282	17	8	13	3	435	402	13				
8	7	-12	216	223	20	8	8	6	676	633	13	8	10	-10	217	191	22	8	11	12	41	38	62*	8	13	4	356	372	15				
8	7	-11	384	369	13	8	8	7	219	173	15	8	10	-9	60	11	65*	8	11	13	561	570	13	8	13	5	73	12	45*				
8	7	-10	409	414	13	8	8	8	0	20	57*	8	10	-8	381	394	15	8	11	14	0	76	68*	8	13	6	394	392	14				

8	7	-9	325	309	14	8	8	9	250	283	15	8	10	-7	421	424	13	8	11	15	263	283	20	8	13	7	309	345	17
8	7	-8	209	195	19	8	8	10	742	738	18	8	10	-6	345	348	15	8	11	16	100	6	43*	8	13	8	691	674	16
8	7	-7	361	367	13	8	8	11	125	21	26*	8	10	-5	824	821	20	8	12	-15	24	158	75*	8	13	9	311	328	16
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8	17	1	103	17	67*	9	1	-15	398	433	13	9	2	1	304	216	11	9	3	17	352	343	14	9	5	-2	557	627	13
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8	18	-5	134	121	75*	9	1	-4	1035	1015	14	9	2	12	94	3	34*	9	4	-10	530	544	13	9	5	9	295	265	13
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9	6	-12	0	136	69*	9	7	6	517	574	12	9	9	-9	431	418	14	9	10	13	0	15	66*	9	12	5	209	200	21
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9	6	-10	0	21	68*	9	7	8	571	521	13	9	9	-7	308	300	17	9	10	15	264	272	20	9	12	7	0	33	63*

9	6	-9	82	20	64*	9	7	9	765	819	18	9	9	-6	256	222	18	9	10	16	229	220	20	9	12	8	131	85	67*
9	6	-8	146	88	26*	9	7	10	70	7	57*	9	9	-5	234	233	19	9	11	-15	255	236	24	9	12	9	342	349	16
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9	6	-6	87	57	60*	9	7	12	415	408	12	9	9	-3	327	317	15	9	11	-13	325	329	19	9	12	11	304	289	17
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9	6	-4	58	47	42*	9	7	14	283	275	16	9	9	-1	75	38	62*	9	11	-11	217	250	25	9	12	13	110	144	56*
9	6	-3	93	138	59*	9	7	15	339	326	15	9	9	0	189	149	23	9	11	-10	277	244	19	9	12	14	137	151	69*
9	6	-2	216	213	16	9	7	16	28	47	63*	9	9	1	652	683	15	9	11	-9	593	586	15	9	13	-14	243	201	26
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9	6	0	176	220	20	9	8	-17	0	38	76*	9	9	3	537	565	14	9	11	-7	412	441	16	9	13	-12	241	195	26
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9	6	2	387	389	11	9	8	-15	0	19	73*	9	9	5	0	84	59*	9	11	-5	407	389	15	9	13	-10	277	289	22
9	6	3	292	410	14	9	8	-14	109	70	68*	9	9	6	648	610	14	9	11	-4	83	33	48*	9	13	-9	318	269	18
9	6	4	0	12	56*	9	8	-13	0	11	69*	9	9	7	635	619	15	9	11	-3	345	336	15	9	13	-8	187	187	29
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9	6	6	76	58	57*	9	8	-11	0	96	66*	9	9	9	200	240	20	9	11	-1	73	69	66*	9	13	-6	87	90	74*
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9	6	12	0	71	61*	9	8	-5	123	8	32*	9	9	15	127	76	31*	9	11	5	24	72	63*	9	13	0	89	8	55*
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9	14	-11	390	403	20	9	16	-2	365	368	17	10	0	16	497	508	11	10	2	-2	384	317	10	10	3	16	191	158	19
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9	14	-8	0	18	80*	9	16	1	0	90	75*	10	1	-17	138	10	28*	10	2	1	475	489	12	10	4	-18	374	389	17
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9	14	-6	356	322	17	9	16	3	190	208	28	10	1	-15	193	193	21	10	2	3	836	875	17	10	4	-16	468	471	13
9	14	-5	576	611	14	9	16	4	377	359	17	10	1	-14	215	240	20	10	2	4	340	243	13	10	4	-15	197	181	23
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9	14	-3	59	117	73*	9	16	6	435	437	16	10	1	-12	433	422	12	10	2	6	208	135	17	10	4	-13	118	60	35*
9	14	-2	371	392	17	9	16	7	96	31	70*	10	1	-11	236	255	19	10	2	7	402	412	12	10	4	-12	791	785	15
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9	15	-10	72	5	74*	9	17	5	99	60	53*	10	1	5	716	703	13	10	3	-14	271	280	18	10	4	4	853	975	18
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14	13	-3	0	63	83*	15	2	-4	278	251	18	15	4	2	106	11	58*	15	6	10	137	109	37*	15	9	4	0	89	78*
14	13	-2	0	134	84*	15	2	-3	102	25	56*	15	4	3	270	306	21	15	7	-10	129	33	76*	15	9	5	220	204	27
14	13	-1	185	212	40*	15	2	-2	0	143	59*	15	4	4	0	94	70*	15	7	-9	203	167	30	15	9	6	263	263	25
14	13	0	103	26	81*	15	2	-1	92	102	69*	15	4	5	121	147	41*	15	7	-8	137	124	76*	15	9	7	165	144	32*
14	13	1	144	207	87*	15	2	0	214	240	25	15	4	6	0	53	70*	15	7	-7	0	3	79*	15	9	8	307	271	20
14	13	2	124	164	84*	15	2	1	0	24	68*	15	4	7	421	432	16	15	7	-6	0	162	81*	15	10	-7	144	226	85*
14	13	3	0	20	82*	15	2	2	384	394	16	15	4	8	102	10	68*	15	7	-5	246	226	26	15	10	-6	0	134	89*
14	13	4	0	174	67*	15	2	3	57	10	67*	15	4	9	138	147	37*	15	7	-4	114	91	75*	15	10	-5	0	25	85*
15	0	-13	373	375	18	15	2	4	0	13	63*	15	4	10	56	14	70*	15	7	-3	171	167	32*	15	10	-4	316	291	23

15	0	-11	0	13	68*	15	2	5	0	29	69*	15	4	11	286	282	20	15	7	-2	227	169	25	15	10	-3	207	177	34*
15	0	-9	429	464	15	15	2	6	435	466	16	15	5	-12	156	163	44*	15	7	-1	128	109	74*	15	10	-2	0	114	83*
15	0	-7	295	314	18	15	2	7	107	61	59*	15	5	-11	126	58	74*	15	7	0	111	33	70*	15	10	-1	112	208	82*
15	0	-5	0	96	65*	15	2	8	480	499	15	15	5	-10	310	270	21	15	7	1	523	491	14	15	10	0	0	112	78*
15	0	-3	260	257	17	15	2	9	62	13	70*	15	5	-9	136	47	76*	15	7	2	375	395	18	15	10	1	189	106	29
15	0	-1	71	11	66*	15	2	10	116	74	69*	15	5	-8	122	159	63*	15	7	3	0	95	75*	15	10	2	235	280	29
15	0	1	371	388	15	15	2	11	14	30	67*	15	5	-7	0	63	73*	15	7	4	153	247	77*	15	10	3	248	214	24
15	0	3	82	179	67*	15	2	12	383	400	16	15	5	-6	224	204	26	15	7	5	154	157	36*	15	10	4	75	61	76*
15	0	5	246	271	21	15	3	-12	119	31	75*	15	5	-5	0	94	73*	15	7	6	0	3	76*	15	10	5	117	181	80*
15	0	7	687	692	17	15	3	-11	261	212	22	15	5	-4	354	392	18	15	7	7	358	340	18	15	10	6	0	163	78*
15	0	9	155	178	33*	15	3	-10	144	165	73*	15	5	-3	225	214	25	15	7	8	391	359	17	15	11	-6	260	285	31
15	0	11	339	323	17	15	3	-9	393	384	17	15	5	-2	0	163	75*	15	7	9	0	149	65*	15	11	-5	267	246	28
15	1	-13	100	102	62*	15	3	-8	212	160	24	15	5	-1	74	121	61*	15	7	10	291	245	20	15	11	-4	0	14	88*
15	1	-12	0	38	73*	15	3	-7	0	91	69*	15	5	0	285	258	20	15	8	-10	62	24	82*	15	11	-3	143	138	83*
15	1	-11	116	123	72*	15	3	-6	142	31	32*	15	5	1	311	336	18	15	8	-9	275	254	26	15	11	-2	325	314	24
15	1	-10	281	290	20	15	3	-5	130	210	72*	15	5	2	299	267	20	15	8	-8	134	145	48*	15	11	-1	81	124	64*
15	1	-9	239	262	22	15	3	-4	314	333	18	15	5	3	406	344	15	15	8	-7	124	8	78*	15	11	0	0	160	83*
15	1	-8	174	131	26	15	3	-3	353	355	16	15	5	4	58	64	49*	15	8	-6	216	155	29	15	11	1	298	328	25
15	1	-7	128	83	34*	15	3	-2	140	211	71*	15	5	5	198	138	25	15	8	-5	335	324	20	15	11	2	70	129	77*
15	1	-6	35	16	65*	15	3	-1	13	64	66*	15	5	6	211	235	27	15	8	-4	168	143	36*	15	11	3	102	52	81*
15	1	-5	175	163	26	15	3	0	0	22	71*	15	5	7	249	270	22	15	8	-3	427	397	17	15	11	4	274	279	25
15	1	-4	336	298	15	15	3	1	253	280	22	15	5	8	310	294	19	15	8	-2	132	186	76*	15	11	5	62	139	78*
15	1	-3	253	286	19	15	3	2	355	353	16	15	5	9	322	310	19	15	8	-1	124	4	74*	15	12	-2	153	171	65*
15	1	-2	137	128	31*	15	3	3	249	214	21	15	5	10	0	19	69*	15	8	0	216	202	28	15	12	-1	0	37	87*
15	1	-1	41	102	70*	15	3	4	195	191	25	15	5	11	83	64	59*	15	8	1	267	211	22	15	12	0	123	170	85*
15	1	0	82	157	69*	15	3	5	116	124	74*	15	6	-11	0	94	76*	15	8	2	197	131	29	15	12	1	136	143	79*
15	1	1	299	269	19	15	3	6	146	84	34*	15	6	-10	180	266	38*	15	8	3	225	252	26	15	12	2	111	71	78*
15	1	2	439	443	14	15	3	7	236	239	24	15	6	-9	26	59	77*	15	8	4	0	120	78*	16	0	-10	0	106	72*
15	1	3	277	371	20	15	3	8	327	329	18	15	6	-8	228	259	28	15	8	5	96	166	76*	16	0	-8	419	418	15
15	1	4	0	64	70*	15	3	9	158	155	33*	15	6	-7	244	241	25	15	8	6	158	111	35*	16	0	-6	541	527	13
15	1	5	55	4	65*	15	3	10	103	134	51*	15	6	-6	0	82	77*	15	8	7	297	270	20	16	0	-4	37	144	59*
15	1	6	320	303	17	15	3	11	105	96	55*	15	6	-5	0	21	76*	15	8	8	106	90	73*	16	0	-2	546	567	13
15	1	7	283	275	21	15	4	-12	168	242	85*	15	6	-4	435	435	16	15	8	9	136	61	73*	16	0	0	556	540	13
15	1	8	300	335	20	15	4	-11	0	156	68*	15	6	-3	0	124	73*	15	9	-9	131	41	80*	16	0	2	24	89	69*
15	1	9	193	202	26	15	4	-10	100	67	74*	15	6	-2	238	256	25	15	9	-8	142	46	84*	16	0	4	528	563	14
15	1	10	113	71	66*	15	4	-9	471	481	16	15	6	-1	294	287	19	15	9	-7	155	99	81*	16	0	6	441	463	16
15	1	11	152	69	30*	15	4	-8	65	107	74*	15	6	0	0	160	75*	15	9	-6	202	176	33	16	0	8	129	86	70*
16	0	10	544	569	14	16	3	0	111	101	44*	16	6	-3	220	202	27	16	10	0	139	9	72*	17	3	4	178	192	33*
16	1	-11	281	258	22	16	3	1	113	7	70*	16	6	-2	0	95	78*	16	10	1	219	200	31	17	3	5	97	27	76*
16	1	-10	125	111	74*	16	3	2	104	51	70*	16	6	-1	422	426	17	16	10	2	145	207	86*	17	3	6	208	191	30
16	1	-9	0	138	73*	16	3	3	115	154	71*	16	6	0	0	63	75*	17	0	-7	145	147	73*	17	3	7	309	274	19
16	1	-8	0	42	74*	16	3	4	209	209	28	16	6	1	287	288	22	17	0	-5	0	29	73*	17	4	-7	0	48	79*
16	1	-7	214	207	25	16	3	5	128	162	73*	16	6	2	0	68	75*	17	0	-3	94	106	71*	17	4	-6	196	160	33*
16	1	-6	269	241	20	16	3	6	175	144	29*	16	6	3	337	315	20	17	0	-1	39	11	73*	17	4	-5	90	60	79*
16	1	-5	143	140	36*	16	3	7	131	114	74*	16	6	4	0	150	79*	17	0	1	130	60	72*	17	4	-4	0	69	73*
16	1	-4	0	18	71*	16	3	8	133	152	40*	16	6	5	502	515	16	17	0	3	160	69	34*	17	4	-3	0	21	78*
16	1	-3	89	42	67*	16	3	9	145	244	73*	16	6	6	0	52	74*	17	0	5	0	124	75*	17	4	-2	82	210	82*
16	1	-2	102	165	60*	16	4	-10	85	107	79*	16	6	7	90	186	72*	17	0	7	147	148	77*	17	4	-1	0	41	74*
16	1	-1	194	182	26	16	4	-9	0	104	80*	16	6	8	142	99	39*	17	1	-8	279	263	22	17	4	0	256	167	23
16	1	0	191	137	28	16	4	-8	320	291	20	16	7	-8	124	43	82*	17	1	-7	215	175	25	17	4	1	111	176	65*
16	1	1	0	44	72*	16	4	-7	0	128	79*	16	7	-7	276	215	25	17	1	-6	90	160	77*	17	4	2	0	28	75*
16	1	2	0	98	70*	16	4	-6	515	535	15	16	7	-6	212	228	34	17	1	-5	347	312	18	17	4	3	84	20	58*
16	1	3	49	71	71*	16	4	-5	0	117	75*	16	7	-5	147	88	81*	17	1	-4	498	507	15	17	4	4	111	122	63*
16	1	4	176	195	30*	16	4	-4	92	127	62*	16	7	-4	0	107	78*	17	1	-3	335	329	18	17	4	5	225	183	27
16	1	5	0	74	71*	16	4	-3	124	66	70*	16	7	-3	300	294	23	17	1	-2	219	268	28	17	4	6	117	165	51*
16	1	6	0	13	75*	16	4	-2	400	382	16	16	7	-2	0	27	76*	17	1	-1	57	71	75*	17	5	-6	146	185	46*
16	1	7	171	137	30*	16	4	-1	74	50	73*	16	7	-1	172	187	35*	17	1	0	233	208	25	17	5	-5	0	185	80*
16	1	8	200	188	27	16	4	0	529	532	14	16	7	0	123	67	73*	17	1	1	308	350	22	17	5	-4	470	464	17
16	1	9	246	266	24	16	4	1	0	15	73*	16	7	1	0	151	77*	17	1	2	466	473	16	17	5	-3	241	186	25
16	1	10	231	213	25	16	4	2	45	28	73*	16	7	2	93	56	75*	17	1	3	426	425	17	17	5	-2	108	278	83*
16	2	-11	263	311	25	16	4	3	127	69	40*	16	7	3	263	262	25	17	1	4	208	225	27	17	5	-1	116	6	76*
16	2	-10	0	18	75*	16	4	4	456	455	16	16	7	4	290	245	22	17	1	5	0	44	77*	17	5	0	140	205	79*
16	2	-9	0	97	79*	16	4	5	0	7	72*	16	7	5	208	131	27	17	1	6	245	287	26	17	5	1	182	252	37*
16	2	-8	0	113	71*	16	4	6	433	444	17	16	7	6	92	144	58*	17	1	7	348	351	20	17	5	2	429	428	17
16	2	-7	481	510	15	16	4	7	0	64	75*	16	7	7	241	247	25	17	2	-8	0	167	82*	17	5	3	332	273	19
16	2	-6	82	66	61*	16	4	8	0	50	63*	16	8	-7	183	175	37*	17	2	-7	148	127	79*	17	5	4	229	260	29
16	2	-5	409	417	16	16	4	9	0	5	71*	16	8	-6	245	233	29	17	2	-6	0	25	75*	17	5	5	0	50	80*
16	2	-4	0	63	72*	16	5	-9	232	238	30	16	8	-5	0	30	82*	17	2	-5	145	103	73*	17	6	-5	130	186	83*
16	2	-3	167	166	31*	16	5	-8	246	228	25	16	8	-4	81	62	61*	17	2	-4	105	19	71*	17	6	-4	141	90	80*
16	2	-2	127	97	40*	16	5	-7	165	104	36*	16	8	-3	134	234	71*	17	2	-3	128	90	41*	17	6	-3	81	126	77*
16	2	-1	628	658	16	16	5	-6	73	165	77*	16	8	-2	243	266	28	17	2	-2	0	10	73*	17	6	-2	0	52	78*
16	2	0	62	20	70*	16	5	-5	209	227	29	16	8	-1	0	41	79*	17	2	-1	177	153	32*	17	6	-1	244	261	27
16	2	1	349	359	17	16	5	-4	234	216	25	16	8	0	314	316	22	17	2	0	0	66	76*	17	6	0	229	181	26
16	2	2	0	66	60*	16	5	-3	0	70	74*	16	8	1	117	53	71*	17	2	1	0	100	76*	17	6	1	96	92	67*
16	2	3	77	178	74*	16	5	-2	329	313	20	16	8	2	95	44	74*	17	2	2	110	99	57*	17	6	2	210	105	26
16	2	4	0	83	74*	16	5	-1	115	81	72*	16	8	3	0	178	82*	17	2	3	69	4	76*	17	6	3	141	57	75*
16	2	5	565	564	14	16	5	0	0	61	78*	16	8	4	399	408	19	17	2	4	129	164	76*	17	6	4	106	131	65*
16	2	6	133	34	69*	16	5	1	0	105	76*	16	8	5	0	40	81*	17	2	5	0	149	78*	17	7	-4	241	184	29
16	2	7	114	231	81*	16	5	2	122	114	62*	16	8	6	409	392	18	17	2	6	132	184	47*	17	7	-3	328	348	23
16	2	8	128	24	69*	16	5	3	50	96	52*	16	9	-5	107	188	65*	17	2	7	63	49	64*	17	7	-2	156	72	80*
16	2	9	282	275	21	16	5	4	245	237	24	16	9	-4	256	220	29	17	3	-8	339	353	21	17	7	-1	0	52	79*
16	2	10	171	58	30*	16	5	5	225	212	26	16	9	-3	62	56	81*	17	3	-7	0	127	83*	17	7	0	65	12	75*
16	3	-10	348	320	20	16	5	6	106	43	52*	16	9	-2	254	260	28	17	3	-6	133	10	77*	17	7	1	298	282	22
16	3	-9	0	32	75*	16	5	7	0	64	56*	16	9	-1	76	87	68*	17	3	-5	444	448	17	17	7	2	268	260	25
16	3	-8	64	64	73*	16	5	8	239	211	25	16	9	0	126	72	48*	17	3	-4	207	247	29	17	7	3	311	320	23
16	3	-7	174	165	34*	16	5	9	70	222	78*	16	9	1	137	119	44*	17	3	-3	442	434	16	18	0	-4	141	34	72*
16	3	-6	155	212	38*	16	6	-9	0	1	79*	16	9	2	248	246	27	17	3	-2	176	156	32*	18	0	-2	489	495	16
16	3	-5	152	44	33*	16	6	-8	149	193	82*	16	9	3	0	42	79*	17	3	-1	125	63	70*	18	0	0	585	601	15
16	3	-4	118	145	72*	16	6	-7	369	365	20	16	9	4	275	245	24	17	3	0	55	137	77*	18	0	2	112	50	76*
16	3	-3	206	247	28	16	6	-6	0	198	84*	16	10	-3	0	85	87*	17	3	1	319	321	20	18	1	-4	75	32	76*
16	3	-2	92	18	50*	16	6	-5	233	239	29	16	10	-2	145	181	50*	17	3	2	395	399	18	18	1	-3	30	137	78*
16	3	-1	222	250	26	16	6	-4	27	92	76*	16	10	-1	0	270	90*	17	3	3	478	484	16	18	1	-2	0	37	72*
18	1	-1	0	4	76*																								
18	1	0	0	46	78*																								
18	1	1	96	15	78*																								
18	1	2	0	129	79*																								
18	1	3	103	34	74*																								
18	2	-3	202	182	31																								
18	2	-2	110	69	65*																								
18	2	-1	564	573	16																								
18	2	0	107	35	59*																								
18	2	1	261	328	28																								
18	2	2	0	32	78*																								
18	3	-2	0	22	80*																								
18	3	-1	0	17	80*																								
18	3	0	26	32	75*																								
18	3	1	223	217	28																								

D. [Me_2SnCl_2(1,10-phenanthroline)].

Crystallographic Data and Refinement details for [Me_2SnCl_2(1,10-phenanthroline)].

Formula	$C_{14}H_{14}Cl_2N_2Sn$
Formula weight	399.9
Crystal morphology	colourless block
Crystal dimensions (mm)	0.10 x 0.13 x 0.31
Crystal system	orthorhombic
Space group	*Cmcm* (D_{2h}^{17}, No. 63)
Temperature (°C)	20.0
a (Å)	11.321(2)
b (Å)	18.889(1)
c (Å)	7.537(1)
V (Å^3)	1611.6(3)
Z	4
D_{calc} (g cm^{-3})	1.648
F(000)	784
Radiation	CuKα (λ = 1.5412Å)
μ (cm^{-1})	155.80
θ limits, data (°)	3.0 to 60.0
hkl range	0 to 6, 0 to 16, 0 to 17
Range of transmission factors	0.843 to 1.000
Scan technique	ω:2θ
Scan width (°)	1.00
No. of data measured	3280
No. of unique data	3280
Program for structure solution	Direct Methods (SHELXS86)
No. of unique data used	1391
No. of parameters	59
R	0.046
R_w	0.057
G.O.F.	3.34
Min./Max. residual electron density (e Å^{-3})	-1.07 to +0.56

Fractional atomic coordinates (Å^2) for the non-hydrogen atoms in [Me_2SnCl_2(1,10-phenathroline)].

Atom	*x*	*y*	*z*
Sn	0.0000	0.25358(3)	0.2500
Cl(1)	0.1780(3)	0.1734(1)	0.2500
N(1)	0.1189(11)	0.3578(3)	0.2500
C(1)	0.0000	0.2556(3)	0.525(1)
C(2)	0.2384(16)	0.3578(5)	0.2500
C(3)	0.3021(11)	0.4194(6)	0.2500
C(4)	0.2425(17)	0.4822(4)	0.2500
C(5)	0.1207(14)	0.4844(4)	0.2500
C(6)	0.0617(7)	0.4204(4)	0.2500
C(7)	0.0570(7)	0.5494(4)	0.2500

Fractional atomic coordinates and B_{eq} values (Å^2) for the hydrogen atoms in Me_2SnCl_2(1,10-phenanthroline)].

Atom	*x*	*y*	*z*	*B*eq
H(1a)	0	0.2075	0.5702	5.9
H(1b)	0.0692	0.2808	0.5668	3.9
H(2a)	0.2800	0.3129	0.2500	5.8
H(3a)	0.3878	0.4184	0.2500	7.4
H(4a)	0.2867	0.5262	0.2500	6.4
H(7a)	0.0996	0.5940	0.2500	4.0

Anisotropic thermal parameters (Å) for the non-hydrogen atoms in Me_2SnCl_2(1,10-phenanthroline)].

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Sn	0.0342(1)	0.0247(5)	0.0318(4)	0.0000	0.0000	0.0000
Cl(1)	0.064(2)	0.048(1)	0.100(2)	0.024(1)	0.000	0.000
N(1)	0.020(8)	0.031(5)	0.047(4)	0.011(5)	0.000	0.000
C(1)	0.069(1)	0.041(5)	0.046(5)	0.000	0.000	-0.001(3)
C(2)	0.024(1)	0.056(7)	0.099(8)	0.002(1)	0.000	0.000
C(3)	0.011(1)	0.061(8)	0.164(1)	-0.023(7)	0.000	0.000
C(4)	0.080(2)	0.026(6)	0.096(7)	-0.020(8)	0.000	0.000
C(5)	0.010(1)	0.043(7)	0.065(6)	-0.010(6)	0.000	0.000
C(6)	0.025(1)	0.026(4)	0.027(4)	-0.009(4)	0.000	0.000
C(7)	0.017(1)	0.027(5)	0.083(6)	-0.004(4)	0.000	0.000

Bond distances (Å) in [Me_2SnCl_2.(1,10-phenathroline)].

Atom - Atom	Distance	Atom - Atom	Distance
Sn - Cl(1)	2.521(3)	C(2) - C(3)	1.37(1)
Sn - Cl(1)'	2.521(3)	C(3) - C(4)	1.37(1)
Sn - N(1)	2.385(9)	C(4) - C(5)	1.38(1)
Sn - N(1)'	2.385(9)	C(5) - C(6)	1.38(1)
Sn - C(1)	2.075(8)	C(5) - C(7)	1.42(1)
Sn - C(1)'	2.075(8)	C(6) - C(6)'	1.40(2)
N(1) - C(2)	1.35(1)	C(7) - C(7)'	1.29(2)
N(1) - C(6)	1.348(9)		

' atom related by a crystallographic mirror plane

Bond angles (°) in [Me_2SnCl_2.(1,10-phenathroline)].

Atom - Atom - Atom	Angle	Atom - Atom - Atom	Angle
Cl(1) - Sn - Cl(1)'	106.1(1)	C(1) - Sn - C(1)'	177.8(4)
Cl(1) - Sn - N(1)	92.6(3)	Sn - N(1) - C(2)	124.3(6)
Cl(1) - Sn - N(1)'	161.3(3)	Sn - N(1) - C(6)	116.9(8)
Cl(1) - Sn - C(1)	90.7(1)	C(2) - N(1) - C(6)	118.8(8)
Cl(1) - Sn - C(1)'	90.7(1)	N(1) - C(2) - C(3)	122(1)
Cl(1)' - Sn - N(1)	161.3(3)	C(2) - C(3) - C(4)	119(1)
Cl(1)' - Sn - N(1)'	92.6(3)	C(3) - C(4) - C(5)	121(1)
Cl(1)' - Sn - C(1)'	90.7(1)	C(4) - C(5) - C(6)	117.1(9)
Cl(1)' - Sn - C(1)	90.7(1)	C(4) - C(5) - C(7)	122.1(9)
N(1) - Sn - N(1)'	68.7(5)	C(6) - C(5) - C(7)	121(1)
N(1) - Sn - C(1)	89.1(1)	N(1) - C(6) - C(5)	122.4(9)
N(1) - Sn - C(1)'	89.1(1)	N(1) - C(6) - C(6)'	118.7(6)
N(1) - Sn - C(1)	89.1(1)	C(5) - C(6) - C(6)'	118.9(7)
N(1) - Sn - C(1)'	89.1(1)	C(5) - C(7) - C(7)'	120.4(6)

' atom related by a crystallographic mirror plane

Observed and calculated structure factors for [Me_2SnCl_2(1,10-phenanthroline)].

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	-8	1000	792	20	0	6	6	560	509	14	0	-8	6	595	561	14	0	12	6	703	685	16	1	-11	4	402	397	10
0	0	-6	1542	1464	24	0	6	8	479	425	11	0	-8	5	211	207	9	0	14	-6	426	430	12	1	-11	5	743	758	15
0	0	-4	3055	3010	27	0	8	-6	575	561	15	0	-8	4	915	897	12	0	14	-5	302	294	14	1	-11	6	187	199	12
0	0	-2	4253	4878	34	0	8	-5	213	207	14	0	-8	3	418	426	10	0	14	-4	706	727	14	1	-11	7	554	567	14
0	-2	8	487	460	12	0	8	-4	882	897	14	0	-8	2	805	767	10	0	14	-3	490	474	12	1	-9	-7	578	549	14
0	-2	6	752	691	14	0	8	-3	390	426	8	0	-8	1	516	506	8	0	14	-2	775	804	14	1	-9	-6	158	147	23
0	-2	5	142	146	11	0	8	-2	758	767	10	0	-8	0	1160	1175	11	0	14	-1	532	544	10	1	-9	-5	749	738	17
0	-2	4	1153	1145	12	0	8	-1	496	506	9	0	-8	-1	504	506	9	0	14	0	1014	1017	15	1	-9	-4	280	285	9
0	-2	3	338	329	9	0	8	0	1111	1175	11	0	-8	-2	764	767	10	0	14	1	501	544	10	1	-9	-3	1146	1163	13
0	-2	2	796	743	8	0	8	1	501	506	8	0	-8	-3	396	426	9	0	14	2	744	804	13	1	-9	-2	285	303	7
0	0	2	4440	4878	35	0	8	2	777	767	10	0	-8	-4	892	897	14	0	14	3	453	474	12	1	-9	-1	1323	1356	13
0	0	4	3160	3010	26	0	8	3	427	426	8	0	-8	-5	201	207	15	0	14	4	724	727	15	1	-9	0	530	520	9
0	0	6	1570	1464	19	0	8	4	929	897	14	0	-8	-6	628	561	16	0	14	5	297	294	11	1	-9	1	1366	1356	13
0	0	8	806	792	16	0	8	5	208	207	13	0	-10	7	212	219	10	0	14	6	458	430	11	1	-9	2	292	303	8
0	2	-8	627	460	16	0	8	6	634	561	13	0	-10	6	664	661	14	0	16	-5	229	250	18	1	-9	3	1227	1163	13
0	2	-6	704	691	16	0	8	7	202	149	14	0	-10	5	402	403	9	0	16	-4	630	622	14	1	-9	4	267	285	8
0	2	-5	137	146	20	0	-2	1	620	599	7	0	-10	4	1120	1126	14	0	16	-3	449	437	12	1	-9	5	718	738	14
0	2	-4	1142	1145	15	0	-2	0	1665	1756	13	0	-10	3	798	787	12	0	16	-2	685	662	17	1	-9	6	151	147	13
0	2	-3	348	329	8	0	-2	-1	646	599	7	0	-10	2	1290	1273	13	0	16	-1	659	657	15	1	-9	7	537	549	13
0	2	-2	768	743	9	0	-2	-2	813	743	10	0	-10	1	972	1000	11	0	16	0	850	824	16	1	-7	-7	724	603	14
0	2	-1	608	599	6	0	-2	-3	362	329	8	0	-10	0	1655	1677	15	0	16	1	641	657	14	1	-7	-5	743	743	16
0	2	0	1671	1756	13	0	-2	-4	1183	1145	17	0	-10	-1	947	1000	11	0	16	2	673	662	15	1	-7	-4	207	207	9
0	2	1	596	599	7	0	-2	-6	854	691	17	0	-10	-2	1229	1273	13	0	16	3	422	437	10	1	-7	-3	1153	1139	13
0	2	2	798	743	10	0	-2	-8	593	460	15	0	-10	-3	748	787	12	0	16	4	594	622	12	1	-7	-2	155	147	7
0	2	3	339	329	8	0	-4	8	440	435	10	0	-10	-4	1110	1126	16	0	16	5	220	250	12	1	-7	-1	1128	1187	11
0	2	4	1111	1145	15	0	-4	6	626	618	13	0	-10	-5	437	403	11	1	-15	-5	409	375	12	1	-7	0	323	324	8
0	2	5	154	146	16	0	-4	5	245	251	8	0	-10	-6	769	661	15	1	-15	-3	553	539	12	1	-7	1	1194	1187	11
0	2	6	771	691	18	0	-4	4	1016	1013	12	0	-10	-7	229	219	16	1	-15	-1	570	589	14	1	-7	2	173	147	6
0	2	8	520	460	12	0	-4	3	549	535	9	0	10	-7	198	219	17	1	-15	1	572	589	14	1	-7	3	1195	1139	12
0	4	-8	578	435	15	0	-4	2	750	724	8	0	10	-6	627	661	15	1	-15	3	512	539	11	1	-7	4	207	207	8
0	4	-6	610	618	13	0	-4	1	1104	1060	10	0	10	-5	383	403	12	1	-15	5	378	375	9	1	-7	5	733	743	13
0	4	-5	229	251	14	0	-4	0	1631	1603	13	0	10	-4	1069	1126	15	1	-13	-6	254	222	15	1	-7	6	138	130	15
0	4	-4	1037	1013	14	0	-4	-1	1103	1060	10	0	10	-3	743	787	13	1	-13	-5	804	705	18	1	-7	7	592	603	14
0	4	-3	551	535	9	0	-4	-2	760	724	9	0	10	-2	1231	1273	13	1	-13	-4	369	341	10	1	-5	-7	635	599	14
0	4	-2	724	724	8	0	-4	-3	539	535	10	0	10	-1	950	1000	11	1	-13	-3	1084	1057	15	1	-5	-5	657	675	16
0	4	-1	1046	1060	9	0	-4	-4	1070	1013	15	0	10	0	1647	1677	15	1	-13	-2	325	328	8	1	-5	-3	1023	1030	11
0	4	0	1593	1603	13	0	-4	-5	252	251	14	0	10	1	933	1000	11	1	-13	-1	1205	1246	14	1	-5	-2	178	164	6
0	4	1	1055	1060	10	0	-4	-6	740	618	16	0	10	2	1265	1273	13	1	-13	0	483	475	12	1	-5	-1	834	856	9
0	4	2	738	724	9	0	-4	-7	165	76	24	0	10	3	776	787	13	1	-13	1	1207	1246	14	1	-5	1	906	856	9
0	4	3	543	535	10	0	-4	-8	519	435	13	0	10	4	1152	1126	15	1	-13	2	325	328	8	1	-5	2	164	164	6
0	4	4	1064	1013	14	0	-6	8	428	425	10	0	10	5	445	403	10	1	-13	3	1086	1057	14	1	-5	3	1056	1030	11
0	4	5	253	251	11	0	-6	6	496	509	11	0	10	6	691	661	17	1	-13	4	335	341	9	1	-5	5	660	675	12
0	4	6	702	618	18	0	-6	5	110	86	13	0	10	7	284	219	10	1	-13	5	716	705	14	1	-5	7	592	599	15
0	4	8	488	435	12	0	-6	4	711	725	11	0	12	-6	648	685	15	1	-13	6	191	222	11	1	-3	-7	693	611	17
0	6	-8	543	425	12	0	-6	3	173	165	7	0	12	-5	292	272	13	1	-11	-7	621	567	14	1	-3	-5	791	790	16
0	6	-6	490	509	12	0	-6	2	340	332	9	0	12	-4	1167	1170	17	1	-11	-6	193	199	22	1	-3	-4	155	148	10
0	6	-4	725	725	13	0	-6	1	439	417	8	0	12	-3	455	474	11	1	-11	-5	819	758	18	1	-3	-3	1496	1486	14
0	6	-3	174	165	8	0	-6	0	837	816	9	0	12	-2	1398	1426	15	1	-11	-4	392	397	9	1	-3	-2	479	452	8
0	6	-2	309	332	7	0	-6	-1	453	417	8	0	12	-1	541	540	12	1	-11	-3	1060	1120	14	1	-3	-1	1617	1605	13
0	6	-1	437	417	8	0	-6	-2	318	332	7	0	12	0	1733	1793	17	1	-11	-2	479	496	12	1	-3	0	585	541	10
0	6	0	797	816	9	0	-6	-3	160	165	9	0	12	1	529	540	11	1	-11	-1	1229	1291	13	1	-3	1	1739	1605	14
0	6	1	422	417	8	0	-6	-4	717	725	14	0	12	2	1414	1426	15	1	-11	0	734	736	11	1	-3	2	464	452	9
0	6	2	322	332	7	0	-6	-6	573	509	13	0	12	3	461	474	11	1	-11	1	1266	1291	13	1	-3	3	1498	1486	14
0	6	3	173	165	9	0	-6	-8	484	425	12	0	12	4	1192	1170	16	1	-11	2	512	496	11	1	-3	4	156	148	9
0	6	4	761	725	13	0	-8	7	156	149	14	0	12	5	271	272	12	1	-11	3	1082	1120	13	1	-3	5	783	790	13
1	-3	7	663	611	15	1	1	-5	1219	1132	18	1	9	-3	1173	1163	14	2	-16	5	211	224	10	2	-6	-3	219	205	7
1	-1	-7	843	817	20	1	1	-4	403	408	9	1	9	-2	289	303	7	2	-14	-6	452	386	11	2	-6	-2	1974	1959	17
1	-1	-5	1164	1132	21	1	1	-3	2161	2122	18	1	9	-1	1376	1356	13	2	-14	-5	238	222	15	2	-6	-1	192	203	5
1	-1	-4	425	408	10	1	1	-2	801	740	9	1	9	0	538	520	11	2	-14	-4	633	603	13	2	-6	0	2632	2815	21
1	-1	-3	2169	2122	19	1	1	-1	2612	2476	21	1	9	1	1358	1356	13	2	-14	-3	330	338	9	2	-6	1	189	203	6
1	-1	-2	782	740	8	1	1	0	927	1044	13	1	9	2	295	303	7	2	-14	-2	615	611	13	2	-6	2	1890	1959	16
1	-1	-1	2529	2476	20	1	1	1	2180	2476	18	1	9	3	1223	1163	14	2	-14	-1	331	351	8	2	-6	3	216	205	6
1	-1	0	1096	1044	10	1	1	2	802	740	12	1	9	4	277	285	10	2	-14	0	852	797	13	2	-6	4	1574	1599	15
0	-12	6	693	685	14	1	1	3	2194	2122	20	1	9	5	777	738	16	2	-14	1	347	351	9	2	-6	5	125	114	13
0	-12	5	270	272	10	1	1	4	457	408	11	1	9	6	150	147	20	2	-14	2	599	611	13	2	-6	6	858	893	14
0	-12	4	1188	1170	15	1	1	5	1213	1132	16	1	9	7	576	549	12	2	-14	3	339	338	8	2	-6	8	603	556	15
0	-12	3	471	474	9	1	1	6	213	215	14	1	11	-7	474	567	11	2	-14	4	585	603	15	2	-4	-8	507	478	11
0	-12	2	1462	1426	15	1	1	7	887	817	17	1	11	-6	159	199	24	2	-14	5	208	222	11	2	-4	-6	680	735	17
0	-12	1	542	540	11	1	3	-7	533	611	13	1	11	-5	741	758	19	2	-14	6	399	386	10	2	-4	-5	227	234	11
0	-12	0	1737	1793	16	1	3	-5	796	790	15	1	11	-4	390	397	10	2	-12	-6	527	482	13	2	-4	-4	1298	1304	15
0	-12	-1	528	540	11	1	3	-4	171	148	9	1	11	-3	1085	1120	15	2	-12	-4	699	708	16	2	-4	-3	571	558	10
0	-12	-2	1409	1426	15	1	3	-3	1507	1486	14	1	11	-2	488	496	12	2	-12	-3	128	144	14	2	-4	-2	1412	1392	13
0	-12	-3	479	474	11	1	3	-2	508	452	9	1	11	-1	1273	1291	14	2	-12	-2	620	642	12	2	-4	-1	920	913	9
0	-12	-4	1233	1170	17	1	3	-1	1687	1605	14	1	11	0	767	736	12	2	-12	-1	144	88	10	2	-4	0	2320	2337	19
0	-12	-5	263	272	16	1	3	0	607	541	13	1	11	1	1272	1291	14	2	-12	0	824	833	12	2	-4	1	931	913	9
0	-12	-6	815	685	19	1	3	1	1716	1605	15	1	11	2	518	496	12	2	-12	2	625	642	11	2	-4	2	1360	1392	12
0	-14	6	453	430	10	1	3	2	445	452	9	1	11	3	1132	1120	15	2	-12	3	102	144	16	2	-4	3	569	558	9
0	-14	5	292	294	9	1	3	3	1382	1486	15	1	11	4	387	397	9	2	-12	4	683	708	14	2	-4	4	1295	1304	14
0	-14	4	714	727	15	1	3	4	157	148	14	1	11	5	785	758	17	2	-12	5	120	104	15	2	-4	5	225	234	9
0	-14	3	466	474	11	1	3	5	809	790	16	1	11	6	209	199	13	2	-12	6	474	482	10	2	-4	6	756	735	14
0	-14	2	751	804	13	1	3	7	668	611	17	1	11	7	560	567	11	2	-10	-6	615	586	14	2	-4	8	517	478	11
0	-14	1	516	544	13	1	5	-7	491	599	13	1	13	-6	176	222	23	2	-10	-5	128	98	19	2	-2	-6	612	648	13
0	-14	0	1016	1017	14	1	5	-5	673	675	15	1	13	-5	708	705	14	2	-10	-4	952	981	16	2	-2	-5	129	120	15
0	-14	-1	523	544	13	1	5	-3	1035	1030	11	1	13	-4	355	341	11	2	-10	-3	182	161	10	2	-2	-4	1165	1102	14
0	-14	-2	748	804	14	1	5	-2	195	164	6	1	13	-3	1075	1057	16	2	-10	-2	1010	1072	12	2	-2	-3	156	131	7
0	-14	-3	483	474	11	1	5	-1	887	856	10	1	13	-2	348	328	9	2	-10	-1	313	317	7	2	-2	-2	969	943	10
0	-14	-4	758	727	18	1	5	0	118	48	13	1	13	-1	1235	1246	15	2	-10	0	1394	1432	14	2	-2	0	1895	1944	16
0	-14	-5	335	294	13	1	5	1	902	856	10	1	13	0	497	475	10	2	-10	1	328	317	8	2	-2	1	96	43	14
0	-14	-6	533	430	12	1	5	2	165	164	9	1	13	1	1242	1246	15	2	-10	2	1047	1072	12	2	-2	2	1064	943	11
0	-16	5	240	250	10	1	5	3	1047	1030	13	1	13	2	347	328	9	2	-10	3	176	161	9	2	-2	3	147	131	9
0	-16	4	609	622	14	1	5	5	680	675	15	1	13	3	1077	1057	16	2	-10	4	941	981	13	2	-2	4	1181	1102	14
0	-16	3	447	437	11	1	5	7	654	599	16	1	13	4	313	341	11	2	-10	6	578	586	14	2	-2	5	151	120	13
0	-16	2	695	662	14	1	7	-7	779	603	18	1	13	5	695	705	17	2	-8	-6	642	606	14	2	-2	6	680	648	15
0	-16	1	675	657	14	1	7	-6	173	130	18	1	13	6	203	222	12	2	-8	-5	176	184	15	2	-2	8	476	448	10
0	-16	0	836	824	15	1	7	-5	721	743	16	1	15	-5	395	375	13	2	-8	-4	1071	1044	15	2	0	-8	370	501	13
0	-16	-1	657	657	15	1	7	-4	209	207	10	1	15	-3	571	539	13	2	-8	-3	300	307	8	2	0	-6	717	664	17
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4	-12	2	659	672	13	4	-2	0	1653	1677	15	4	8	0	1260	1246	15	5	-13	-3	890	872	16	5	-5	3	886	896	13
4	-12	3	219	213	10	4	-2	1	204	203	8	4	8	1	175	169	11	5	-13	-2	150	130	15	5	-5	5	620	631	15
4	-12	4	701	672	14	4	-2	2	1093	1085	12	4	8	2	929	899	13	5	-13	-1	995	996	15	5	-5	7	489	518	10
4	-12	5	141	133	15	4	-2	4	1182	1103	15	4	8	3	184	164	12	5	-13	0	229	195	11	5	-3	-5	848	868	19

5	-3	-4	172	171	17	5	5	1	1001	911	14	5	15	-3	963	900	20	6	-8	5	212	242	12	6	2	6	654	704	14
5	-3	-3	1380	1387	17	5	5	2	104	76	14	5	15	-2	172	111	19	6	-8	6	425	433	11	6	4	-6	404	537	16
5	-3	-2	334	329	8	5	5	3	919	896	13	5	15	-1	1036	1045	18	6	-6	-6	545	429	13	6	4	-4	836	837	16
5	-3	-1	1672	1670	16	5	5	5	609	631	14	5	15	0	159	173	18	6	-6	-4	717	672	13	6	4	-3	269	277	16
5	-3	0	403	432	9	5	5	7	446	518	9	5	15	1	1126	1045	17	6	-6	-3	127	131	19	6	4	-2	862	832	18
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5	-3	2	322	329	8	5	7	-5	440	517	14	5	15	3	885	900	14	6	-6	-1	153	189	13	6	4	0	1187	1112	15
5	-3	3	1411	1387	15	5	7	-4	198	205	21	5	15	4	149	155	12	6	-6	0	941	899	13	6	4	1	450	415	11
5	-3	4	178	171	12	5	7	-3	689	701	18	6	-16	-3	218	215	13	6	-6	1	174	189	12	6	4	2	830	832	13
5	-3	5	894	868	15	5	7	-2	159	201	17	6	-16	-2	494	520	12	6	-6	2	638	649	13	6	4	3	262	277	8
5	-3	7	568	626	14	5	7	-1	696	675	14	6	-16	-1	172	211	15	6	-6	3	164	131	13	6	4	4	825	837	14
5	-1	-5	807	818	17	5	7	0	225	204	10	6	-16	0	609	644	12	6	-6	4	676	672	15	6	4	6	495	537	13
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5	-1	1	1582	1527	16	5	7	6	140	123	12	6	-14	0	1053	1070	16	6	-4	-2	869	832	15	6	6	1	178	189	12
5	-1	2	699	677	12	5	7	7	382	451	9	6	-14	2	892	870	15	6	-4	-1	401	415	10	6	6	2	638	649	13
5	-1	3	1334	1314	15	5	9	-6	273	176	18	6	-14	4	690	743	14	6	-4	0	1168	1112	14	6	6	3	143	131	12

5	-1	4	390	365	9
5	-1	5	844	818	15
5	-1	6	162	175	15
5	-1	7	527	582	14
5	1	-7	228	582	25
5	1	-5	753	818	20
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5	1	-3	1246	1314	19
5	1	-2	650	677	12
5	1	-1	1469	1527	16
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5	1	1	1530	1527	16
5	1	2	641	677	12
5	1	3	1269	1314	15
5	1	4	363	365	9
5	1	5	802	818	14
5	1	6	151	175	15
5	1	7	518	582	13
5	3	-7	528	626	14
5	3	-5	777	868	19
5	3	-3	1430	1387	19
5	3	-2	320	329	11
5	3	-1	1735	1670	18
5	3	0	410	432	9
5	3	1	1761	1670	17
5	3	2	328	329	8
5	3	3	1392	1387	15
5	3	4	159	171	13
5	3	5	845	868	15
5	3	7	540	626	13
5	5	-7	661	518	14
5	5	-5	543	631	13
5	5	-3	891	896	17
5	5	-1	927	911	14
5	5	0	156	114	16
6	12	2	948	904	15
6	12	3	274	252	10
6	12	4	735	757	14
6	12	5	137	162	12
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6	14	0	1066	1070	17
6	14	2	908	870	15
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6	16	-1	201	211	15
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6	16	2	506	520	10
6	16	3	194	215	9

5	9	-5	465	517	14
5	9	-4	324	352	16
5	9	-3	781	764	19
5	9	-2	481	475	13
5	9	-1	886	839	15
5	9	0	626	583	15
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5	9	2	494	475	10
5	9	3	801	764	14
5	9	4	378	352	9
5	9	5	520	517	11
5	9	6	166	176	11
5	11	-6	179	183	23
5	11	-5	536	576	13
5	11	-4	370	360	15
5	11	-3	894	851	20
5	11	-2	533	478	13
5	11	-1	1005	941	16
5	11	0	629	608	16
5	11	1	1051	941	16
5	11	2	511	478	11
5	11	3	937	851	15
5	11	4	387	360	10
5	11	5	570	576	14
5	11	6	175	183	10
5	13	-5	554	578	14
5	13	-3	902	872	20
5	13	-1	1040	996	17
5	13	0	213	195	14
5	13	1	1075	996	16
5	13	2	166	130	14
5	13	3	906	872	15
5	13	4	194	154	11
5	13	5	550	578	13
5	15	-4	196	155	22

6	-12	-5	159	162	19
6	-12	-4	748	757	18
6	-12	-3	272	252	12
6	-12	-2	965	904	16
6	-12	-1	300	297	10
6	-12	0	1139	1144	16
6	-12	1	339	297	9
6	-12	2	952	904	15
6	-12	3	292	252	10
6	-12	4	743	757	15
6	-12	5	176	162	11
6	-10	-6	401	453	9
6	-10	-5	211	251	16
6	-10	-4	742	693	17
6	-10	-3	421	376	11
6	-10	-2	773	715	15
6	-10	-1	472	467	10
6	-10	0	987	922	14
6	-10	1	475	467	12
6	-10	2	757	715	14
6	-10	3	405	376	10
6	-10	4	715	693	15
6	-10	5	240	251	11
6	-10	6	420	453	9
6	-8	-6	527	433	12
6	-8	-5	211	242	17
6	-8	-4	646	623	14
6	-8	-3	443	428	10
6	-8	-2	594	553	15
6	-8	-1	584	614	14
6	-8	0	732	743	13
6	-8	1	659	614	13
6	-8	2	565	553	14
6	-8	3	433	428	11
6	-8	4	628	623	15

6	-4	1	432	415	11
6	-4	2	848	832	13
6	-4	3	272	277	8
6	-4	4	844	837	15
6	-4	6	528	537	11
6	-2	-6	596	704	15
6	-2	-4	1207	1204	21
6	-2	-3	425	423	11
6	-2	-2	1446	1441	18
6	-2	-1	619	584	14
6	-2	0	1812	1876	18
6	-2	1	649	584	14
6	-2	2	1405	1441	16
6	-2	3	402	423	9
6	-2	4	1171	1204	16
6	-2	5	206	219	12
6	-2	6	637	704	15
6	0	-6	431	527	18
6	0	-4	905	898	18
6	0	-2	956	956	17
6	0	0	1238	1293	16
6	0	2	915	956	14
6	0	4	865	898	14
6	0	6	527	527	10
6	2	-6	532	704	16
6	2	-4	1191	1204	24
6	2	-3	425	423	13
6	2	-2	1417	1441	19
6	2	-1	621	584	15
6	2	0	1805	1876	18
6	2	1	644	584	14
6	2	2	1362	1441	15
6	2	3	418	423	10
6	2	4	1152	1204	15
6	2	5	201	219	11

6	6	4	668	672	13
6	6	5	102	107	16
6	6	6	383	429	10
6	8	-6	689	433	17
6	8	-5	269	242	18
6	8	-4	617	623	14
6	8	-3	426	428	13
6	8	-2	572	553	13
6	8	-1	613	614	12
6	8	0	809	743	15
6	8	1	661	614	15
6	8	2	571	553	14
6	8	3	422	428	10
6	8	4	594	623	15
6	8	5	203	242	11
6	8	6	393	433	9
6	10	-6	346	453	14
6	10	-5	252	251	20
6	10	-4	711	693	17
6	10	-3	414	376	13
6	10	-2	791	715	19
6	10	-1	493	467	11
6	10	0	981	922	16
6	10	1	507	467	12
6	10	2	758	715	14
6	10	3	392	376	9
6	10	4	702	693	14
6	10	5	253	251	8
6	10	6	391	453	9
6	12	-4	795	757	17
6	12	-3	271	252	19
6	12	-2	1006	904	19
6	12	-1	319	297	12
6	12	0	1168	1144	17
6	12	1	337	297	10

Chapter 4

Examination of the Effect of Crystal Packing Forces on Geometric Parameters: A Crystallographic and Theoretical Study of Diimine Adducts of R_2SnCl_2

Chapter 4 (Section I)

Examination of the Effect of Crystal Packing Forces on Geometric Parameters: A Crystallographic and Theoretical Study of 2,2'-Bipyridyl Adducts of R_2SnCl_2

4.1 Introduction

This chapter reports crystal structure determinations for a series of diimine adducts of diorganotindichlorides; R_2SnCl_2(2,2'-bipyridyl) (Section I of this chapter) and R_2SnCl_2(1,10-phenanthroline) (Section II of this chapter) and the correlation of the variation in the Sn-ligand parameters with the Lewis acidity of the tin atom. The influence of solid state effects (i.e. intermolecular forces or crystal packing effects) on molecular geometry has been determined by comparing the crystallographic results with those calculated (employing *ab initio* molecular orbital theory) for the theoretical gas phase structures. It has been shown by this combined study that intermolecular forces do indeed influence the Sn-ligand parameters in the crystalline state.

As indicated in chapter 1 and 3, it is likely that a subtle combination of electronic and/or steric effects of the tin metal centre and/or ligand and intermolecular forces i.e. crystal packing effects are operating in organotin systems giving rise to the structural diversity that is know to exist [1]. Different coordination geometries and even coordination numbers may be found even when only small changes in a remote organic substituent are made. A related phenomenon has been highlighted in recent surveys of the variation of crystallographically determined geometric parameters for transition metal complexes [2,3]. The conclusion of these studies is that crystal packing effects may exert an influence on metal-ligand parameters, even in heavy element-containing complexes.

Our previous work [4] has indicated that a joint crystallographic/theoretical approach is a potent combination to study the influence of crystal packing on molecular geometry and hence, geometric parameters about a heavy element center. A hindrance to systematic studies of this type is the non-availability of suitable crystals for X-ray structure analysis [5]. This obstacle has been overcome in the present study as suitable crystals of diimine adducts of diorganotindichlorides; R_2SnCl_2(2,2'-bipyridyl) and R_2SnCl_2(1,10-phenanthroline) have been obtained. In section I, crystals of R_2SnCl_2(2,2'-bipyridyl), R = Me, ^nBu, ^iPr and Bz, have been obtained, characterised

crystallographically and their derived interatomic parameters compared with three literature structures, i.e. R = Vin [4], Ph/Me [4], and Ph (two polymorphs) [6,7]. In Section II of this chapter we look at R_2SnCl_2(1,10-phenanthroline) adducts.

Thus, seven R_2SnCl_2(2,2'-bipyridyl) structures, representing a broad range of diorganotin centers, are available for systematic analysis. The availability of a series of closely related R_2SnCl_2(2,2'-bipyridyl) structures enables an investigation of the influence of moderating the Lewis acidity of the diorganotin center (i.e. by varying the nature of R) upon geometric parameters about the tin centers (primarily Sn-Cl and Sn-N distances) in the crystalline state, i.e. an electronic factor. The "crystal packing effects" factor can be removed by employing *ab initio* theoretical methods to investigate molecular structure of the isolated gas-phase molecules. To this end, geometry optimisations have been conducted on the same series of R_2SnCl_2(2,2'-bipyridyl) compounds and these results compared with the crystallographically determined structures. This study will enable the determination of the influence of both Lewis Acidity and intermolecular forces in the crystalline state on the geometric parameters in the R_2SnCl_2(2,2'-bipyridyl) adducts.

The calculations reported in this chapter have been conducted at the Hartree-Fock (HF) level of theory. Recent work [4, 8, 9] has shown that for studies examining molecular geometries of heavy metal-containing species, HF is an appropriate theoretical approach. Although the HF approach does not take into account electron correlation in the geometry optimisations, it has been shown that good agreement between theory and experiment is obtained [4, 8, 9].

4.2 Results

Details of the experimental procedure employed in the synthesis of the compounds reported in this chapter are provided in Chapter 2. Spectroscopic characterizations are also provided in Chapter 2.

4.2.1. Crystallographic Studies

A series of structurally similar molecules, R_2SnCl_2(2,2'-bipyridyl), as determined by X-ray crystallography, are described and then compared to analogous literature structures.

The experimental procedure employed in the data collection and the structure determinations is described in Chapter 2. Presented below are the experimental details unique to the R_2SnCl_2(2,2'-bipyridyl) adducts which are crystallographically examined in this chapter. A summary of each structures crystallographic data is detailed in Table 4.1. Crystal data and refinement details specific for these molecular structure determinations are provided in Appendix A of this chapter. All diagrams are drawn with ORTEP [10] at the 35% probability level.

In this section, the crystal and molecular structures of four R_2SnCl_2(2,2'-bipyridyl) R = Me, ^{n}Bu, ^{i}Pr and Bz, compounds are described; brief comments on three literature structures R = Ph [6,7], Vin [4] and Ph/Me [4] are also given. Selected interatomic parameters for all crystal structures described herein are collected in Table 4.2. A summary of, and a conclusion based on, the crystallographic studies is given in section 4.3.1.

TABLE 4.1: Crystallographic Data for R_2SnCl_2(2,2'-bipyridyl) for R=Me, ^{n}Bu, ^{i}Pr and Bz

	R_2SnCl_2(2,2'-bipyridyl)			
Crystallographic Data	**R = Me**	**R = ^{n}Bu**	**R = ^{i}Pr**	**R = Bz**
Formula	$C_{12}H_{14}Cl_2N_2Sn$	$C_{18}H_{26}Cl_2N_2Sn$	$C_{16}H_{22}Cl_2N_2Sn$	$C_{24}H_{22}Cl_2N_2Sn$
Formula weight	375.9	460.0	432.0	528.1
Crystal system	Monoclinic	monoclinic	monoclinic	triclinic
Space group	*C*2/*c*	*P*2$_1$/*n*	*P*2$_1$/*n*	$P\bar{1}$
a, Å	6.633(6)	9.521(1)	9.415(4)	10.547(3)
b, Å	16.99(1)	16.364(3)	15.049(5)	13.152(3)
c, Å	13.211(8)	13.771(2)	13.082(4)	9.363(2)
α, (°)	90	90	90	98.66(2)
β, (°)	104.5(1)	105.20(1)	91.28(3)	111.74(2)
γ, (°)	90	90	90	67.71(2)
V, Å^3	1441(2)	2070.6(5)	1853(1)	1116.1(5)
Z	4	4	4	2
D_{calcd}, g cm^{-3}	1.731	1.476	1.548	1.571
Radiation, Å	Mo, 0.7107	Cu, 1.5418	Mo, 0.7107	Mo, 0.7107
μ, cm^{-1}	21.22	121.97	16.62	14.02
Trans coeff	0.992 – 1	0.908 - 1	0.919 - 1	0.969 - 1
2θ range, (°)	6.0 - 55.0	6.0 - 120.0	6.0 - 55.0	6.0 - 55.0
No. reflns meas	3461	3425	4704	5415
No. unique reflns	3317	3212	4446	5137
No of reflns used [a]	2953	2079	1650	4403
No. of variables	78	209	190	262
R	0.022	0.052	0.049	0.028
R_W	0.028	0.055	0.044	0.031
Residual e$^-$/Å^3	0.29	1.05	0.77	0.55

[a] $I \geq 3.0\sigma(I)$

TABLE 4.2: Crystallographically Determined Interatomic Parameters (Å, deg.) for R_2SnCl_2(2,2'-bipyridyl) for R= Me, ^nBu, ^iPr, Bz Ph [7,8], Vin [5] and the mixed species Ph(Me) [5].

	R_2SnCl_2(2,2'-bipyridyl)								
Bond Distance	R = Me [a] (y = 1')	R = ^nBu (y = 5)	R = ^iPr (y = 4)	R= Ph/Me (y = C(Ph))		R= Bz (y = 8)	R= Ph (y = 7)		R= Vin (y = 3)
				Molecule *a*	Molecule *b*		Monoclinic	Tetragonal	
Sn-Cl(1)	2.532(1)	2.573(4)	2.569(4)	2.488(2)	2.500(2)	2.504(1)	2.511(2)	2.478(2)	2.529(1)
Sn-Cl(2)	2.532(1)	2.490(3)	2.546(3)	2.492(2)	2.481(2)	2.525(1)	2.508(2)	2.468(2)	2.463(1)
Sn-N(1)	2.396(2)	2.397(9)	2.400(9)	2.389(5)	2.388(5)	2.383(2)	2.345(6)	2.325(5)	2.360(3)
Sn-N(2)	2.396(2)	2.404(7)	2.377(9)	2.401(5)	2.391(5)	2.372(2)	2.376(6)	2.333(5)	2.396(3)
Sn-C(1)	2.118(2)	2.13(1)	2.13(1)	2.139(7)	2.110(8)	2.165(3)	2.151(7)	2.102(7)	2.119(3)
Sn-C(y)	2.118(2)	2.11(1)	2.18(2)	2.154(7)	2.142(7)	2.166(3)	2.153(8)	2.114(7)	2.119(4)
Bond Angle									
Cl(1)-Sn-Cl(2)	104.83(4)	104.6(1)	106.1(1)	101.89(7)	103.14(7)	104.37(3)	103.47(7)	105.81(8)	104.74(3)
Cl(1)-Sn-N(1)	162.06(4)	163.2(2)	160.7(2)	161.7(1)	164.7(1)	162.05(6)	161.0(1)	163.4(1)	161.50(7)
Cl(1)-Sn-N(2)	93.11(5)	95.0(2)	93.6(2)	93.1(1)	95.5(1)	93.54(6)	92.0(1)	94.0(2)	92.47(7)
Cl(1)-Sn-C(1)	90.46(8)	85.8(4)	90.3(4)	93.7(2)	90.1(3)	90.33(8)	92.9(2)	89.2(2)	89.71(9)
Cl(1)-Sn-C(y)	92.08(8)	90.1(4)	91.2(4)	93.2(2)	91.4(2)	91.27(8)	92.3(2)	90.9(2)	89.2(1)
Cl(2)-Sn-N(1)	93.11(5)	92.2(2)	92.9(2)	96.4(1)	92.2(1)	93.29(6)	95.6(1)	90.8(2)	93.72(7)
Cl(2)-Sn-N(2)	162.06(4)	160.4(2)	160.2(2)	165.0(1)	161.3(1)	162.08(6)	164.5(1)	160.2(1)	162.79(7)
Cl(2)-Sn-C(1)	92.08(8)	93.8(3)	88.8(4)	91.7(2)	93.1(3)	92.24(9)	92.4(2)	91.3(2)	94.2(1)
Cl(2)-Sn-C(y)	90.46(8)	95.5(3)	88.6(4)	91.4(2)	92.9(2)	87.70(8)	90.2(2)	91.0(2)	94.3(1)
N(1)-Sn-N(2)	68.96(8)	68.2(3)	67.4(3)	68.5(2)	69.2(2)	68.88(8)	69.0(2)	69.4(2)	69.1(1)
N(1)-Sn-C(1)	88.77(8)	93.4(4)	93.1(5)	85.2(2)	88.5(3)	92.2(1)	85.5(2)	89.9(2)	90.2(1)
N(1)-Sn-C(y)	87.80(8)	88.0(4)	86.2(4)	86.9(2)	88.4(2)	86.2(1)	88.3(2)	89.3(2)	88.1(1)
N(2)-Sn-C(1)	87.80(8)	86.7(4)	89.4(5)	86.9(2)	85.6(3)	86.9(1)	87.0(3)	88.7(2)	85.4(1)
N(2)-Sn-C(y)	88.77(8)	85.1(4)	92.8(4)	88.1(2)	87.7(2)	92.6(1)	88.9(2)	88.9(2)	86.1(1)
C(1)-Sn-C(y)	175.8(1)	170.5(5)	177.2(6)	171.8(3)	173.3(3)	178.4(1)	173.5(3)	177.6(2)	171.4(2)

[a] molecule has crystallographic two-fold symmetry

4.2.1a. [Me_2SnCl_2(2,2'-bipyridyl)]

Transparent crystals were obtained from the slow evaporation of an acetonitrile/chloroform (9/1 *v/v*) solution of [Me_2SnCl_2(2,2'-bipyridyl)]; melting point: 235-237°C.

The molecular structure of [Me_2SnCl_2(2,2'-bipyridyl)], with crystallographically imposed twofold symmetry, is shown in Figure 4.1. The tin atom approximates an octahedral geometry with the organic substituents occupying axial positions above and below the equatorial plane that is defined by a N_2Cl_2 donor set. There are no non-hydrogen interactions in the lattice < 3.6 Å, however, short Cl...H contacts are noted with Cl(1)...H(4)^{i} of 2.86 Å being the shortest (symmetry operation *i*: -0.5 - *x*, -0.5 + *y*, 0.5 - *z*). The basic structural motif found for [Me_2SnCl_2(2,2'-bipyridyl)] is found in all other structures described in this chapter. The molecular structures of [$^{n}Bu_2SnCl_2$(2,2'-bipyridyl)], [$^{i}Pr_2SnCl_2$(2,2'-bipyridyl)] and [Bz_2SnCl_2(2,2'-bipyridyl)] are shown in Figures 4.2, 4.3 and 4.4, respectively; in each of these examples there is no crystallographically imposed symmetry.

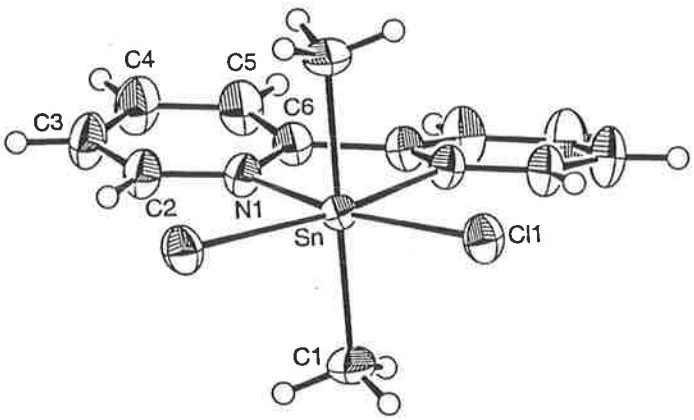


Figure 4.1
The molecular structure of [Me_2SnCl_2(2,2'-bipyridyl)]

4.2.1b [$^nBu_2SnCl_2$(2,2'-bipyridyl)]

White crystals were obtained from the slow evaporation of an acetonitrile/chloroform (4/1 *v/v*) solution of [$^nBu_2SnCl_2$(2,2'-bipyridyl)]; melting point: 180 - 181 °C.

The molecular structure of [$^nBu_2SnCl_2$(2,2'-bipyridyl)] is shown in Figure 4.2. In the lattice of [$^nBu_2SnCl_2$(2,2'-bipyridyl)], the closest non-hydrogen contact of 3.57(2) Å occurs between the C(15) and C(16)^i atoms (symmetry operation *i*: 1 - x, - y, - z) and is one of a number of contacts associated with base stacking between isolated pairs of 2,2'-bipyridyl residues. A key feature of the molecular structure is the large disparity in the Sn-Cl bond distances, i.e. Sn-Cl(1) is 2.573(4) Å and Sn-Cl(2) is 2.490(3) Å; the Sn-N distances are equal within experimental error. Using similar arguments invoked in an earlier contribution [5], and by others [11], the disparity may be traced to three close Cl(1)...H intermolecular contacts less than 3.1 Å (Cl(1)...H(15)^{ii} 2.67 Å, Cl(1)...H(12)^{ii} 2.87 Å, and Cl(1)...H(10)^{iii} 3.03 Å; *ii*: -1 + *x*, *y*, *z*, *iii*: -0.5 + *x*, - 0.5 - *y*, 0.5 + *z*) compared to one such Cl(2)...H contact (Cl(2)...H(11)^{ii} 2.89 Å); the *intra*molecular Cl(1)...H(18) and Cl(2)...H(9) contacts are 2.92 Å and 2.72 Å, respectively.

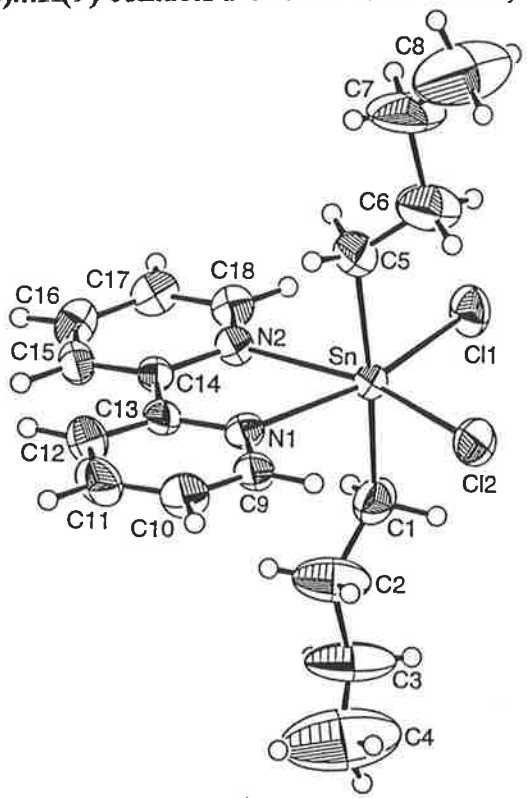


Figure 4.2

The molecular structure of [$^nBu_2SnCl_2$(2,2'-bipyridyl)]

4.2.1c [$^{i}Pr_2SnCl_2$(2,2'-bipyridyl)]

Colourless crystals were obtained from the slow evaporation of an acetonitrile/chloroform (9/1 *v/v*) solution of [$^{i}Pr_2SnCl_2$(2,2'-bipyridyl)]; melting point: 201 - 202 °C

The molecular structure of [$^{i}Pr_2SnCl_2$(2,2'-bipyridyl)] is illustrated in Figure 4.3. No evidence for base-stacking was found in the crystal structure of [$^{i}Pr_2SnCl_2$(2,2'-bipyridyl)]; indeed, there were no non-hydrogen intermolecular contacts < 3.6 Å. A small disparity exists between the Sn-Cl distances, which again may be traced to close intermolecular Cl...H interactions < 3.1 Å; Cl(1)...H(14)^{i}, H(15)^{ii} and H(8)^{iii} of 2.78 Å, 2.89 Å and 2.96 Å, respectively (*i*: -1 + *x*, *y*, *z*; *ii*: - *x*, - *y*, 1 - *z*; *iii*: -0.5 - *x*, -0.5 + *y*, 1.5 - *z*) *cf* Cl(2)...H(10)^{i} 2.70 Å. The *intra*molecular Cl...H contacts of 2.83 Å and 2.79 Å are indistinguishable.

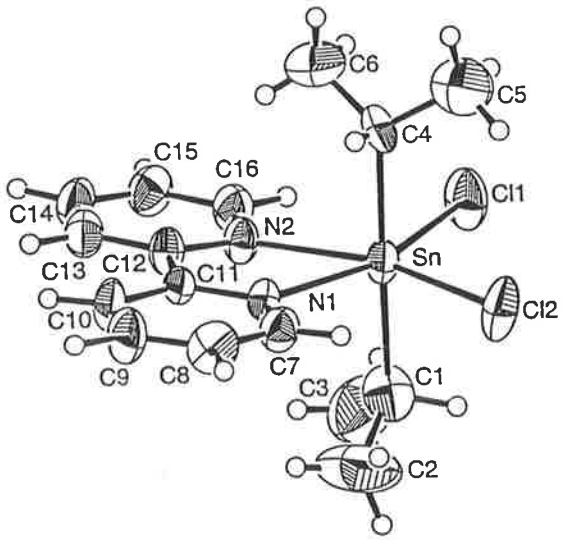


Figure 4.3

The molecular structure of [$^{i}Pr_2SnCl_2$(2,2'-bipyridyl)]

4.2.1d [Bz_2SnCl_2(2,2'-bipyridyl)]

Orange crystals were obtained from the slow evaporation of an acetonitrile/chloroform (4/1 *v/v*) solution of [Bz_2SnCl_2(2,2'-bipyridyl)]; melting point: 215 - 217 °C

The molecular structure of [Bz_2SnCl_2(2,2'-bipyridyl)] is shown in Figure 4.4. No base stacking occurs in the lattice of [Bz_2SnCl_2(2,2'-bipyridyl)] although an isolated contact of 3.512(5) Å is noted between the C(14) and C(15)^{i} atoms (*i*: *x*, 1 - *y*, 1 - *z*). The Sn-Cl distances are experimentally distinct, however, there are no major differences in the nature of the Cl...H intermolecular contacts formed in the lattice, i.e. Cl(1)...H(22)^{ii} 2.97 Å, Cl(1)...H(7)^{iii} 3.02 Å, Cl(2)...H(21)^{ii} 2.86 Å and Cl(2)...H(11)^{iv} 3.10 Å (*ii*: *x*, *y*, 1 + *z*; *iii*: - *x*, - *y*, 1 - *z*; *iv*: -1 + *x*, *y*, *z*). Similarly, the *intra*molecular Cl...H(2,2'-bipyridyl) contacts are indistinguishable at 2.81 Å and 2.80 Å, respectively.

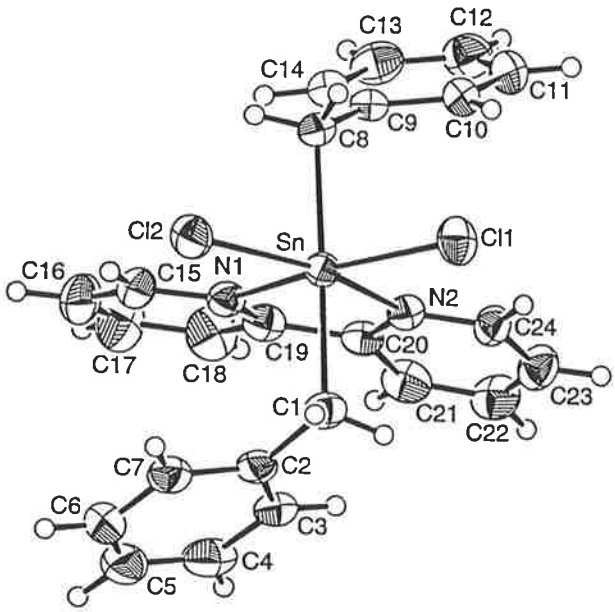


Figure 4.4

The molecular structure of [Bz_2SnCl_2(2,2'-bipyridyl)]

4.2.1e Other R_2SnCl_2(2,2'-bipyridyl) Structures: [Vin_2SnCl_2(2,2'-bipyridyl)] [4], [Ph_2SnCl_2(2,2'-bipyridyl)] [6,7] and [Ph(Me)$SnCl_2$(2,2'-bipyridyl)] [4].

The crystal structures of R_2SnCl_2(2,2'-bipyridyl), R = Ph (two polymorphs), [6,7] Vin,[4] and the mixed species Ph/Me[4] are available in the literature. These structures conform to the motif described above and selected interatomic parameters are included in Table 4.2. Differences in geometric parameters have been correlated with intermolecular interactions for R = Vin and Ph/Me [4, chapter 3]; discussion of the R = Ph polymorphs appear below.

[Ph_2SnCl_2(2,2'-bipyridyl)], as illustrated in Figure 4.5, crystallises in the tetragonal space group $P4_2/n$ after vapor diffusion of diethylether into an acetonitrile solution of the compound,[6] and in the monoclinic space group $P2_1/n$ after recrystallisation from a benzene solution.[7]

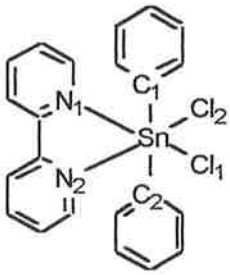


Figure 4.5

[Ph_2SnCl_2(2,2'-bipyridyl)]

The molecular structures in the two polymorphs are, to a first approximation, similar and feature a distorted octahedral environment about the tin atom as described above. Some experimentally significant differences between comparable parameters involving the tin atom can be noted from the listing of selected bond distances and angles in Table 4.2. Particularly noteworthy is the observation that there is a systematic expansion in the Sn-ligand bond distances in the monoclinic form compared with those found in tetragonal form, with the largest discrepancy being 0.040(3) Å for the Sn-Cl(2) bond distance. While there is generally close agreement between comparable bond angles,

there are also some notable differences with the greatest being 4.8° for the Cl(2)-Sn-N(1) angle (larger angle for the monoclinic form). In summary, the two polymorphs reported for [Ph_2SnCl_2(2,2'-bipyridyl)] have some crystallographically distinct parameters and these differences arise, presumably, as a result of the different crystal packing rather than any chemical reason. It is noteworthy that both structures would be described, conventionally, as molecular as there are no 'significant' intermolecular contacts in the lattice. The closest contacts involving non-hydrogen atoms in the lattice of tetragonal [Ph_2SnCl_2(2,2'-bipyridyl)] are 3.50(1) Å for two separate 2,2'-bipyridyl C...C contacts that occur between centrosymmetrically related pairs. Similarly, in monoclinic [Ph_2SnCl_2(2,2'-bipyridyl)], C...C contacts of 3.49(1) Å are noted between centrosymmetrically related 2,2'-bipyridyl ligands. While the above contacts in each of [Ph_2SnCl_2(2,2'-bipyridyl)] may be indicative of some π-π interactions, the contacts are restricted to isolated pairs of atoms and do not extend throughout the lattice. Thus, it can be concluded from the above discussion that noteworthy differences in geometric parameters about the tin atom are found for the polymorphs of [Ph_2SnCl_2(2,2'-bipyridyl)], i.e. with the same molecule existing in different crystalline environments. This result is consistent with the results of surveys of the geometric parameters for series of closely related transition metal systems which indicated that the variation of interatomic parameters was much greater than the errors indicated for those parameters [2,3]. In other words, geometric parameters, while determined accurately for a given structure, can show significant variations when found in different crystalline environments.

4.2.2. Geometry Optimisations

Experimental details pertaining to the geometry optimisation calculations presented below are discussed in Chapter 2. The results of the optimisations are discussed below.

In order that the influence of intermolecular forces on the relevant molecular geometries and geometric parameters of [R_2SnCl_2(2,2'-bipyridyl)] adducts be determined, geometry optimisation calculations have been conducted for [Me_2SnCl_2(2,2'-bipyridyl)], [$^nBu_2SnCl_2$(2,2'-bipyridyl)], [$^iPr_2SnCl_2$(2,2'-bipyridyl)], [Bz_2SnCl_2(2,2'-bipyridyl)] and [Ph_2SnCl_2(2,2'-bipyridyl)]. These, coupled with previously reported calculations for [Vin_2SnCl_2(2,2'-bipyridyl)] and [Ph(Me)$SnCl_2$(2,2'-bipyridyl)] [4, chapter 3] enable a comparison between the solid and theoretical (gas phase) structures.

Geometry optimisations for [Me_2SnCl_2(2,2'-bipyridyl)], [$^nBu_2SnCl_2$(2,2'-bipyridyl)], [Bz_2SnCl_2(2,2'-bipyridyl)], [Ph_2SnCl_2(2,2'-bipyridyl)], [Vin_2SnCl_2(2,2'-bipyridyl)] and [Ph(Me)$SnCl_2$(2,2'-bipyridyl)] all of which converged to symmetrical gas phase structures, are discussed next and finally, the calculated structure of [$^iPr_2SnCl_2$(2,2'-bipyridyl)] is described which, in contrast to the other compounds, has a non-symmetrical structure.

In section 4.2.1e it was noted that there was a significant spread of Sn-Cl and Sn-N values for the [Ph_2SnCl_2(2,2'-bipyridyl)] compound which is known to crystallise in two polymorphs [6,7]. Accordingly, this system was chosen first for geometry optimisation calculations at the HF level of theory employing the LanL2DZ basis set [12] which has been demonstrated previously to be appropriate for investigations of this type [4].

A list of selected interatomic parameters obtained from the geometry optimisation calculations for structures [R_2SnCl_2(2,2'-bipyridyl)], R= Me, ^{n}Bu, ^{i}Pr, Bz, Ph, Vin and the mixed species Ph(Me) are found in Table 4.3.

TABLE 4.3: Interatomic Parameters (Å, deg.) for R_2SnCl_2(2,2'-bipyridyl) for R= Me, ^{n}Bu, ^{i}Pr, Bz Ph, Vin [4] and the mixed species Ph(Me) [4] Derived from Geometry Optimisation Calculations

	R_2SnCl_2(2,2'-bipyridyl)						
Bond Distance	R = Me [a] (y = 2)	R = ^{n}Bu (y = 5)	R = ^{i}Pr (y = 4)	R= Ph/Me (y = C(Ph))	R= Bz (y = 8)	R= Ph (y = 7)	R= Vin (y = 3)
Sn-Cl(1)	2.549	2.562	2.626	2.536	2.573	2.522	2.525
Sn-Cl(2)	2.549	2.562	2.576	2.536	2.573	2.521	2.525
Sn-N(1)	2.416	2.439	2.415	2.404	2.350	2.367	2.404
Sn-N(2)	2.416	2.439	2.416	2.404	2.350	2.367	2.404
Sn-C(1)	2.114	2.137	2.168	2.115	2.155	2.137	2.111
Sn-C(y)	2.114	2.137	2.168	2.140	2.155	2.147	2.111
Bond Angle							
Cl(1)-Sn-Cl(2)	110.5	112.6	115.0	110.0	108.0	106.9	109.7
Cl(1)-Sn-N(1)	158.8	157.4	156.8	159.3	160.8	161.2	159.5
Cl(1)-Sn-N(2)	90.7	90.0	88.8	90.7	91.1	91.9	90.8
Cl(1)-Sn-C(1)	91.2	92.0	86.5	90.4	87.2	91.5	91.3
Cl(1)-Sn-C(y)	91.2	92.0	86.5	93.5	90.6	92.7	94.4
Cl(2)-Sn-N(1)	90.7	90.0	88.1	90.7	91.1	91.9	90.8
Cl(2)-Sn-N(2)	158.8	157.4	156.2	159.3	160.8	161.2	159.5
Cl(2)-Sn-C(1)	91.2	92.0	92.9	90.4	90.6	91.5	94.4
Cl(2)-Sn-C(y)	91.2	92.0	92.9	93.5	87.2	92.7	91.3
N(1)-Sn-N(2)	68.1	67.4	68.0	68.6	69.9	69.3	68.7
N(1)-Sn-C(1)	88.3	87.0	92.6	88.2	94.4	89.0	86.9
N(1)-Sn-C(y)	88.3	87.1	92.6	86.2	88.7	85.2	84.9
N(2)-Sn-C(1)	88.3	87.0	88.4	88.2	88.7	89.0	84.9
N(2)-Sn-C(y)	88.3	87.0	88.4	86.2	94.4	85.2	86.9
C(1)-Sn-C(y)	176.0	172.9	172.3	173.3	176.2	173.0	170.1

[a] molecule has crystallographic two-fold symmetry

4.2.2a The Two Polymorphs of [Ph_2SnCl_2(2,2'-bipyridyl)]

The first significant result of the geometry optimisation calculations for the two polymorphs of [Ph_2SnCl_2(2,2'-bipyridyl)] is the observation that the starting point geometries of each of the crystallographically determined structures converged to the same optimised structure and energy. The energy of tetragonal [Ph_2SnCl_2(2,2'-bipyridyl)] was calculated to be 557.1 kJ mol^{-1} less stable than that of the optimised geometry and the calculations also show that monoclinic [Ph_2SnCl_2(2,2'-bipyridyl)] is more stable than tetragonal [Ph_2SnCl_2(2,2'-bipyridyl)] by 103.7 kJ mol^{-1}; a further discussion of energy considerations is given in 4.2.3 for all systems studied.

An examination of the calculated interatomic parameters involving the tin atom shows a number of interesting trends; the optimised structure is illustrated in Figure 4.6. From Table 4.3, it can be seen that the optimised structure is more symmetrical with individual pairs of Sn-Cl, Sn-N distances being equivalent. Further, there is a general expansion in the Sn-Cl and Sn-N distances compared with the crystallographically determined structures, Table 4.2. By contrast, the Sn-C distances lie between the Sn-C distances determined for tetragonal and monoclinic [Ph_2SnCl_2(2,2'-bipyridyl)]. The small disparity in the Sn-C distances in the optimised geometry is ascribed to the different orientations of the phenyl groups, which results in slightly different *intra*molecular Cl...H interactions. There is, in general, good agreement between the experimental and calculated bond angles with the major differences involving the *ipso* C atoms. The distinctive feature of the three geometries relates to the relative disposition of the phenyl groups.

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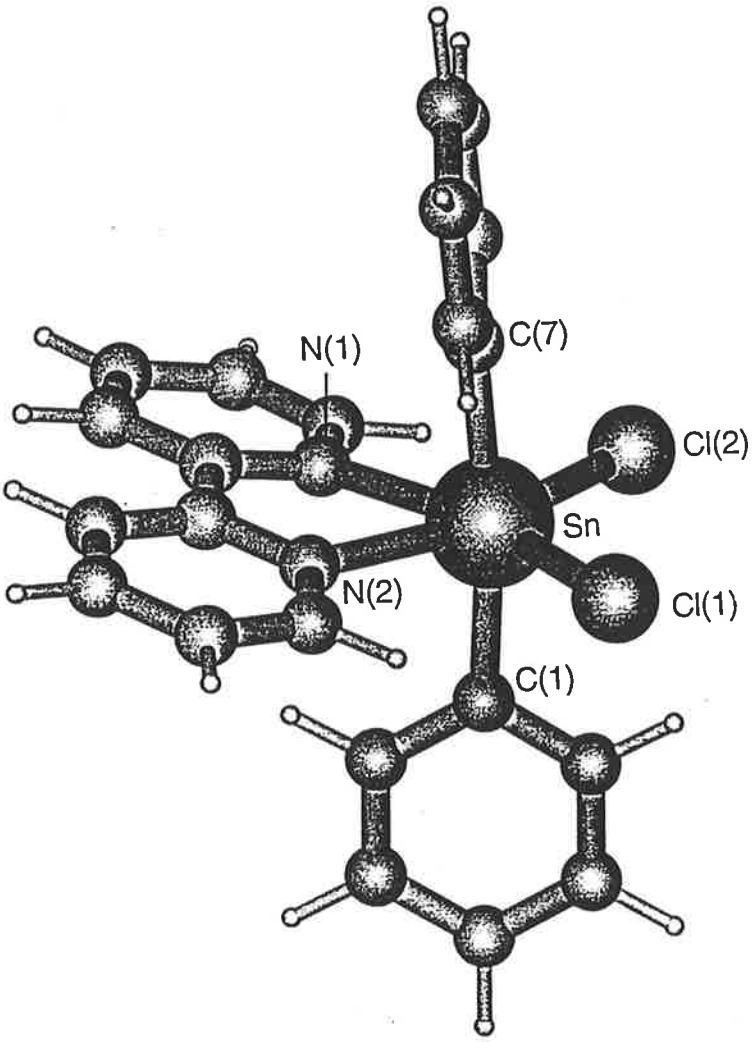


Figure 4.6

The optimised structure of [Ph_2SnCl_2(2,2'-bipyridyl)]

In the calculated structure, the phenyl groups are virtually anti-parallel, indicating no interaction between the two π-systems. A small twist of approximately 6° is observed in the structure of monoclinic [Ph_2SnCl_2(2,2'-bipyridyl)] and this increases to 25° in tetragonal [Ph_2SnCl_2(2,2'-bipyridyl)]. An increase in the interactions between the phenyl π-systems reduces the electron density available to the Sn atom and consequently results in the formation of stronger Sn-Cl and Sn-N interactions. Hence, it may be concluded that the chief influence of the crystal packing in the two polymorphs of [Ph_2SnCl_2(2,2'-bipyridyl)] is to alter the relative positions of the phenyl groups, which in turn influences the geometric parameters about the tin atom.

4.2.2b [Me_2SnCl_2(2,2'-bipyridyl)]

The geometry optimised structure of [Me_2SnCl_2(2,2'-bipyridyl)] is shown in Figure 4.7. The structure has crystallographic twofold symmetry in the solid state but has *mm*2 symmetry in the gas phase where the Sn/Cl/2,2'-bipyridyl entities define one plane, the $(HC)_2Sn$ atoms of the Me_2Sn entity define another mirror plane and the two-fold axis bisects the $SnCl_2$ atoms. Besides the symmetrisation of the structure, the other key result is the elongation of the Sn-Cl and Sn-N distances in the gas phase. The gas phase structure was calculated to be 380.2 kJ mol^{-1} more stable than the crystallographically determined structure.

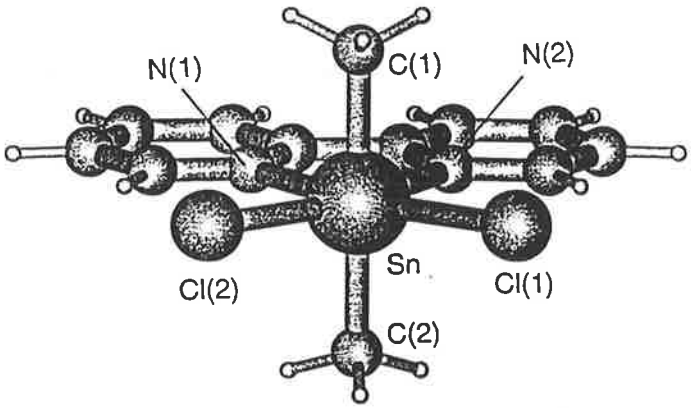


Figure 4.7
The optimised structure of [Me_2SnCl_2(2,2'-bipyridyl)]

4.2.2c [$^nBu_2SnCl_2$(2,2'-bipyridyl)]

A symmetrical optimised structure was also found for [$^nBu_2SnCl_2$(2,2'-bipyridyl)] as shown in Figure 4.8. The significant difference between the solid state and gas phase structures relates to a rotation about the Sn-C(1) bond so that both *n*-butyl groups occupy a position between the Cl atoms and away from the 2,2'-bipyridyl ligand in the calculated structure. All chemically equivalent geometric parameters are identical indicating that the gas phase structure of [$^nBu_2SnCl_2$(2,2'-bipyridyl)] has *mm*2 symmetry as found for the R = Me analog. The gas phase structure was calculated to be 1249.5 kJ mol^{-1} more stable than the solid state structure.

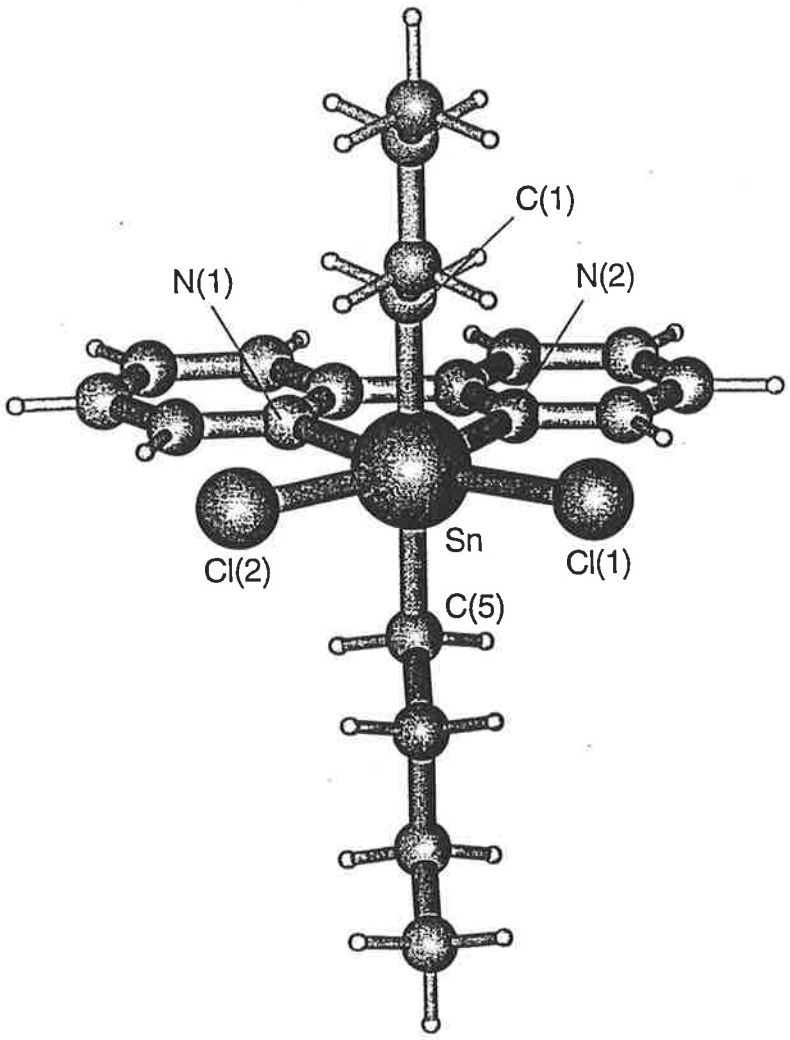


Figure 4.8

The optimised structure of [$^nBu_2SnCl_2$(2,2'-bipyridyl)]

4.2.2d [Bz_2SnCl_2(2,2'-bipyridyl)]

The optimised structure of [$(Bz)_2SnCl_2$(2,2'-bipyridyl)] is shown in Figure 4.9. By contrast to the crystallographically determined structure, the optimised structure of [$(Bz)_2SnCl_2$(2,2'-bipyridyl)] is symmetrical having a twofold axis that bisects the $SnCl_2$ atoms so that the phenyl rings lie on either side of the molecule. The optimised geometry is 591.2 kJ mol^{-1} more stable than the solid state structure.

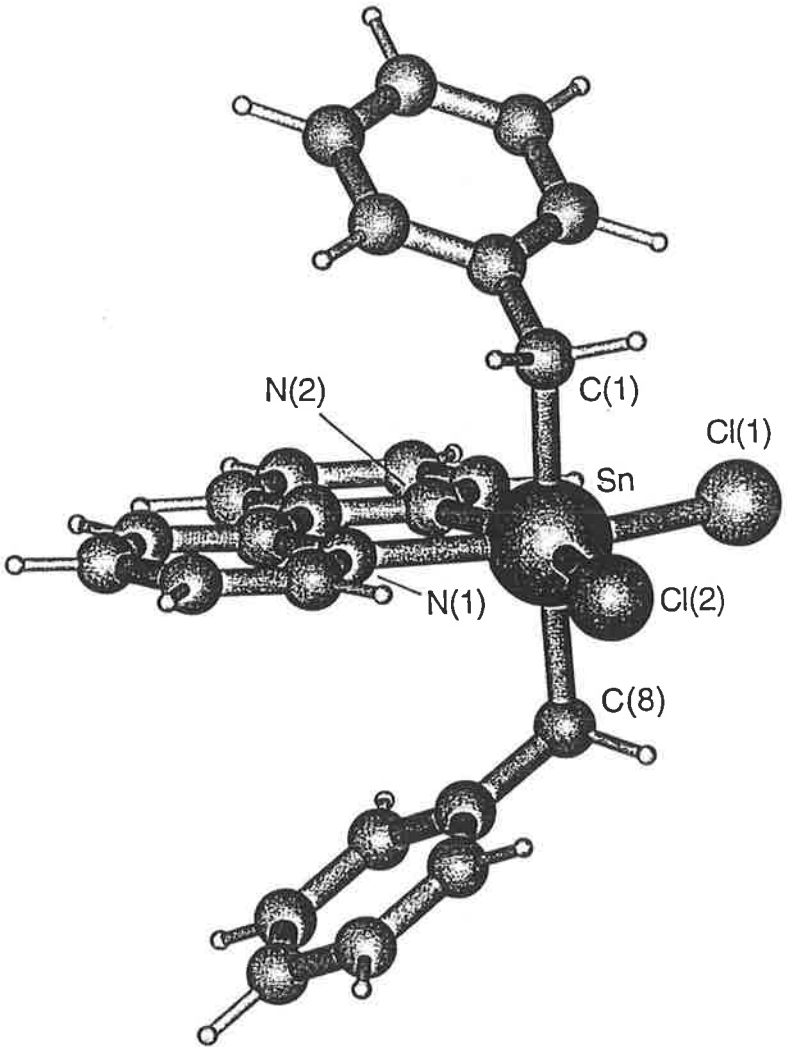


Figure 4.9
The optimised structure of [Bz_2SnCl_2(2,2'-bipyridyl)]

4.2.2e Other R_2SnCl_2(2,2'-bipyridyl) geometry optimisations: [Ph(Me)$SnCl_2$(2,2'-bipyridyl)] and [Vin_2SnCl_2(2,2'-bipyridyl)]

The geometry optimisations of [Ph(Me)$SnCl_2$(2,2'-bipyridyl)] and [Vin_2SnCl_2(2,2'-bipyridyl)] have been discussed previously [4, chapter 3]. Two molecules of [Ph(Me)$SnCl_2$(2,2'-bipyridyl)] comprise the crystallographic asymmetric unit; these converged to the one optimised geometry. The general trends as reported above hold in these structures in that there is a general elongation of the Sn-ligand parameters and symmetrisation of their respective molecular geometries.

4.2.2f [$^iPr_2SnCl_2$(2,2'-bipyridyl)]

The geometry optimisation of [$^iPr_2SnCl_2$(2,2'-bipyridyl)] proceeded in a manner different to those for the other R_2SnCl_2(2,2'-bipyridyl) structures in that a non-symmetrical structure proved to have the lowest energy. Whereas symmetrical structures were found to have lowest energy for each of the other systems investigated in this chapter, the symmetrical *mm*2 structures for [$^iPr_2SnCl_2$(2,2'-bipyridyl)] (with both methine-*H* atoms directed towards the 2,2'-bipyridyl or both directed away from the 2,2'-bipyridyl ligand) were of higher energy. The most stable structure, illustrated in Figure 4.10, is the one with both methine-*H* atoms lying over to one side of the molecule; the structure with a two-fold axis bisecting the $SnCl_2$ atoms was also of higher energy. The most stable structure was 1061.8 kJ mol^{-1} lower in energy compared with the crystallographic structure. The important geometric consequence of the non-symmetrical structure determined for [$^iPr_2SnCl_2$(2,2'-bipyridyl)] is that the Sn-Cl distances are no longer equivalent (i.e. 2.626 Å and 2.576 Å) owing to the presence of two Cl(1)...H interactions of 2.84 Å; analogous Cl(2)...H interactions do not exist. Interestingly, despite the relatively large disparity in the Sn-Cl bond distances, the Sn-N distances are equivalent.

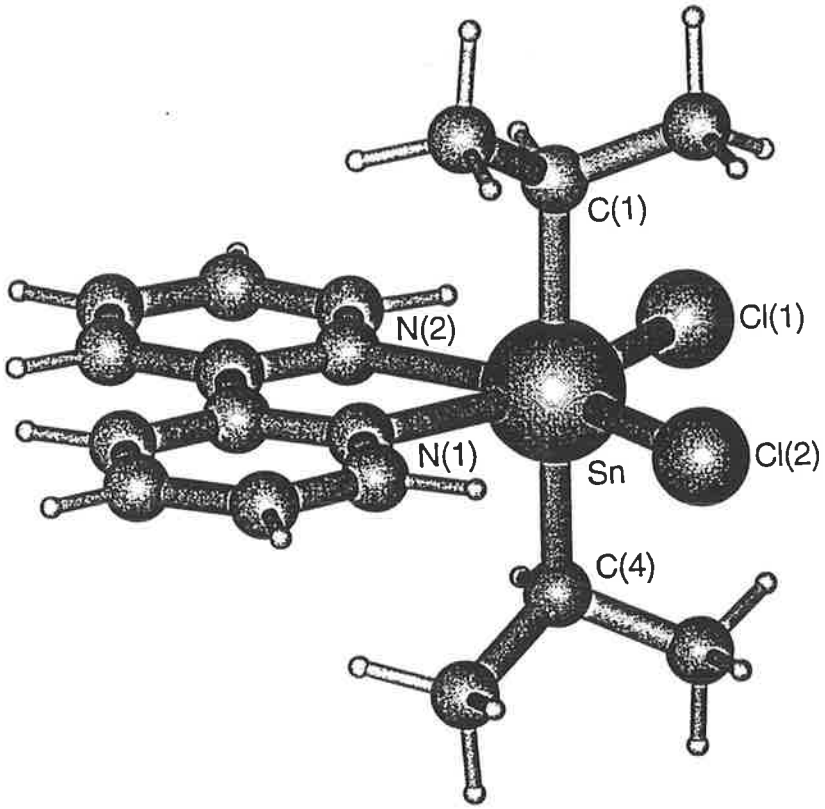


Figure 4.10

The optimised structure of [$^{i}Pr_2SnCl_2$(2,2'-bipyridyl)]

4.2.3. Energy Considerations.

A summary of the energies calculated for the crystallographically determined structures (single point) and the optimised geometries is given in Table 4.4. The differences in energy between the experimental and calculated structures range from 380.2 to 1249.5 kJ mol^{-1} with the optimised geometries being more stable. As has been noted in an earlier contribution, the reported energy differences are exaggerated owing to a number of factors [4, chapter 3]. These factors include treatment of H atoms in the model, systematic errors in the data and inadequacies in the refinement of the X-ray structure [4]. Nonetheless, the qualitative relative energy differences calculated give a general indication of the relative stabilities of the gas phase structures compared with the solid state structures. Particularly noteworthy is that the energy difference between the two

molecules that comprise the crystallographic asymmetric unit of [Vin$_2$SnCl$_2$(2,2'-bipyridyl)] of 17.6 kJ mol^{-1}. The crystal packing influence on both molecules would be similar, however it is significantly smaller than the energy difference calculated for the two polymorphs of [Ph$_2$SnCl$_2$(2,2'-bipyridyl)] where distinct crystalline environments are evident (103.7 kJ mol^{-1}). Thus, the quantitative energy differences are consistent with the qualitative notion that intermolecular forces exerted on the two molecules existing in the one crystalline lattice are more similar than is the case when two molecules exist in distinct crystalline environments such as for the polymorphs of [Ph$_2$SnCl$_2$(2,2'-bipyridyl)].

TABLE 4.4: Calculated Energies (hartrees, kJ mol^{-1}) for R_2SnCl_2(2,2'-bipyridyl) Employing the LanL2DZ Basis Set

	Calculated Energies		
R_2SnCl_2(2,2'-bipyridyl)	**Single point** (Hartrees)	**Optimised geometry** (Hartrees)	**Δ** (kJ mol^{-1})
[Me_2SnCl_2(2,2'-bipyridyl)]	-603.9503	-604.0951	380.2
[$^{n}Bu_2SnCl_2$(2,2'-bipyridyl)]	-837.7430	-838.2189	1249.5
[$^{i}Pr_2SnCl_2$(2,2'-bipyridyl)]	-759.7562	-760.1606	1061.8
[Ph(Me)SnCl$_2$(2,2'-bipyridyl)] *molecule a[4]*	-794.3827	-794.5436	422.4
[Ph(Me)SnCl$_2$(2,2'-bipyridyl)] *molecule b[4]*	-794.3760	-794.5436	440.0
[Bz$_2$SnCl$_2$(2,2'-bipyridyl)]	-1062.8342	-1063.0594	591.2
[Ph$_2$SnCl$_2$(2,2'-bipyridyl)] *monoclinic polymorph[7]*	-985.2441	-984.9924	660.8
[Ph$_2$SnCl$_2$(2,2'-bipyridyl)] *tetragonal polymorph[6]*	-985.2046	-984.9924	557.1
[Vin$_2$SnCl$_2$(2,2'-bipyridyl)] [4]	-679.5857	-679.7460	420.9

4.3 Discussion

Descriptions of both the crystal structures and the gas phase structures of the R_2SnCl_2(2,2'-bipyridyl) adducts for R= Me, ^nBu, ^iPr, Bz Ph, Vin [4] and the mixed species Ph(Me) [4] have been presented in the previous sections. Crystallographically no significant change in the structural motif was found but significant changes in Sn-ligand parameters are noted. Significant differences that are found between the solid state structures and the gas phase structures are correlated with the crystal packing effects.

The geometric optimisation calculations show, in general, that more symmetrical structures are found in the gas phase. This result indicates that crystal packing effects do indeed influence molecular geometry of the R_2SnCl_2(2,2'-bipyridyl) compounds. Further, a comparison of the calculated geometric parameters with those derived from the crystallographic studies reveals two important observations; see Tables 4.2 and 4.3. The first conclusion is that there is, generally, an elongation in the Sn-Cl and Sn-N parameters (see below for further discussion on this point). Also, and significantly, the disparity in the Sn-Cl and Sn-N parameters that are sometimes found in a solid state structure no longer pertains in the absence of crystal packing effects.

In principle, the changes in geometric parameters should be correlated with systematic changes in Lewis acidity of the tin atom as the R substituents are varied rather than with a change in structure. The focus of the analysis is on the Sn-Cl and Sn-N parameters as i) these are most likely to be influenced by changes at the tin center owing to their proximity and ii) these parameters are determined at relatively high levels of precision.

This study examines a series of closely related compounds and attempts to correlate the variation of crystallographically determined Sn-ligand parameters with the Lewis acidity of the tin atoms in R_2SnCl_2. In section 4.3.1, some correlations are made between the seven crystallographically determined R_2SnCl_2(2,2'-bipyridyl) structures specifically a correlation between the Sn-Cl and Sn-N bond distances and the Lewis acidity at the tin atom has been established, however, a large spread of bond distances is found. In

section 4.3.2 crystal packing effects have been removed as a contributing factor to the spread of Sn-Cl and Sn-N bond distances by considering the gas phase theoretical structures. Correlations have been made between the gas phase Sn-Cl and Sn-N bond lengths and Lewis acidity. A good correlation between the Sn-Cl and Sn-N bond distances of the gas phase structures and Lewis acidity is found.

4.3.1 Structural Correlations Based on Crystal Structures.

The availability of several crystallographically determined structures of R_2SnCl_2(2,2'-bipyridyl) affords the opportunity to ascertain how the derived interatomic parameters, particularly Sn-Cl and Sn-N, vary as the nature of R is altered, i.e. as the Lewis acidity of tin is changed. As an independent indication of Lewis acidity, the ^{119}Sn NMR chemical shifts of the R_2SnCl_2 precursors, obtained in a non-coordinating solvent, i.e. in the absence of intermolecular associations, have been measured as these are an indication of the electron density (to a first approximation) at the tin centers. In Figure 4.11, a graph is presented showing the variation of the Sn-Cl and Sn-N distances for each of [R_2SnCl_2(2,2'-bipyridyl)] where R = Me, ^{n}Bu, ^{i}Pr, Vin, Bz, Ph, and the mixed species Ph(Me) versus the measured $\delta(^{119}Sn)$ for R_2SnCl_2, i.e. a measure of Lewis acidity of the tin atom in the diorganotin precursors.

Examining first the relationship between the Sn-Cl distances in each of [R_2SnCl_2(2,2'-bipyridyl)] where R = Me, ^{n}Bu, ^{i}Pr, Vin, Bz, Ph and the mixed species Ph(Me) versus $\delta(^{119}Sn)$ for R_2SnCl_2, a general trend to longer distances is evident as the Lewis acidity at tin decreases. However, a significant spread of values is noted. The spread of Sn-Cl at the high Lewis acidity region may be correlated with the presence of the two polymorphs of [Ph_2SnCl_2(2,2'-bipyridyl)] which have some significantly different geometric parameters (see above), emphasising that influence of crystal packing

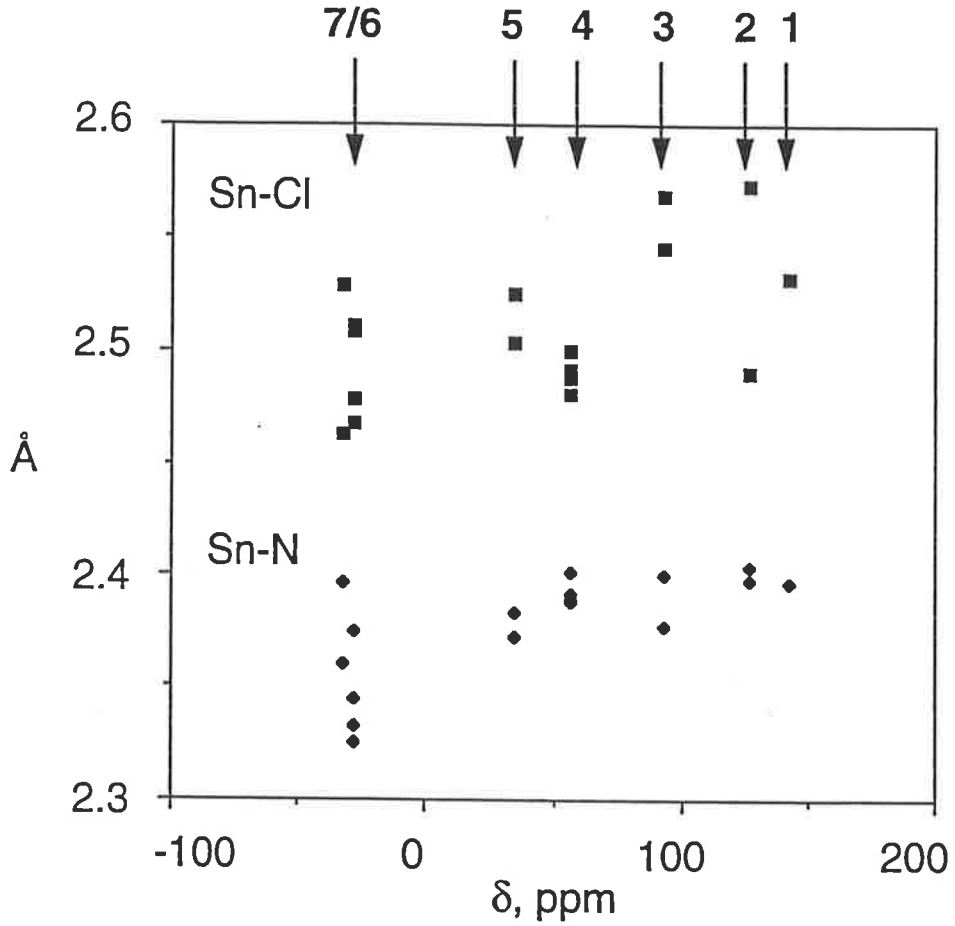


Figure 4.11

Variation of the experimental Sn-Cl and Sn-N (Å) bond lengths of [R_2SnCl_2(2,2'-bipyridyl)] where R = Me (1), R = ^{n}Bu(2), R = ^{i}Pr(3), R_2 = Ph(Me)(4), R = Bz(5), R = Ph(6) and R = Vin(7) versus the experimental chemical shift δ(^{119}Sn) for R_2SnCl_2 (ppm)

effects on geometric parameters about the tin atom [6,7]. Further, there is no indication for an inverse relationship between the Sn-Cl and Sn-N bond distances that would exist if a *trans* influence was in effect. Indeed, the Sn-N bond distances tend to increase as the Lewis acidity of the tin atom decreases, i.e. mimicking the trend in the Sn-Cl distances. The large spread in the Sn-N distances in the high Lewis acidity region reflects, in part, the existence of two polymorphs for [Ph_2SnCl_2(2,2'-bipyridyl)].

The results plotted in Figure 4.11 reflect the foregoing description of crystallographic structures where it was shown that *intra-* and inter- molecular Cl...H interactions can influence the magnitude of Sn-Cl. Similarly, that both Sn-Cl and Sn-N are influenced by the crystalline environment as evidenced, at least, by the disparity in these parameters

within the polymorphs of [Ph_2SnCl_2(2,2'-bipyridyl)]. In summary, while there is no intrinsic chemical reason for the observed variation of the Sn-ligand parameters in individual structures, it would seem that variations from a correlation of these parameters with the Lewis acidity of the tin atom may be rationalised in terms of intermolecular forces, i.e. crystal packing effects.

4.3.2 Structural Correlations Based on Geometry Optimisations.

Crystal packing effects were removed as a contributing factor to the size Sn-ligand parameters through determination of the gas phase structures of these compounds using *ab initio* methods.

A good correlation between the theoretically determined Sn-Cl and Sn-N bond distances and the Lewis acidity at the tin atom is found, i.e. after intermolecular forces have been factored out. Deviations from the correlations are ascribed to the presence of *intra*molecular Cl..H interactions.

A graph showing the variation of the Sn-Cl and Sn-N distances for each of the calculated structures for [R_2SnCl_2(2,2'-bipyridyl)] where R = Me, ^{n}Bu, ^{i}Pr, Vin, Bz, Ph, and the mixed species Ph(Me) in the gas phase, versus $\delta(^{119}Sn)$ measured for R_2SnCl_2 is shown in Figure 4.12; for [^{i}Pr $_2SnCl_2$(2,2'-bipyridyl)], the average Sn-Cl bond distance is used. The obvious difference between Figure 4.12 and the analogous graph plotting the values obtained from the X-ray crystallographic studies (Figure 4.11) is the narrower spread of values. There are two primary reasons for this observation: i) in the geometry optimisations described above, the presence of multiple molecules for a given R_2SnCl_2(2,2'-bipyridyl) structure [i.e. two molecules in the asymmetric unit [Vin_2SnCl_2(2,2'-bipyridyl)] and polymorphs [Ph_2SnCl_2(2,2'-bipyridyl)] in the solid state converge to a single gas phase structure; and ii) the disparity in the individual pairs of Sn-Cl and Sn-N distances as found in the crystalline state are largely removed upon symmetrisation of the structure.

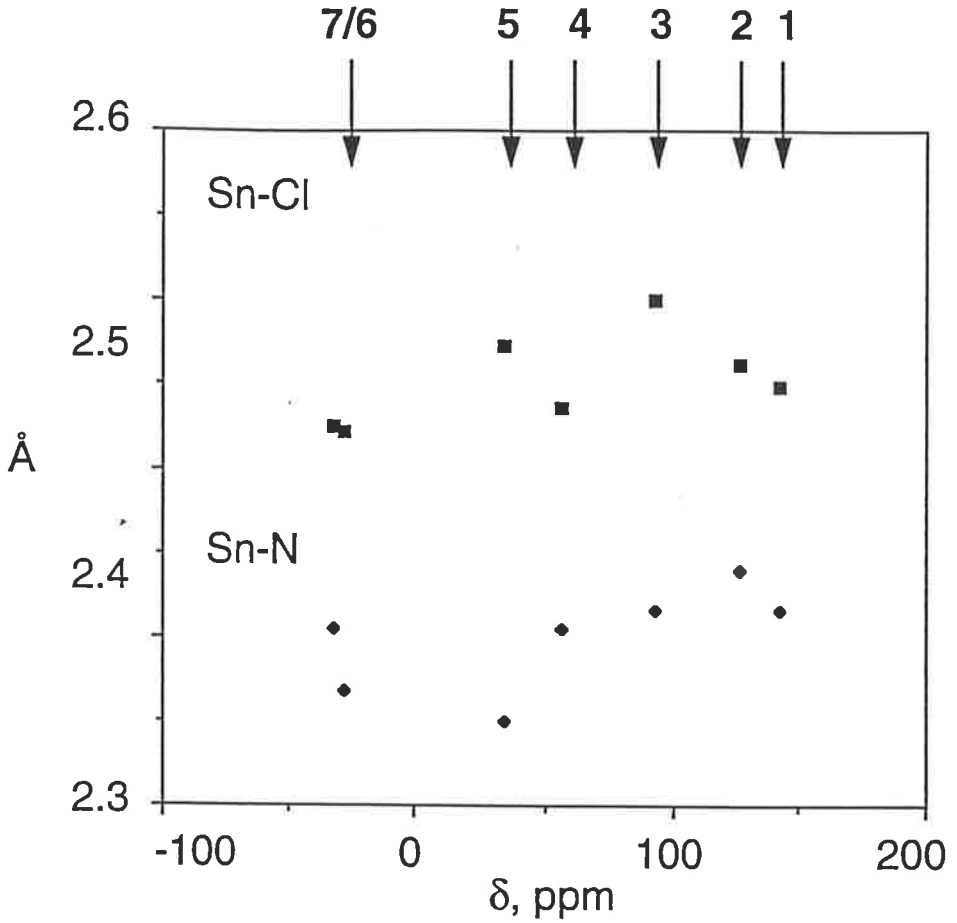


Figure 4.12

Variation of the calculated Sn-Cl and Sn-N (Å) bond lengths of [R_2SnCl_2(2,2'-bipyridyl)] where R = Me (**1**), R = ^{n}Bu(**2**), R = ^{i}Pr(**3**), R_2 = Ph(Me)(**4**), R = Bz(**5**), R = Ph(**6**) and R = Vin(**7**) versus the experimental chemical shift δ(^{119}Sn) for R_2SnCl_2 (ppm)

It may be thus concluded from the results of the theoretical calculations that there is no inherent chemical reason to explain the presence of multiple molecules found in each of [Vin_2SnCl_2(2,2'-bipyridyl)] and [Ph_2SnCl_2(2,2'-bipyridyl)] and their existence may be ascribed to crystal packing effects. Further, it may be surmised that the differences in the pairs of Sn-Cl and Sn-N distances within a particular structure can similarly be ascribed to intermolecular forces. With the exception of [$^{i}Pr_2SnCl_2$(2,2'-bipyridyl)], the crystalline structures uniformly converge to symmetrical structures in the gas phase. As a consequence, in the absence of crystal packing effects, chemically equivalent

parameters in a given structure (e.g. Sn-Cl bond distances) have equal values indicating that intermolecular forces, notably Cl...H interactions, can influence the magnitude of geometric parameters about the tin center in the solid state. It may appear incongruous that crystal packing effects/intermolecular forces can influence the derived interatomic parameters about a heavy metal center such as tin, however, recent bibliographic surveys have described similar effects in transition metal systems [2,3].

The Sn-ligand parameters in the gas phase are longer than the equivalent average parameters in the crystalline state, with one exception that is discussed in detail below. This generalisation is true also for the structure of [$^{i}Pr_2SnCl_2$(2,2'-bipyridyl)] for which a disparity in Sn-Cl is evident (see above). The exception to the above generalisation is found for [Bz_2SnCl_2(2,2'-bipyridyl)]. In the gas phase structure of [Bz_2SnCl_2(2,2'-bipyridyl)] the Sn-N distance of 2.350 Å is shorter than the Sn-N distances found in the solid state of 2.383(2) and 2.372(2) Å. It is noted that the Sn-Cl distance has elongated significantly in the gas phase (up to 0.07 Å) and it is argued that the shortening of Sn-N reflects this elongation. The reason for the elongation of the Sn-Cl distance may be traced to *intra*molecular Cl...H interactions. In the experimental (X-ray) structure, Cl...H the closest contacts are 3.10 Å (x2) and the next closest are at 3.20 and 3.25 Å. By contrast, in the optimised geometry the analogous contacts are 3.07 Å (x2) and 3.11 Å (x2) which arise as a result of the symmetrisation of the structure. It is proposed that the presence of the more significant Cl...H interactions in the optimised structure is responsible for the greater than expected elongation of the Sn-Cl bond distances in [Bz_2SnCl_2(2,2'-bipyridyl)].

Another important feature of Figure 4.12 relates to the relationship of the Sn-Cl and Sn-N distances to $\delta(^{119}Sn)$ of R_2SnCl_2. There is a general trend to increasing Sn-Cl distances as the $\delta(^{119}Sn)$ of R_2SnCl_2 shifts downfield. This trend is consistent with decreasing Lewis acidity, i.e. as the Lewis acidity of the tin atom in R_2Sn decreases, as in Me_2Sn, the length of Sn-Cl increases. A similar trend is found in the Sn-N distances. These results give confidence in the assumption that ^{119}Sn data recorded for R_2SnCl_2 in

non-coordinating solvent is a reliable indicator for the Lewis acidity of tin atom in R_2SnCl_2. However, it should be noted again that $\delta(^{119}Sn)$ of R_2SnCl_2 is only an approximate measure of the Lewis acidity of the tin atom and that an absolute scale of Lewis acidities does not exist. Allowing for this caveat, and having factored out crystal packing effects by considering the theoretical structures, any deviations from a correlation between the Sn-Cl distances, for example, and the Lewis acidity of the tin center (i.e. electronic effects) may be ascribed to *intra*molecular interactions.

Referring to Figure 4.12, outlying points for the Sn-Cl distances are found for [$^{i}Pr_2SnCl_2$(2,2'-bipyridyl)] and [Bz_2SnCl_2(2,2'-bipyridyl)]; the outlying point in the Sn-N distances for [Bz_2SnCl_2(2,2'-bipyridyl)] is related to the exceptionally long Sn-Cl distances in this molecule as discussed above. The structure of [$^{i}Pr_2SnCl_2$(2,2'-bipyridyl)] has already been highlighted as exceptional in that there is a lack of molecular symmetry and that one of the Sn-Cl bond distances has been significantly elongated owing to substantial *intra*molecular Cl...H interactions involving the methine-*H* atoms. Similarly, additional *intra*molecular Cl...H interactions have been noted in the optimised structure of [Bz_2SnCl_2(2,2'-bipyridyl)]. Hence, it may be concluded that the deviations in the Sn-Cl distances found in [$^{i}Pr_2SnCl_2$(2,2'-bipyridyl)] and [Bz_2SnCl_2(2,2'-bipyridyl)] from the established correlations may be ascribed to *intra*molecular interactions, i.e. the proximity of hydrogen atoms on the organic residues.

4.4 Conclusions

The molecular geometries of a series of structurally similar molecules, R_2SnCl_2(2,2'-bipyridyl), have been determined by X-ray crystallographic methods and their theoretical structures calculated employing *ab initio* geometry optimisations (HF with the LanL2DZ basis set). For the solid state structures, it has been demonstrated that geometric parameters about the tin centers can be influenced by crystal packing effects. The influence of crystal packing effects were factored out as a contributing factor to any perturbation of molecular geometry by performing geometry optimisation calculations, i.e. by investigating the theoretical gas phase structures. Anomalies found

in the solid state, such as two molecules in the crystallographic asymmetric unit and polymorphs, no longer pertain in the gas phase. Plotting the calculated Sn-Cl and Sn-N distances against an electronic factor, i.e. a measure of the Lewis acidities of the Sn centers in R_2Sn, showed that increasing Sn-Cl and Sn-N bond distances could be correlated with decreasing Lewis acidity at the tin atom. Furthermore, deviations from these correlations could be explained in terms of *intra*molecular Cl...H interactions.

In summary, it has been demonstrated in this combined crystallographic/theoretical study that crystal packing effects and electronic effects (relating to the tin center as moderated by R and *intra*molecular interactions relating to R_2Sn) both exert an influence on the geometric parameters about the tin center. To our knowledge this is the first occasion that such a systematic delineation of intermolecular interactions contributing to molecular structure in heavy-atom systems has been achieved.

Section II of this chapter describes the results of an analogous study of selected 1,10-phenanthroline adducts.

4.5 References (section I)

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Appendix - Chapter 4, Section I

Crystal data and refinement details for:

A. [Me_2SnCl_2(2,2'-bipyridyl)]

B. [$^{n}Bu_2SnCl_2$(2,2'-bipyridyl)]

C. [$^{i}Pr_2SnCl_2$(2,2'-bipyridyl)]

D. [Bz_2SnCl_2(2,2'-bipyridyl)]

A. [Me_2SnCl_2(2,2'-bipyridyl)]

Crystallographic Data and Refinement details for $[Me_2SnCl_2(2,2'\text{-bipyridyl})]$.

Formula	$C_{12}H_{14}Cl_2N_2Sn$
Formula weight	375.9
Crystal morphology	colourless block
Crystal dimensions (mm)	0.15 x 0.23 x 0.24
Crystal system	monoclinic
Space group	$C2/c$ (C_{2h}^6, No. 15)
Temperature (°C)	20.0
a (Å)	6.633(6)
b (Å)	16.99(1)
c (Å)	13.211(8)
β (°)	104.5(1)
V (Å^3)	1441(2)
Z	4
D_{calc} (g cm^{-3})	1.731
$F(000)$	736
Radiation	MoKα (λ = 0.7107Å)
μ (cm^{-1})	21.22
θ limits, data (°)	3.0 to 27.5
hkl range	0 to 17, -12 to 12, -9 to 9
Range of transmission factors	0.992 to 1
Scan technique	ω:2θ
Scan width (°)	1.21
No. of data measured	3461
No. of unique data	3317
R_{amal}	0.028
Program for structure solution	Direct Methods (SHELXS86)
No. of unique data used	2953
No. of parameters	78
R	0.022
R_w	0.028
G.O.F.	1.68
Min./Max. residual electron density (e Å^{-3})	-0.28 to +0.29

Fractional atomic coordinates ($Å^2$) for the non-hydrogen atoms in $[Me_2SnCl_2(2,2'\text{-bipyridyl})]$.

Atom	*x*	*y*	*z*
Sn	0.0000	0.0255(1)	0.2500
Cl(1)	0.2586(1)	-0.0654(1)	0.3675(1)
N(1)	-0.1745(3)	0.1417(1)	0.1703(1)
C(1)	0.1897(4)	0.0301(2)	0.1428(2)
C(2)	-0.3530(3)	0.1381(2)	0.0971(2)
C(3)	-0.4676(4)	0.2046(2)	0.0602(2)
C(4)	-0.3978(4)	0.2759(2)	0.1024(2)
C(5)	-0.2115(4)	0.2804(2)	0.1773(2)
C(6)	-0.1011(3)	0.2121(2)	0.2099(2)

Anisotropic thermal parameters ($Å^2$) for the non-hydrogen atoms in $[Me_2SnCl_2(2,2'\text{-bipyridyl})]$.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Sn	0.0344(1)	0.0348(1)	0.0348(1)	0.0000	0.0095(7)	0.0000
Cl(1)	0.055(3)	0.047(3)	0.052(3)	0.007(2)	0.003(2)	0.008(2)
N(1)	0.038(8)	0.037(8)	0.048(9)	0.001(7)	0.004(7)	-0.001(7)
C(1)	0.05(1)	0.08(2)	0.05(1)	0.01(1)	0.03(1)	0.01(1)
C(2)	0.04(1)	0.05(1)	0.06(1)	0.003(9)	-0.001(9)	-0.001(9)
C(3)	0.05(1)	0.06(1)	0.07(2)	0.01(1)	-0.01(1)	-0.01(1)
C(4)	0.07(2)	0.05(1)	0.09(2)	0.02(1)	-0.01(1)	-0.01(1)
C(5)	0.07(2)	0.04(1)	0.07(2)	0.01(1)	-0.01(2)	-0.01(1)
C(6)	0.05(1)	0.039(9)	0.05(1)	0.003(8)	0.005(9)	-0.001(8)

Fractional atomic coordinates and *B*eq values ($Å^2$) for the hydrogen atoms in $[Me_2SnCl_2(2,2'\text{-bipyridyl})]$.

Atom	*x*	*y*	*z*	B_{eq}
H(1a)	0.2856	-0.0140	0.1552	5.3
H(1b)	0.1022	0.0270	0.0719	5.3
H(1c)	0.2669	0.0789	0.1517	5.9
H(2)	-0.4043	0.0873	0.0688	4.6
H(3)	-0.5952	0.2008	0.0052	5.7
H(4)	-0.4785	0.3232	0.0799	6.5
H(5)	-0.1587	0.3309	0.2066	5.7

Bond distances (Å) for $[Me_2SnCl_2(2,2'\text{-bipyridyl})]$.

Atom - Atom	Distance	Atom - Atom	Distance
Sn - Cl(1)	2.532(1)	N(1) - C(6)	1.347(3)
Sn - Cl(1)'	2.532(1)	C(2) - C(3)	1.380(3)
Sn - N(1)	2.396(2)	C(3) - C(4)	1.366(4)
Sn - N(1)'	2.396(2)	C(4) - C(5)	1.379(3)
Sn - C(1)	2.118(2)	C(5) - C(6)	1.382(3)
Sn - C(1)'	2.118(2)	C(6) - C(6)'	1.487(4)
N(1) - C(2)	1.331(3)		

' atom related by a crystallographic two-fold axis

Bond angles (°) for [Me_2SnCl_2(2,2'-bipyridyl)].

Atom - Atom - Atom	Angle	Atom - Atom - Atom	Angle
Cl(1) - Sn - Cl(1)'	104.83(5)	N(1)' - Sn - C(1)'	88.77(8)
Cl(1) - Sn - N(1)	162.06(4)	C(1) - Sn - C(1)'	175.8(1)
Cl(1) - Sn - N(1)'	93.11(5)	Sn - N(1) - C(2)	121.8(1)
Cl(1) - Sn - C(1)	90.46(8)	Sn - N(1) - C(6)	118.3(1)
Cl(1) - Sn - C(1)'	92.08(8)	C(2) - N(1) - C(6)	119.5(2)
Cl(1)' - Sn - N(1)	93.11(5)	N(1) - C(2) - C(3)	122.1(2)
Cl(1)' - Sn - N(1)'	162.06(4)	C(2) - C(3) - C(4)	118.7(2)
Cl(1)' - Sn - C(1)	92.08(8)	C(3) - C(4) - C(5)	119.6(2)
Cl(1)' - Sn - C(1)'	90.46(8)	C(4) - C(5) - C(6)	119.2(2)
N(1) - Sn - N(1)'	68.96(8)	N(1) - C(6) - C(5)	120.8(2)
N(1) - Sn - C(1)	88.77(8)	N(1) - C(6) - C(6)	116.8(1)
N(1) - Sn - C(1)'	87.80(8)	C(5) - C(6) - C(6)	122.4(1)
N(1)' - Sn - C(1)	87.80(8)		

' atom related by a crystallographic two-fold axis

Observed and calculated structure factors for [Me_2SnCl_2(2,2'-bipyridyl)].

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	-16	346	343	9	0	6	-1	578	597	6	0	-6	-7	614	625	7	0	12	-12	126	127	6	0	20	0	419	432	9
0	0	-14	334	318	8	0	6	0	371	398	5	0	-6	-8	199	191	5	0	12	-11	320	323	8	0	22	-1	98	107	9
0	0	-12	414	423	7	0	8	-15	276	281	6	0	-6	-9	562	556	7	0	12	-10	79	82	9	0	22	0	290	301	7
0	0	-10	887	891	9	0	8	-14	219	229	5	0	-6	-10	325	316	7	0	12	-9	743	731	9	1	-21	-5	0	19	32*
0	0	-8	1251	1242	11	0	8	-13	487	481	8	0	-6	-11	521	526	8	0	12	-8	80	77	8	1	-21	-4	277	283	7
0	0	-6	996	973	9	0	8	-12	369	362	8	0	-6	-12	476	470	8	0	12	-7	742	764	9	1	-21	-3	170	162	6
0	0	-4	263	228	4	0	8	-11	601	596	8	0	-6	-13	262	259	6	0	12	-6	283	283	7	1	-21	-2	304	309	7
0	0	-2	2178	2301	19	0	8	-10	44	14	24*	0	-6	-14	311	291	6	0	12	-5	406	417	7	1	-19	-8	246	255	6
0	2	-16	341	340	9	0	8	-9	723	736	8	0	-6	-15	185	188	6	0	12	-4	282	281	7	1	-19	-7	143	144	8
0	2	-15	75	88	10	0	8	-8	97	92	6	0	-6	-16	103	94	8	0	12	-3	483	478	7	1	-19	-6	295	300	7
0	2	-14	296	293	6	0	8	-7	823	835	8	0	-8	-1	1738	1691	15	0	12	-2	340	341	7	1	-19	-5	145	147	7
0	2	-13	340	326	8	0	8	-6	332	336	6	0	-8	-2	400	383	5	0	12	-1	1120	1132	11	1	-19	-4	336	343	7
0	2	-12	406	402	7	0	8	-5	447	488	6	0	-8	-3	832	829	8	0	12	0	664	669	8	1	-19	-3	97	92	9
0	2	-11	330	310	7	0	8	-4	647	662	7	0	-8	-4	641	662	7	0	14	-12	231	234	6	1	-19	-2	377	364	8
0	2	-10	1001	1014	10	0	8	-3	846	829	8	0	-8	-5	428	488	7	0	14	-11	236	235	5	1	-17	-10	159	160	7
0	2	-9	89	78	6	0	8	-2	391	383	5	0	-8	-6	324	336	6	0	14	-10	228	236	6	1	-17	-9	130	140	9
0	2	-8	1595	1539	14	0	8	-1	1716	1691	15	0	-8	-7	833	835	9	0	14	-9	473	476	8	1	-17	-8	403	390	10
0	2	-7	81	76	5	0	8	0	209	190	5	0	-8	-8	83	92	7	0	14	-8	244	256	6	1	-17	-7	245	246	6
0	2	-6	953	935	9	0	-2	-2	1724	1647	15	0	-8	-9	738	736	8	0	14	-7	484	488	8	1	-17	-6	515	500	9
0	2	-5	862	851	8	0	-2	-3	618	602	6	0	-8	-10	38	14	24*	0	14	-6	454	453	7	1	-17	-5	168	167	6
0	2	-4	693	687	7	0	-2	-4	677	687	7	0	-8	-11	612	596	8	0	14	-5	336	337	7	1	-17	-4	448	448	8
0	2	-3	603	602	6	0	-2	-5	872	851	8	0	-8	-12	369	362	8	0	14	-4	720	723	8	1	-17	-3	42	25	19*
0	2	-2	1718	1647	15	0	-2	-6	947	935	9	0	-8	-13	478	481	8	0	14	-3	509	496	7	1	-17	-2	427	431	8
0	4	-16	245	243	6	0	-2	-7	66	76	6	0	-8	-14	225	229	6	0	14	-2	305	307	7	1	-15	-12	173	166	7
0	4	-15	188	198	5	0	-2	-8	1581	1539	14	0	-8	-15	262	281	6	0	14	-1	567	571	8	1	-15	-11	165	168	8
0	4	-14	265	266	6	0	-2	-9	34	78	24*	0	-10	-1	1600	1560	14	0	14	0	246	255	6	1	-15	-10	165	170	7
0	4	-13	517	510	8	0	-2	-10	999	1014	10	0	-10	-2	121	107	4	0	16	-11	137	135	7	1	-15	-9	266	267	6
0	4	-12	341	340	7	0	-2	-11	292	310	6	0	-10	-3	803	766	8	0	16	-10	196	203	5	1	-15	-8	407	420	9
0	4	-11	480	484	7	0	-2	-12	400	402	7	0	-10	-4	448	434	7	0	16	-9	53	81	28*	1	-15	-7	283	289	7
0	4	-10	591	585	7	0	-2	-13	310	326	8	0	-10	-5	571	587	7	0	16	-8	151	135	5	1	-15	-6	685	689	9
0	4	-9	228	227	5	0	-2	-14	300	293	6	0	-10	-6	120	98	6	0	16	-7	217	213	5	1	-15	-5	361	364	9
0	4	-8	790	770	8	0	-2	-15	83	88	9	0	-10	-7	842	853	9	0	16	-6	399	384	8	1	-15	-4	254	247	7
0	4	-7	482	484	6	0	-2	-16	343	340	9	0	-10	-8	245	258	6	0	16	-5	319	332	8	1	-15	-3	683	687	9
0	4	-6	1003	996	9	0	-4	-1	247	247	4	0	-10	-9	864	845	9	0	16	-4	631	620	8	1	-15	-2	104	107	8
0	4	-5	1044	1080	10	0	-4	-2	1372	1370	12	0	-10	-10	47	50	24*	0	16	-3	251	242	6	1	-13	-13	241	244	6
0	4	-4	1230	1231	11	0	-4	-3	1369	1341	12	0	-10	-11	445	445	8	0	16	-2	531	536	8	1	-13	-12	78	78	12
0	4	-3	1386	1341	12	0	-4	-4	1237	1231	11	0	-10	-12	0	8	26*	0	16	-1	456	455	8	1	-13	-11	530	524	10
0	4	-2	1415	1370	12	0	-4	-5	1075	1081	10	0	-10	-13	196	191	5	0	16	0	421	442	8	1	-13	-10	147	143	8
0	4	-1	241	247	4	0	-4	-6	1018	996	9	0	-10	-14	8	35	28*	0	18	-9	0	8	29*	1	-13	-9	536	536	9
0	4	0	1720	1738	15	0	-4	-7	473	484	6	0	10	-14	37	35	26*	0	18	-8	251	247	7	1	-13	-8	401	402	9
0	6	-16	74	94	11	0	-4	-8	785	770	8	0	10	-13	193	191	5	0	18	-7	41	59	21*	1	-13	-7	397	388	8
0	6	-15	190	188	5	0	-4	-9	216	227	5	0	10	-12	2	8	25*	0	18	-6	335	347	8	1	-13	-6	460	475	8
0	6	-14	290	291	6	0	-4	-10	594	585	7	0	10	-11	446	445	8	0	18	-5	200	206	5	1	-13	-5	483	486	8
0	6	-13	257	259	6	0	-4	-11	465	484	7	0	10	-10	48	50	25*	0	18	-4	446	434	8	1	-13	-4	297	300	6
0	6	-12	468	470	8	0	-4	-12	345	340	7	0	10	-9	858	845	9	0	18	-3	190	205	5	1	-13	-3	483	468	8
0	6	-11	514	526	7	0	-4	-13	516	510	8	0	10	-8	268	258	7	0	18	-2	381	397	8	1	-13	-2	162	166	5
0	6	-10	316	316	7	0	-4	-14	278	266	6	0	10	-7	833	853	9	0	18	-1	105	97	7	1	-11	-14	54	41	14*
0	6	-9	555	556	7	0	-4	-15	191	198	5	0	10	-6	114	98	5	0	18	0	381	382	8	1	-11	-13	294	294	7
0	6	-8	206	191	5	0	-4	-16	245	243	6	0	10	-5	573	587	7	0	20	-7	26	57	27*	1	-11	-12	43	48	28*
0	6	-7	607	625	7	0	-6	-1	601	597	6	0	10	-4	443	434	6	0	20	-6	262	252	7	1	-11	-11	571	564	9
0	6	-6	690	688	7	0	-6	-2	770	771	7	0	10	-3	804	766	8	0	20	-5	146	150	7	1	-11	-10	125	125	7
0	6	-5	1661	1631	15	0	-6	-3	1616	1629	14	0	10	-2	108	107	5	0	20	-4	240	247	6	1	-11	-9	686	662	9
0	6	-4	1174	1180	11	0	-6	-4	1148	1180	11	0	10	-1	1556	1560	14	0	20	-3	116	117	8	1	-11	-8	139	136	7
0	6	-3	1667	1629	15	0	-6	-5	1644	1631	15	0	10	0	356	341	6	0	20	-2	385	373	8	1	-11	-7	524	523	8
0	6	-2	759	771	7	0	-6	-6	694	688	7	0	12	-13	137	139	6	0	20	-1	174	170	6	1	-11	-6	40	59	27*
1	-11	-5	613	623	8	1	-3	-9	337	345	6	0	-16	-7	207	213	6	-1	15	-6	193	207	5	-1	7	-3	1364	1324	12
1	-11	-4	176	168	5	1	-3	-8	933	935	9	0	-16	-8	130	135	8	-1	15	-7	213	208	5	-1	7	-4	481	489	6
1	-11	-3	1403	1388	13	1	-3	-7	1008	1028	10	0	-16	-9	95	81	10	-1	15	-8	255	252	6	-1	7	-5	681	685	7
1	-11	-2	377	392	7	1	-3	-6	1152	1130	11	0	-16	-10	207	203	6	-1	15	-9	220	215	6	-1	7	-6	100	99	5
1	-9	-15	297	309	7	1	-3	-5	836	869	8	0	-16	-11	149	135	7	-1	15	-10	337	340	8	-1	7	-7	668	677	7
1	-9	-14	79	100	11	1	-3	-4	1104	1146	10	0	-18	-1	105	97	7	-1	15	-11	224	227	6	-1	7	-8	147	156	5
1	-9	-13	373	382	9	1	-3	-3	881	846	8	0	-18	-2	395	397	8	-1	13	1	619	616	8	-1	7	-9	668	675	8
1	-9	-12	86	13	9	1	-3	-2	693	737	7	0	-18	-3	191	205	5	-1	13	0	299	296	7	-1	7	-10	796	796	9
1	-9	-11	602	616	9	1	-1	-17	41	52	29*	0	-18	-4	419	434	8	-1	13	-1	572	603	8	-1	7	-11	493	491	8
1	-9	-10	135	132	6	1	-1	-16	291	283	7	0	-18	-5	192	206	6	-1	13	-2	627	637	8	-1	7	-12	416	432	8
1	-9	-9	726	711	9	1	-1	-15	140	135	6	0	-18	-6	346	347	8	-1	13	-3	477	467	7	-1	7	-13	317	321	8
1	-9	-8	289	296	6	1	-1	-14	327	331	8	0	-18	-7	0	59	32*	-1	13	-4	428	428	7	-1	7	-14	11	8	25*
1	-9	-7	518	510	8	1	-1	-13	26	43	25*	0	-18	-8	242	247	6	-1	13	-5	774	808	9	-1	7	-15	201	208	5
1	-9	-6	588	586	7	1	-1	-12	675	646	8	0	-18	-9	0	8	33*	-1	13	-6	82	85	9	-1	5	1	266	303	5
1	-9	-5	797	844	8	1	-1	-11	178	175	5	0	-20	-1	178	170	6	-1	13	-7	705	732	9	-1	5	0	1203	1252	11
1	-9	-4	39	27	15*	1	-1	-10	1048	1046	10	0	-20	-2	349	373	9	-1	13	-8	150	149	5	-1	5	-1	1968	1979	17
1	-9	-3	1316	1310	12	1	-1	-9	92	69	5	0	-20	-3	121	117	7	-1	13	-9	282	282	6	-1	5	-2	2161	2108	19
1	-9	-2	374	397	6	1	-1	-8	983	994	9	0	-20	-4	239	247	6	-1	13	-10	254	275	6	-1	5	-3	1835	1792	16
1	-7	-16	261	276	6	1	-1	-7	362	360	5	0	-20	-5	146	150	7	-1	13	-11	166	164	5	-1	5	-4	961	942	9
1	-7	-15	324	318	7	1	-1	-6	689	696	7	0	-20	-6	242	252	6	-1	13	-12	201	219	5	-1	5	-5	497	477	6
1	-7	-14	359	342	9	1	-1	-5	237	235	5	0	-20	-7	80	57	12	-1	11	1	1275	1302	12	-1	5	-6	410	421	6
1	-7	-13	406	411	8	1	-1	-4	1595	1579	14	0	-22	-1	109	107	8	-1	11	0	314	313	7	-1	5	-7	261	258	6
1	-7	-12	76	62	9	1	-1	-3	1775	1716	15	-1	21	1	148	134	7	-1	11	-1	670	665	8	-1	5	-8	496	506	7
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1	-7	-10	54	60	11*	0	-12	-1	1138	1132	11	-1	21	-1	0	39	29*	-1	11	-3	680	651	8	-1	5	-10	374	379	7
1	-7	-9	679	670	8	0	-12	-2	349	341	7	-1	21	-2	300	280	6	-1	11	-4	151	145	5	-1	5	-11	550	560	8
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1	-7	-7	1124	1112	11	0	-12	-4	278	281	7	-1	21	-4	254	272	6	-1	11	-6	149	148	5	-1	5	-13	258	262	6
1	-7	-6	657	633	8	0	-12	-5	393	417	8	-1	19	1	97	79	9	-1	11	-7	806	833	9	-1	5	-14	195	207	5
1	-7	-5	1036	1090	10	0	-12	-6	271	283	6	-1	19	0	371	393	9	-1	11	-8	60	50	10	-1	5	-15	108	118	8
1	-7	-4	539	560	6	0	-12	-7	745	764	9	-1	19	-1	141	153	7	-1	11	-9	384	392	7	-1	3	1	128	113	3
1	-7	-3	775	796	8	0	-12	-8	64	77	12*	-1	19	-2	325	330	6	-1	11	-10	24	52	24*	-1	3	0	1663	1656	14
1	-7	-2	237	212	5	0	-12	-9	744	731	9	-1	19	-3	148	150	6	-1	11	-11	189	186	5	-1	3	-1	1783	1771	15
1	-5	-16	200	197	6	0	-12	-10	70	82	10	-1	19	-4	315	311	6	-1	11	-12	84	82	8	-1	3	-2	1308	1304	11
1	-5	-15	315	308	7	0	-12	-11	315	323	6	-1	19	-5	0	26	28*	-1	11	-13	315	316	6	-1	3	-3	1304	1287	11
1	-5	-14	283	278	6	0	-12	-12	123	127	7	-1	19	-6	282	296	7	-1	9	1	1439	1473	13	-1	3	-4	1303	1293	12
1	-5	-13	317	301	6	0	-12	-13	132	139	7	-1	19	-7	94	84	9	-1	9	0	264	261	6	-1	3	-5	321	306	5
1	-5	-12	305	299	8	0	-14	-1	560	571	7	-1	17	1	46	72	28*	-1	9	-1	847	873	8	-1	3	-6	1251	1270	11
1	-5	-11	217	211	6	0	-14	-2	297	307	7	-1	17	0	455	466	8	-1	9	-2	905	891	9	-1	3	-7	76	65	6
1	-5	-10	349	357	7	0	-14	-3	489	496	7	-1	17	-1	268	281	6	-1	9	-3	628	622	7	-1	3	-8	774	778	8
1	-5	-9	549	558	7	0	-14	-4	718	723	9	-1	17	-2	641	638	9	-1	9	-4	209	207	5	-1	3	-9	565	561	7
1	-5	-8	969	950	10	0	-14	-5	344	337	7	-1	17	-3	310	315	6	-1	9	-5	1001	1019	10	-1	3	-10	523	535	7
1	-5	-7	1391	1399	13	0	-14	-6	443	453	8	-1	17	-4	393	403	8	-1	9	-6	245	243	5	-1	3	-11	595	612	8
1	-5	-6	1370	1343	12	0	-14	-7	495	488	8	-1	17	-5	128	143	6	-1	9	-7	782	809	8	-1	3	-12	452	461	8
1	-5	-5	1345	1340	12	0	-14	-8	257	256	6	-1	17	-6	134	123	6	-1	9	-8	35	18	18*	-1	3	-13	166	167	5
1	-5	-4	617	644	7	0	-14	-9	468	476	9	-1	17	-7	76	68	9	-1	9	-9	626	628	8	-1	3	-14	376	394	8
1	-5	-3	77	100	5	0	-14	-10	233	236	6	-1	17	-8	266	257	6	-1	9	-10	124	115	6	-1	3	-15	0	25	27*
1	-5	-2	356	355	5	0	-14	-11	236	235	6	-1	17	-9	149	151	6	-1	9	-11	525	527	8	-1	1	1	922	914	8
1	-3	-16	282	278	7	0	-14	-12	247	234	6	-1	15	1	612	628	8	-1	9	-12	50	29	26*	-1	1	0	1897	1851	16
1	-3	-15	345	350	9	0	-16	-1	447	455	8	-1	15	0	556	573	8	-1	9	-13	327	331	8	-1	1	-1	45	44	5
1	-3	-14	306	304	6	0	-16	-2	532	536	8	-1	15	-1	329	327	8	-1	9	-14	54	49	13*	-1	1	-2	984	988	9
1	-3	-13	287	278	6	0	-16	-3	252	242	6	-1	15	-2	822	813	9	-1	7	1	962	1006	9	-1	1	-3	708	697	7
1	-3	-12	535	539	8	0	-16	-4	601	620	8	-1	15	-3	349	344	8	-1	7	0	573	597	6	-1	1	-4	1328	1346	12
1	-3	-11	82	72	8	0	-16	-5	325	332	6	-1	15	-4	443	434	8	-1	7	-1	1619	1651	14	-1	1	-5	373	357	5
1	-3	-10	899	890	9	0	-16	-6	389	384	8	-1	15	-5	310	301	8	-1	7	-2	614	647	6	-1	1	-6	1458	1468	13
-1	1	-7	392	388	6	1	5	-3	86	100	4	1	13	-6	469	475	8	2	-16	-8	496	491	9	2	-8	-3	1069	1082	10
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-5	-1	-9	121	130	7	-5	-9	-2	194	183	5	-6	14	0	268	263	7	-6	6	-8	214	214	6	-6	-4	5	173	176	6				
-5	-1	-10	179	180	6	-5	-9	-3	403	399	8	-6	14	-1	248	239	6	-6	4	6	480	462	8	-6	-4	4	497	501	8				
-5	-1	-11	67	62	13*	-5	-9	-4	96	94	8	-6	14	-2	226	222	6	-6	4	5	158	176	7	-6	-4	3	346	342	8				
-5	-3	5	446	447	8	-5	-9	-5	422	421	8	-6	12	6	58	75	34*	-6	4	4	485	501	8	-6	-4	2	358	355	8				
-5	-3	4	811	805	9	-5	-9	-6	110	104	8	-6	12	5	511	520	10	-6	4	3	340	342	9	-6	-4	1	612	605	8				
-5	-3	3	93	84	8	-5	-9	-7	403	420	8	-6	12	4	74	57	15*	-6	4	2	338	355	8	-6	-4	0	327	313	8				
-5	-3	2	986	962	10	-5	-9	-8	100	76	8	-6	12	3	410	418	10	-6	4	1	602	605	8	-6	-4	-1	373	365	8				
-5	-3	1	179	174	5	-5	-9	-9	202	213	6	-6	12	2	98	106	11	-6	4	0	318	313	8	-6	-4	-2	439	435	8				
-5	-3	0	763	763	9	-5	-11	4	99	82	8	-6	12	1	169	156	7	-6	4	-1	359	365	8	-6	-4	-3	177	176	6				
-5	-3	-1	758	754	9	-5	-11	3	674	674	9	-6	12	0	182	180	7	-6	4	-2	437	435	8	-6	-4	-4	340	354	9				
-5	-3	-2	409	423	7	-5	-11	2	0	27	29*	-6	12	-1	243	227	6	-6	4	-3	162	176	6	-6	-4	-5	85	109	10				
-5	-3	-3	514	552	8	-5	-11	1	641	633	9	-6	12	-2	73	101	14*	-6	4	-4	342	354	9	-6	-4	-6	270	278	7				
-5	-3	-4	449	465	8	-5	-11	0	19	29	28*	-6	12	-3	435	419	9	-6	4	-5	99	109	9	-6	-4	-7	228	230	6				
-5	-3	-5	67	85	12*	-5	-11	-1	251	242	6	-6	12	-4	46	26	31*	-6	4	-6	283	278	7	-6	-4	-8	284	274	7				
-5	-3	-6	572	596	8	-5	-11	-2	152	137	6	-6	10	6	68	69	16*	-6	4	-7	228	230	6	-6	-6	5	342	335	8				
-5	-3	-7	10	55	28*	-5	-11	-3	284	273	7	-6	10	5	476	463	9	-6	4	-8	284	274	7	-6	-6	4	119	107	7				
-5	-3	-8	325	325	6	-5	-11	-4	110	133	9	-6	10	4	48	43	27*	-6	2	6	732	718	9	-6	-6	3	270	269	6				
-5	-3	-9	225	217	6	-5	-11	-5	397	417	9	-6	10	3	385	378	9	-6	2	5	44	64	22*	-6	-6	2	389	377	8				
-5	-3	-10	225	227	6	-5	-11	-6	63	48	14*	-6	10	2	23	43	30*	-6	2	4	648	642	9	-6	-6	1	354	341	8				
-5	-5	4	394	384	7	-5	-11	-7	387	403	9	-6	10	1	326	319	7	-6	2	3	54	63	29*	-6	-6	0	596	584	9				
-5	-5	3	354	332	7	-5	-11	-8	0	30	30*	-6	10	0	48	8	31*	-6	2	2	497	507	8	-6	-6	-1	529	529	9				
-5	-5	2	433	424	8	-5	-13	4	173	158	6	-6	10	-1	418	405	9	-6	2	1	425	429	8	-6	-6	-2	268	266	7				
-5	-5	1	563	553	8	-5	-13	3	602	614	9	-6	10	-2	90	66	11	-6	2	0	467	471	8	-6	-6	-3	294	299	7				
-5	-5	0	315	313	8	-5	-13	2	196	194	6	-6	10	-3	417	425	9	-6	2	-1	361	358	8	-6	-6	-4	23	52	24*				
-5	-5	-1	589	595	8	-5	-13	1	457	467	9	-6	10	-4	87	89	11	-6	2	-2	606	619	8	-6	-6	-5	253	257	6				
-5	-5	-2	444	443	8	-5	-13	0	258	251	6	-6	10	-5	362	358	9	-6	2	-3	0	45	29*	-6	-6	-6	180	180	6				
-5	-5	-3	386	401	8	-5	-13	-1	185	183	6	-6	10	-6	58	80	16*	-6	2	-4	582	594	9	-6	-6	-7	377	380	9				
-5	-5	-4	479	473	8	-5	-13	-2	242	240	6	-6	8	6	72	35	13*	-6	2	-5	47	24	29*	-6	-6	-8	195	214	6				
-5	-5	-5	221	217	5	-5	-13	-3	232	227	6	-6	8	5	452	455	9	-6	2	-6	269	273	7	-6	-8	5	461	455	8				
-5	-5	-6	201	191	5	-5	-13	-4	144	147	7	-6	8	4	24	41	31*	-6	2	-7	181	179	6	-6	-8	4	56	41	14*				
-5	-5	-7	194	214	5	-5	-13	-5	461	447	9	-6	8	3	561	552	9	-6	2	-8	190	191	6	-6	-8	3	552	552	9				
-5	-5	-8	290	291	6	-5	-13	-6	0	69	31*	-6	8	2	323	311	7	-6	0	6	610	602	9	-6	-8	2	317	311	7				
-5	-5	-9	345	349	9	-5	-15	4	248	252	6	-6	8	1	618	622	9	-6	0	4	715	726	9	-6	-8	1	618	622	9				
-5	-5	-10	310	304	7	-5	-15	3	200	197	6	-6	8	0	342	351	7	-6	0	2	540	543	8	-6	-8	0	346	351	9				
-5	-7	4	185	181	5	-5	-15	2	163	165	6	-6	8	-1	400	401	9	-6	0	0	448	455	8	-6	-8	-1	411	401	8				
-5	-7	3	555	562	8	-5	-15	1	250	244	6	-6	8	-2	77	55	12	-6	0	-2	544	535	8	-6	-8	-2	74	55	11				
-5	-7	2	0	10	28*	-5	-15	0	303	292	7	-6	8	-3	363	369	9	-6	0	-4	553	547	8	-6	-8	-3	377	369	9				
-5	-7	1	624	618	8	-5	-15	-1	240	245	6	-6	8	-4	0	45	29*	-6	0	-6	374	391	9	-6	-8	-4	24	45	29*				
-5	-7	0	658	638	8	-5	-15	-2	361	346	9	-6	8	-5	316	316	7	-6	0	-8	117	134	8	-6	-8	-5	303	316	7				
-5	-7	-1	605	607	8	-5	-15	-3	217	211	6	-6	8	-6	59	54	30*	-6	-2	6	701	718	9	-6	-8	-6	42	54	23*				
-5	-7	-2	748	749	9	-5	-15	-4	216	209	6	-6	8	-7	191	183	6	-6	-2	5	50	64	29*	-6	-8	-7	175	183	6				
-5	-7	-3	561	549	8	-5	-15	-5	169	157	6	-6	6	6	207	215	6	-6	-2	4	648	642	9	-6	-10	5	459	463	9				
-5	-7	-4	107	100	8	-5	-17	4	178	161	6	-6	6	5	340	335	6	-6	-2	3	0	63	28*	-6	-10	4	66	43	13*				
-5	-7	-5	339	335	8	-5	-17	3	78	72	11	-6	6	4	119	107	8	-6	-2	2	504	507	8	-6	-10	3	379	378	9				
-5	-7	-6	0	33	28*	-5	-17	2	191	195	6	-6	6	3	274	269	7	-6	-2	1	437	429	8	-6	-10	2	45	43	19*				
-5	-7	-7	329	322	8	-5	-17	1	68	44	13*	-6	6	2	366	377	9	-6	-2	0	467	471	8	-6	-10	1	323	319	7				
-5	-7	-8	63	79	14*	-5	-17	0	309	304	7	-6	6	1	347	341	8	-6	-2	-1	343	358	8	-6	-10	0	0	8	25*				
-5	-7	-9	326	350	7	-5	-17	-1	180	183	7	-6	6	0	587	584	9	-6	-2	-2	611	619	8	-6	-10	-1	420	405	9				
-5	-7	-10	140	155	7	-5	-17	-2	315	315	7	-6	6	-1	517	529	8	-6	-2	-3	31	45	24*	-6	-10	-2	51	66	31*				
-5	-9	4	0	28	29*	-6	14	6	219	215	7	-6	6	-2	265	266	7	-6	-2	-4	581	594	8	-6	-10	-3	423	425	9				
-6	-10	-4	92	89	10	-7	5	5	311	304	7	-7	-3	5	226	217	6	-8	8	4	153	151	9	-8	-4	2	262	268	7				
-6	-10	-5	341	358	7	-7	5	4	230	218	6	-7	-3	4	353	370	7	-8	8	3	266	254	6	-8	-4	1	128	114	8				
-6	-10	-6	80	80	12	-7	5	3	288	280	7	-7	-3	3	421	434	9	-8	6	8	124	105	10	-8	-4	0	235	225	6				
-6	-12	5	507	520	9	-7	5	2	344	342	7	-7	-3	2	237	231	5	-8	6	7	164	178	9	-8	-4	-1	97	85	11				
-6	-12	4	76	57	12	-7	5	1	261	266	6	-7	-3	1	259	265	6	-8	6	6	253	249	7	-8	-6	8	106	105	10				

Crystallographic Data and Refinement details for [$^{n}Bu_2SnCl_2$(2,2'-bipyridyl)].

Formula	$C_{18}H_{26}Cl_2N_2Sn$
Formula weight	460.0
Crystal morphology	colourless needle
Crystal dimensions (mm)	0.07 x 0.15 x 0.50
Crystal system	monoclinic
Space group	$P2_1/n$ (C_{2h}^5, No. 14)
Temperature (°C)	20.0
a (Å)	9.521(1)
b (Å)	16.364(3)
c (Å)	13.771(2)
β (°)	105.20(1)
V (Å^3)	2070.6(5)
Z	4
D_{calc} (g cm^{-3})	1.476
F(000)	928
Radiation	CuKα (λ = 1.5418Å)
μ (cm^{-1})	121.97
θ limits, data (°)	3.0 to 60.0
hkl range	0 to 11, 0 to 18, -15 to 15
Range of transmission factors	0.908 to 1
Scan technique	ω:2θ
Scan width (°)	1.21
No. of data measured	3425
No. of unique data	3212
R_{amal}	0.030
Program for structure solution	Direct Methods (SHELXS86)
No. of unique data used	2079
No. of parameters	209
R	0.052
R_w	0.055
G.O.F.	2.05
Min./Max. residual electron density (e Å^{-3})	-0.67 to +1.05

Fractional atomic coordinates ($Å^2$) for the non-hydrogen atoms in [$^nBu_2SnCl_2$(2,2'-bipyridyl)].

Atom	*x*	*y*	*z*
Sn	-0.05699(7)	0.15468(4)	0.15634(6)
Cl(1)	0.1051(3)	0.1157(2)	0.0406(3)
Cl(2)	0.1152(3)	0.2096(2)	0.3110(3)
N(1)	-0.2623(9)	0.1759(4)	0.2235(6)
N(2)	-0.2810(8)	0.1146(5)	0.0391(6)
C(1)	-0.0832(12)	0.2694(7)	0.0805(11)
C(2)	-0.1657(20)	0.3326(9)	0.1072(13)
C(3)	-0.1579(25)	0.4147(9)	0.0546(15)
C(4)	-0.1858(39)	0.4804(14)	0.0937(21)
C(5)	-0.0494(12)	0.0328(7)	0.2082(11)
C(6)	0.0838(18)	-0.0042(9)	0.2652(12)
C(7)	0.0706(23)	-0.0952(9)	0.2962(17)
C(8)	0.1757(31)	-0.1280(13)	0.3594(19)
C(9)	-0.2444(11)	0.2050(6)	0.3188(9)
C(10)	-0.3549(14)	0.2138(7)	0.3607(9)
C(11)	-0.4928(14)	0.1944(8)	0.3053(12)
C(12)	-0.5138(11)	0.1643(7)	0.2072(9)
C(13)	-0.3947(10)	0.1575(6)	0.1693(8)
C(14)	-0.4077(10)	0.1274(5)	0.0650(8)
C(15)	-0.5379(11)	0.1127(6)	-0.0057(10)
C(16)	-0.5417(13)	0.0861(7)	-0.1001(9)
C(17)	-0.4126(14)	0.0718(7)	-0.1225(9)
C(18)	-0.2856(12)	0.0877(6)	-0.0517(9)

Anisotropic thermal parameters ($Å^2$) for the non-hydrogen atoms in $[^nBu_2SnCl_2(2,2'\text{-bipyridyl})]$.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Sn	0.0402(4)	0.0405(3)	0.0514(4)	-0.0013(3)	0.0119(3)	0.0001(4)
Cl(1)	0.061(2)	0.092(2)	0.080(2)	-0.004(2)	0.035(2)	-0.004(2)
Cl(2)	0.063(2)	0.081(2)	0.074(2)	-0.004(1)	-0.002(2)	-0.021(2)
N(1)	0.054(5)	0.044(5)	0.044(6)	-0.002(4)	0.014(5)	-0.006(4)
N(2)	0.048(5)	0.055(5)	0.038(6)	0.003(4)	0.010(4)	-0.006(4)
C(1)	0.064(8)	0.069(8)	0.085(1)	-0.011(6)	-0.005(7)	0.002(7)
C(2)	0.207(2)	0.067(1)	0.095(1)	0.032(1)	0.035(1)	0.024(1)
C(3)	0.279(2)	0.052(9)	0.105(1)	0.033(1)	0.037(2)	0.017(1)
C(4)	0.501(5)	0.111(2)	0.194(3)	0.012(3)	0.075(3)	0.054(2)
C(5)	0.065(8)	0.067(8)	0.090(1)	0.009(6)	0.015(8)	0.010(8)
C(6)	0.138(1)	0.078(1)	0.095(1)	0.026(1)	-0.010(1)	-0.008(1)
C(7)	0.203(2)	0.053(9)	0.186(2)	0.039(1)	-0.043(2)	0.017(1)
C(8)	0.328(3)	0.117(2)	0.207(3)	-0.006(2)	-0.145(3)	0.021(2)
C(9)	0.058(7)	0.053(6)	0.055(8)	0.002(5)	0.016(6)	-0.018(6)
C(10)	0.077(1)	0.075(8)	0.054(8)	0.000(7)	0.019(7)	-0.023(7)
C(11)	0.074(1)	0.087(1)	0.094(1)	0.015(7)	0.050(9)	-0.007(9)
C(12)	0.056(7)	0.083(8)	0.055(8)	0.006(6)	0.026(6)	0.001(7)
C(13)	0.047(6)	0.041(5)	0.060(7)	0.005(5)	0.016(6)	0.009(6)
C(14)	0.042(6)	0.037(5)	0.051(7)	0.004(4)	0.009(5)	0.016(5)
C(15)	0.043(6)	0.060(7)	0.067(9)	0.004(5)	0.015(6)	0.019(6)
C(16)	0.062(8)	0.075(8)	0.042(8)	-0.013(6)	-0.007(7)	0.014(6)
C(17)	0.079(9)	0.064(7)	0.048(8)	-0.008(6)	0.018(7)	-0.001(6)
C(18)	0.062(7)	0.061(7)	0.048(7)	-0.001(5)	0.020(7)	0.008(6)

Fractional atomic coordinates and *B*eq values ($Å^2$) for the hydrogen atoms in [$^nBu_2SnCl_2$(2,2'-bipyridyl)].

Atom	*x*	*y*	*z*	B_{eq}
H(1a)	-0.1269	0.2577	0.0097	6.4
H(1b)	0.0141	0.2912	0.0882	6.4
H(2a)	-0.1313	0.3409	0.1792	10.1
H(2b)	-0.2668	0.3151	0.0905	10.1
H(3a)	-0.2261	0.4110	-0.0115	11.7
H(4a)	-0.1644	0.5263	0.0557	20.6
H(4b)	-0.1276	0.4837	0.1627	20.6
H(4c)	-0.2887	0.4815	0.0925	12.0
H(5a)	-0.0853	-0.0011	0.1498	6.4
H(5b)	-0.1161	0.0301	0.2512	6.4
H(6a)	0.1205	0.0274	0.3262	9.3
H(6b)	0.1531	-0.0020	0.2247	9.3
H(7a)	0.0520	-0.1277	0.2352	12.0
H(7b)	-0.0128	-0.0986	0.3242	11.7
H(8a)	0.1469	-0.1811	0.3792	17.3
H(8b)	0.2073	-0.0935	0.4180	17.3
H(8c)	0.2568	-0.1357	0.3288	21.9
H(9a)	-0.1472	-0.1811	0.3792	5.0
H(10a)	-0.3377	0.2336	0.4293	6.5
H(11a)	-0.5752	0.2016	0.3336	7.3
H(12a)	-0.6098	0.1487	0.1673	5.6
H(13b)	-0.0600	0.4196	0.0475	11.7
H(15a)	-0.6286	0.1217	0.0122	4.7
H(16a)	-0.6337	0.0777	-0.1498	5.7
H(17a)	-0.4110	0.0506	-0.1880	5.6
H(18a)	-0.1944	0.0789	-0.0691	5.2

Bond distances (Å) for [$^{n}Bu_2SnCl_2$(2,2'-bipyridyl)].

Atom - Atom	Distance	Atom - Atom	Distance
Sn - Cl(1)	2.573(4)	C(5) - C(6)	1.44(2)
Sn - Cl(2)	2.490(3)	C(6) - C(7)	1.56(2)
Sn - N(1)	2.397(9)	C(7) - C(8)	1.26(2)
Sn - N(2)	2.404(7)	C(9) - C(10)	1.33(1)
Sn - C(1)	2.13(1)	C(10) - C(11)	1.37(2)
Sn - C(5)	2.11(1)	C(11) - C(12)	1.40(2)
N(1) - C(9)	1.36(1)	C(12) - C(13)	1.37(1)
N(1) - C(13)	1.32(1)	C(13) - C(14)	1.49(1)
N(2) - C(14)	1.36(1)	C(14) - C(15)	1.38(1)
N(2) - C(18)	1.32(1)	C(15) - C(16)	1.36(2)
C(1) - C(2)	1.40(2)	C(16) - C(17)	1.37(2)
C(2) - C(3)	1.54(2)	C(17) - C(18)	1.36(1)
C(3) - C(4)	1.26(3)		

Bond angles (°) for [$^{n}Bu_2SnCl_2$(2,2'-bipyridyl)].

Atom - Atom - Atom	Angle	Atom - Atom - Atom	Angle
Cl(1) - Sn - Cl(2)	104.6(1)	Sn - C(1) - C(2)	121(1)
Cl(1) - Sn - N(1)	163.2(2)	C(1) - C(2) - C(3)	115(2)
Cl(1) - Sn - N(2)	95.0(2)	C(2) - C(3) - C(4)	120(2)
Cl(1) - Sn - C(1)	85.8(4)	Sn - C(5) - C(6)	122(1)
Cl(1) - Sn - C(5)	90.1(4)	C(6) - C(7) - C(8)	119(2)
Cl(2) - Sn - N(1)	92.2(2)	N(1) - C(9) - C(10)	123(1)
Cl(2) - Sn - N(2)	160.4(2)	C(9) - C(10) - C(11)	119(1)
Cl(2) - Sn - C(1)	93.8(3)	C(10) - C(11) - C(12)	119(1)
Cl(2) - Sn - C(5)	95.5(4)	C(5) - C(6) - C(7)	115(1)
N(1) - Sn - N(2)	68.2(3)	C(11) - C(12) - C(13)	118(1)
N(1) - Sn - C(1)	93.4(4)	N(1) - C(13) - C(12)	122(1)
N(1) - Sn - C(5)	88.0(4)	N(1) - C(13) - C(14)	116.4(9)
N(2) - Sn - C(1)	86.7(4)	C(12) - C(13) - C(14)	122(1)
N(2) - Sn - C(5)	85.1(4)	N(2) - C(14) - C(13)	116.6(9)
C(1) - Sn - C(5)	170.5(5)	N(2) - C(14) - C(15)	119(1)
Sn - N(1) - C(9)	120.8(7)	C(13) - C(14) - C(15)	125(1)
Sn - N(1) - C(13)	120.2(7)	C(14) - C(15) - C(16)	122(1)
C(9) - N(1) - C(13)	118.9(9)	C(15) - C(16) - C(17)	118(1)
Sn - N(2) - C(14)	118.3(7)	C(16) - C(17) - C(18)	119(1)
Sn - N(2) - C(18)	122.1(7)	N(2) - C(18) - C(17)	123(1)
C(14) - N(2) - C(18)	119.3(9)		

Observed and calculated structure factors for [$^{n}Bu_2SnCl_2$(2,2'-bipyridyl)].

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	816	865	13	0	4	5	1117	1094	15	0	8	3	214	209	9	0	12	7	158	194	17	1	0	-5	412	427	13
0	0	4	1016	942	15	0	4	6	825	828	13	0	8	4	234	220	9	0	12	8	61	126	47*	1	0	-3	1264	1335	15
0	0	6	1392	1297	18	0	4	7	667	660	13	0	8	5	751	806	13	0	12	9	120	143	24*	1	0	-1	164	113	14
0	0	8	567	509	14	0	4	8	0	43	43*	0	8	6	53	22	32*	0	12	10	202	223	17	1	0	1	1649	1637	17
0	0	10	610	632	15	0	4	9	60	104	38*	0	8	7	294	298	9	0	12	11	258	259	12	1	0	3	353	419	11
0	0	12	107	170	26*	0	4	10	670	656	15	0	8	8	0	17	45*	0	13	1	269	233	12	1	0	5	522	527	15
0	0	14	0	37	48*	0	4	11	315	313	11	0	8	9	333	332	11	0	13	2	224	256	13	1	0	7	876	816	16
0	1	1	1241	1463	14	0	4	12	0	145	53*	0	8	10	207	186	13	0	13	3	907	933	16	1	0	9	611	566	15
0	1	2	1655	1600	18	0	4	13	0	51	48*	0	8	11	501	493	16	0	13	4	290	318	13	1	0	11	506	500	13
0	1	3	287	272	10	0	4	14	88	37	26*	0	8	12	35	2	41*	0	13	5	75	76	46*	1	0	13	350	402	11
0	1	4	95	82	22*	0	5	1	1476	1285	16	0	8	13	0	59	48*	0	13	6	141	94	16	1	1	-15	58	88	54*
0	1	5	362	318	10	0	5	2	2160	2125	23	0	9	1	309	322	8	0	13	7	477	491	13	1	1	-14	91	91	55*
0	1	6	115	102	18	0	5	3	164	202	10	0	9	2	1210	1222	15	0	13	8	79	25	49*	1	1	-13	189	237	25
0	1	7	480	458	13	0	5	4	1096	1054	14	0	9	3	1571	1587	18	0	13	9	321	344	12	1	1	-12	248	208	20
0	1	8	844	816	14	0	5	5	37	89	37*	0	9	4	532	535	12	0	13	10	0	6	49*	1	1	-11	426	427	15
0	1	9	469	442	15	0	5	6	215	255	10	0	9	5	347	342	10	0	14	0	329	340	12	1	1	-10	423	397	16
0	1	10	0	56	46*	0	5	7	186	188	12	0	9	6	124	96	16	0	14	1	346	329	12	1	1	-9	145	161	34*
0	1	11	208	222	14	0	5	8	920	937	15	0	9	7	354	365	11	0	14	2	262	252	13	1	1	-8	234	206	21
0	1	12	412	445	12	0	5	9	152	92	15	0	9	8	449	467	15	0	14	3	0	122	49*	1	1	-7	537	563	15
0	1	13	163	165	17	0	5	10	133	143	21	0	9	9	248	259	12	0	14	4	414	380	13	1	1	-6	736	731	18
0	1	14	295	323	11	0	5	11	24	58	47*	0	9	10	162	200	19	0	14	5	597	599	17	1	1	-5	681	661	16
0	2	0	1142	1207	14	0	5	12	288	294	12	0	9	11	0	10	47*	0	14	6	250	278	13	1	1	-4	823	696	15
0	2	1	1847	2110	19	0	5	13	206	214	15	0	9	12	44	81	49*	0	14	7	120	128	24*	1	1	-3	193	141	12
0	2	2	952	965	12	0	5	14	235	235	11	0	9	13	281	254	11	0	14	8	0	26	50*	1	1	-2	1061	960	12
0	2	3	248	163	10	0	6	0	1156	1227	14	0	10	0	391	393	10	0	14	9	185	180	17	1	1	-1	1973	1915	20
0	2	4	609	581	12	0	6	1	158	132	8	0	10	1	0	56	39*	0	15	1	173	150	19	1	1	0	935	844	10
0	2	5	944	894	14	0	6	2	1423	1324	16	0	10	2	378	395	10	0	15	2	402	355	14	1	1	1	627	633	8
0	2	6	893	826	14	0	6	3	993	927	13	0	10	3	291	278	10	0	15	3	360	340	11	1	1	2	801	654	11
0	2	7	1348	1273	17	0	6	4	765	771	12	0	10	4	724	761	13	0	15	4	409	377	12	1	1	3	1162	1268	15
0	2	8	265	286	10	0	6	5	148	133	11	0	10	5	376	384	10	0	15	5	254	212	14	1	1	4	742	850	13
0	2	9	472	428	15	0	6	6	965	935	14	0	10	6	558	577	14	0	15	6	258	267	14	1	1	5	1053	1014	15
0	2	10	110	84	22*	0	6	7	196	185	11	0	10	7	106	86	21*	0	15	7	134	121	23*	1	1	6	587	605	14
0	2	11	469	511	13	0	6	8	80	57	42*	0	10	8	126	144	20	0	15	8	308	313	12	1	1	7	632	611	15
0	2	12	165	162	17	0	6	9	413	424	11	0	10	9	0	45	48*	0	16	0	566	568	18	1	1	8	39	22	45*
0	2	13	18	58	47*	0	6	10	434	408	12	0	10	10	392	400	13	0	16	1	0	78	53*	1	1	9	482	466	16
0	2	14	20	43	45*	0	6	11	312	291	11	0	10	11	179	179	17	0	16	2	261	280	14	1	1	10	478	457	12
0	3	1	1315	1291	14	0	6	12	332	360	11	0	10	12	263	263	13	0	16	3	0	32	49*	1	1	11	328	336	12
0	3	2	1245	1130	15	0	6	13	49	5	49*	0	11	1	151	138	15	0	16	4	369	350	12	1	1	12	0	82	49*
0	3	3	590	652	11	0	6	14	146	120	17	0	11	2	863	869	14	0	16	5	162	185	22	1	1	13	0	23	50*
0	3	4	653	615	12	0	7	1	1149	1074	14	0	11	3	155	185	16	0	16	6	399	387	13	1	1	14	130	137	20
0	3	5	353	315	9	0	7	2	454	465	11	0	11	4	1001	1009	15	0	16	7	65	50	39*	1	2	-15	119	102	22*
0	3	6	682	634	13	0	7	3	1364	1357	16	0	11	5	0	60	43*	0	17	1	66	66	50*	1	2	-14	285	362	15
0	3	7	703	705	14	0	7	4	730	730	12	0	11	6	266	278	10	0	17	2	347	320	11	1	2	-13	209	209	20
0	3	8	486	492	14	0	7	5	762	746	13	0	11	7	147	189	17	0	17	3	286	278	11	1	2	-12	194	177	23
0	3	9	666	638	14	0	7	6	416	415	13	0	11	8	439	460	12	0	17	4	219	241	14	1	2	-11	0	26	63*
0	3	10	76	89	45*	0	7	7	412	448	11	0	11	9	124	170	23*	0	17	5	0	71	52*	1	2	-10	396	364	16
0	3	11	319	305	11	0	7	8	0	59	44*	0	11	10	280	291	13	0	18	0	150	131	19	1	2	-9	379	344	17
0	3	12	89	29	28*	0	7	9	647	695	15	0	11	11	28	9	49*	0	18	1	408	364	13	1	2	-8	1061	997	21
0	3	13	430	455	13	0	7	10	85	56	29*	0	12	0	366	377	12	0	18	2	53	27	36*	1	2	-7	520	498	17
0	3	14	0	12	49*	0	7	11	0	34	48*	0	12	1	454	490	15	0	18	3	72	51	44*	1	2	-6	0	16	61*
0	4	-1	2330	2385	25	0	7	12	152	157	18	0	12	2	265	254	11	1	0	-15	327	328	18	1	2	-5	199	198	17
0	4	0	2165	2251	23	0	7	13	276	242	11	0	12	3	106	54	21*	1	0	-13	359	319	19	1	2	-4	1015	1048	15
0	4	2	731	679	11	0	8	0	228	232	9	0	12	4	421	385	12	1	0	-11	0	45	65*	1	2	-3	474	469	16
0	4	3	28	17	35*	0	8	1	1072	1052	14	0	12	5	558	582	15	1	0	-9	1004	969	21	1	2	-2	994	986	12
0	4	4	441	449	12	0	8	2	559	567	11	0	12	6	165	160	15	1	0	-7	855	903	19	1	2	-1	86	36	11
1	2	0	1016	949	11	1	4	-4	453	543	16	1	6	-6	184	188	19	1	8	-6	132	106	26*	1	10	-2	219	195	12
1	2	1	943	894	11	1	4	-3	463	568	14	1	6	-5	426	418	13	1	8	-5	89	85	49*	1	10	-1	100	128	23*
1	2	2	2167	2137	23	1	4	-2	127	122	16	1	6	-4	455	476	12	1	8	-4	965	960	17	1	10	0	256	232	10
1	2	3	267	273	9	1	4	-1	127	57	12	1	6	-3	1422	1324	18	1	8	-3	292	262	11	1	10	1	925	896	14
1	2	4	256	261	9	1	4	0	427	422	8	1	6	-2	582	567	13	1	8	-2	620	578	14	1	10	2	435	412	14
1	2	5	425	459	13	1	4	1	623	708	9	1	6	-1	65	32	28*	1	8	-1	265	266	11	1	10	3	876	872	15
1	2	6	765	775	14	1	4	2	388	483	11	1	6	0	358	349	11	1	8	0	580	542	13	1	10	4	232	213	11
1	2	7	392	365	11	1	4	3	957	965	14	1	6	1	1468	1396	16	1	8	1	113	53	12	1	10	5	0	15	46*
1	2	8	900	843	16	1	4	4	206	194	10	1	6	2	786	788	12	1	8	2	1114	1146	15	1	10	6	204	199	13
1	2	9	0	62	51*	1	4	5	81	43	41*	1	6	3	1136	1070	15	1	8	3	0	16	42*	1	10	7	611	617	15
1	2	10	267	261	12	1	4	6	704	649	14	1	6	4	119	90	18	1	8	4	694	680	14	1	10	8	44	101	48*
1	2	11	237	233	14	1	4	7	694	654	14	1	6	5	239	261	11	1	8	5	54	89	44*	1	10	9	234	271	13
1	2	12	328	347	13	1	4	8	540	538	15	1	6	6	122	61	17	1	8	6	519	511	15	1	10	10	103	82	26*
1	2	13	158	166	17	1	4	9	483	451	16	1	6	7	849	824	15	1	8	7	0	129	46*	1	10	11	154	137	18
1	2	14	133	189	18	1	4	10	113	64	23*	1	6	8	515	524	15	1	8	8	667	674	15	1	10	12	60	46	47*
1	3	-15	51	42	46*	1	4	11	272	257	13	1	6	9	240	226	13	1	8	9	167	132	16	1	11	-12	99	28	30*
1	3	-14	68	87	39*	1	4	12	389	395	13	1	6	10	43	95	50*	1	8	10	157	148	17	1	11	-11	397	413	12
1	3	-13	0	44	63*	1	4	13	184	197	15	1	6	11	144	160	22	1	8	11	94	42	28*	1	11	-10	0	33	54*
1	3	-12	395	431	17	1	4	14	118	139	19	1	6	12	160	84	17	1	8	12	305	338	12	1	11	-9	113	164	60*
1	3	-11	120	151	65*	1	5	-14	54	36	56*	1	6	13	191	217	15	1	9	-13	91	97	55*	1	11	-8	96	118	56*
1	3	-10	618	536	19	1	5	-13	274	279	19	1	7	-14	0	2	52*	1	9	-12	346	401	15	1	11	-7	319	339	13
1	3	-9	193	178	28	1	5	-12	183	166	28	1	7	-13	92	115	59*	1	9	-11	230	192	18	1	11	-6	239	210	15
1	3	-8	344	307	17	1	5	-11	610	567	18	1	7	-12	407	384	15	1	9	-10	313	321	17	1	11	-5	677	698	17
1	3	-7	225	209	20	1	5	-10	0	22	70*	1	7	-11	261	287	21	1	9	-9	61	137	61*	1	11	-4	196	199	16
1	3	-6	1095	1159	19	1	5	-9	436	398	16	1	7	-10	464	459	15	1	9	-8	56	122	57*	1	11	-3	124	67	19
1	3	-5	333	299	13	1	5	-8	75	53	47*	1	7	-9	128	146	35*	1	9	-7	402	433	13	1	11	-2	275	260	11
1	3	-4	444	478	12	1	5	-7	815	845	19	1	7	-8	180	146	24	1	9	-6	544	557	19	1	11	-1	834	834	15
1	3	-3	498	568	14	1	5	-6	179	211	20	1	7	-7	248	211	15	1	9	-5	507	514	17	1	11	0	311	323	10
1	3	-2	869	963	12	1	5	-5	916	1000	17	1	7	-6	685	691	17	1	9	-4	413	419	13	1	11	1	288	291	10
1	3	-1	613	567	10	1	5	-4	0	35	51*	1	7	-5	524	581	17	1	9	-3	375	316	12	1	11	2	33	32	39*
1	3	0	1067	1106	12	1	5	-3	341	347	10	1	7	-4	689	644	16	1	9	-2	324	334	10	1	11	3	510	530	14
1	3	1	57	41	18*	1	5	-2	203	224	11	1	7	-3	592	511	15	1	9	-1	569	540	14	1	11	4	59	100	47*
1	3	2	468	464	10	1	5	-1	689	780	12	1	7	-2	796	730	14	1	9	0	457	450	13	1	11	5	654	657	15
1	3	3	431	469	12	1	5	0	353	358	10	1	7	-1	835	732	14	1	9	1	429	422	13	1	11	6	207	191	14
1	3	4	1500	1586	18	1	5	1	447	470	9	1	7	0	1273	1165	16	1	9	2	268	240	10	1	11	7	122	133	24*
1	3	5	34	61	36*	1	5	2	153	157	11	1	7	1	245	223	7	1	9	3	227	205	12	1	11	8	0	78	51*
1	3	6	1067	1049	16	1	5	3	859	838	13	1	7	2	358	381	9	1	9	4	725	699	14	1	11	9	371	395	11
1	3	7	94	68	22*	1	5	4	241	233	10	1	7	3	452	374	13	1	9	5	442	414	12	1	11	10	39	85	41*
1	3	8	230	186	12	1	5	5	1116	1120	16	1	7	4	880	826	14	1	9	6	389	404	12	1	11	11	225	259	13
1	3	9	449	441	12	1	5	6	526	509	14	1	7	5	768	763	14	1	9	7	105	58	24*	1	12	-11	68	61	49*
1	3	10	711	697	16	1	5	7	206	167	13	1	7	6	368	355	12	1	9	8	301	318	12	1	12	-10	154	209	25
1	3	11	0	70	48*	1	5	8	0	34	48*	1	7	7	0	13	45*	1	9	9	264	277	12	1	12	-9	257	294	15
1	3	12	118	145	26*	1	5	9	707	679	16	1	7	8	486	480	15	1	9	10	374	370	13	1	12	-8	407	428	12
1	3	13	75	22	47*	1	5	10	86	48	51*	1	7	9	0	116	43*	1	9	11	171	227	18	1	12	-7	192	206	19
1	3	14	155	146	16	1	5	11	417	435	13	1	7	10	571	545	16	1	9	12	149	132	16	1	12	-6	135	153	24*
1	4	-14	291	269	14	1	5	12	48	66	40*	1	7	11	209	252	16	1	10	-12	0	42	56*	1	12	-5	249	246	14
1	4	-13	156	128	31*	1	5	13	90	61	45*	1	7	12	0	23	48*	1	10	-11	0	153	59*	1	12	-4	564	604	17
1	4	-12	237	188	23	1	6	-14	110	123	56*	1	7	13	87	61	44*	1	10	-10	0	140	61*	1	12	-3	414	406	12
1	4	-11	89	38	69*	1	6	-13	248	275	21	1	8	-13	103	52	52*	1	10	-9	388	423	14	1	12	-2	443	431	12
1	4	-10	428	372	18	1	6	-12	0	47	71*	1	8	-12	149	128	29*	1	10	-8	71	39	55*	1	12	-1	27	13	43*
1	4	-9	718	611	23	1	6	-11	0	101	63*	1	8	-11	15	1	47*	1	10	-7	306	296	14	1	12	0	211	228	13
1	4	-8	870	761	21	1	6	-10	211	164	24	1	8	-10	413	393	15	1	10	-6	0	112	51*	1	12	1	517	465	15
1	4	-7	454	453	13	1	6	-9	476	482	15	1	8	-9	74	67	50*	1	10	-5	440	447	13	1	12	2	429	424	12
1	4	-6	185	217	20	1	6	-8	288	291	19	1	8	-8	534	550	15	1	10	-4	141	107	20	1	12	3	388	381	11
1	4	-5	555	593	17	1	6	-7	590	600	19	1	8	-7	102	19	56*	1	10	-3	956	906	16	1	12	4	126	135	22*
1	12	5	60	84	47*	1	15	1	263	283	14	2	1	-13	201	185	24	2	2	13	256	233	12	2	4	10	259	298	17
1	12	6	482	500	16	1	15	2	0	21	51*	2	1	-12	0	64	65*	2	3	-15	268	297	13	2	4	11	90	105	52*
1	12	7	304	332	11	1	15	3	273	234	14	2	1	-11	253	274	24	2	3	-14	86	76	57*	2	4	12	48	54	47*
1	12	8	322	356	11	1	15	4	219	258	12	2	1	-10	566	565	17	2	3	-13	287	255	19	2	4	13	107	20	20*
1	12	9	205	236	15	1	15	5	370	407	10	2	1	-9	359	320	15	2	3	-12	0	7	70*	2	5	-14	276	327	20

1	12	10	60	19	46*	1	15	6	107	97	23*	2	1	-8	1040	1019	20	2	3	-11	432	411	19	2	5	-13	104	12	65*
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6	3	1	348	357	11	6	5	9	32	92	48*	6	8	-3	888	920	16	6	11	-6	489	489	13	7	0	-13	351	335	23
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6	3	4	119	139	28*	6	6	-11	88	94	51*	6	8	0	133	144	18	6	11	-3	0	45	47*	7	0	-7	871	837	19
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6	4	-14	82	129	69*	6	6	-5	212	220	13	6	8	6	105	52	25*	6	11	3	0	62	52*	7	0	5	363	400	16
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8	5	-6	455	465	14	8	8	-2	65	6	39*	9	1	-7	167	164	27	9	4	1	154	148	22	9	9	-3	77	32	31*
8	5	-5	0	18	51*	8	8	-1	511	489	16	9	1	-6	297	265	15	9	4	2	359	353	13	9	9	-2	176	165	15
8	5	-4	292	298	12	8	8	0	113	105	24*	9	1	-5	496	465	15	9	4	3	313	280	14	9	9	-1	258	242	12
8	5	-3	258	265	13	8	8	1	505	451	16	9	1	-4	196	189	19	9	5	-10	0	75	63*	9	9	0	439	406	11
10	0	-8	108	90	56*																								
10	0	-6	456	392	15																								
10	0	-4	299	255	16																								
10	0	-2	383	383	15																								
10	0	0	244	255	18																								

10	1	-9	202	144	25
10	1	-8	0	154	64*
10	1	-7	0	91	65*
10	1	-6	0	11	59*
10	1	-5	65	133	52*
10	1	-4	421	418	13
10	1	-3	323	302	15
10	1	-2	113	181	63*
10	1	-1	0	46	58*
10	1	0	242	229	18
10	1	1	151	161	26*
10	2	-8	0	24	58*
10	2	-7	104	179	64*
10	2	-6	142	157	30*
10	2	-5	447	406	13
10	2	-4	108	98	56*
10	2	-3	33	126	53*
10	2	-2	0	57	57*
10	2	-1	312	348	15
10	2	0	0	92	55*
10	2	1	65	132	47*
10	3	-8	158	12	24
10	3	-7	151	159	28*
10	3	-6	64	111	58*
10	3	-5	255	230	16
10	3	-4	105	120	53*
10	3	-3	425	412	14
10	3	-2	0	67	57*
10	3	-1	51	29	52*
10	3	0	0	6	51*
10	4	-7	236	228	18
10	4	-6	233	246	19
10	4	-5	227	209	16
10	4	-4	0	131	55*
10	4	-3	29	25	53*
10	4	-2	305	299	13
10	4	-1	206	207	16
10	4	0	206	191	15
10	5	-7	62	38	45*
10	5	-6	97	39	52*
10	5	-5	0	121	57*
10	5	-4	400	383	14
10	5	-3	0	22	50*
10	5	-2	251	222	13
10	5	-1	0	27	52*
10	6	-5	227	193	15
10	6	-4	61	61	38*
10	6	-3	157	127	18
10	6	-2	233	220	13

C. [$^{i}Pr_2SnCl_2$(2,2'-bipyridyl)]

Crystallographic Data and Refinement details for [$^{i}Pr_2SnCl_2$(2,2'-bipyridyl)].

Formula	$C_{16}H_{22}Cl_2N_2Sn$
Formula weight	432.0
Crystal morphology	colourless block
Crystal dimensions (mm)	0.03 x 0.16 x 0.32
Crystal system	monoclinic
Space group	$P2_1/n$ (C_{2h}^5, No. 14)
Temperature (°C)	20.0
a (Å)	9.415(4)
b (Å)	15.049(5)
c (Å)	13.082(2)
β (°)	91.28(3)
V (Å^3)	1853(1)
Z	4
D_{calc} (g cm^{-3})	1.548
F(000)	864
Radiation	MoKα (λ = 0.7107Å)
μ (cm^{-1})	16.62
θ limits, data (°)	3.0 to 27.5
hkl range	0 to 12, 0 to 17, -20 to 20
Range of transmission factors	0.919 to 1
Scan technique	ω:2θ
Scan width (°)	1.10
No. of data measured	4704
No. of unique data	4446
R_{amal}	0.049
Program for structure solution	Direct Methods (SHELXS86)
No. of unique data used	1650
No. of parameters	190
R	0.049
R_w	0.044
G.O.F.	2.15
Min./Max. residual electron density (e Å^{-3})	-0.58 to +0.77

Fractional atomic coordinates ($Å^2$) for the non-hydrogen atoms in [$^iPr_2SnCl_2$(2,2'-bipyridyl)].

Atom	*x*	*y*	*z*
Sn	-0.19152(8)	0.25374(7)	0.63540(7)
Cl(1)	-0.3168(4)	0.1191(3)	0.5534(3)
Cl(2)	-0.3851(3)	0.3458(3)	0.7175(3)
N(1)	-0.0057(9)	0.3508(7)	0.6968(7)
N(2)	0.0366(9)	0.2103(6)	0.5770(8)
C(1)	-0.2251(15)	0.3278(11)	0.4983(10)
C(2)	-0.1873(23)	0.4287(12)	0.5097(15)
C(3)	-0.1834(20)	0.2941(14)	0.4058(15)
C(4)	-0.1634(14)	0.1829(10)	0.7798(12)
C(5)	-0.2879(19)	0.1516(12)	0.8281(12)
C(6)	-0.0509(20)	0.1101(14)	0.7751(15)
C(7)	-0.0346(13)	0.4207(9)	0.7559(9)
C(8)	0.0688(15)	0.4757(9)	0.7973(10)
C(9)	0.2064(13)	0.4577(11)	0.7742(11)
C(10)	0.2371(11)	0.3851(10)	0.7131(10)
C(11)	0.1301(11)	0.3303(8)	0.6734(9)
C(12)	0.1528(10)	0.2501(10)	0.6085(8)
C(13)	0.2849(12)	0.2242(9)	0.5826(10)
C(14)	0.3011(13)	0.1511(11)	0.5223(11)
C(15)	0.1851(14)	0.1088(9)	0.4897(10)
C(16)	0.0526(13)	0.1377(9)	0.5195(10)

Anisotropic thermal parameters ($Å^2$) for the non-hydrogen atoms in [$^iPr_2SnCl_2$(2,2'-bipyridyl)].

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Sn	0.0348(3)	0.0558(5)	0.0681(5)	-0.0014(8)	0.0006(3)	-0.0079(9)
Cl(1)	0.066(2)	0.081(3)	0.133(4)	-0.018(2)	0.000(2)	-0.034(3)
Cl(2)	0.043(2)	0.110(3)	0.127(4)	0.015(2)	0.000(2)	-0.036(3)
N(1)	0.036(5)	0.061(7)	0.063(7)	-0.001(5)	-0.006(5)	0.004(6)
N(2)	0.039(5)	0.055(6)	0.068(7)	-0.006(5)	-0.003(5)	-0.017(6)
C(1)	0.09(1)	0.12(1)	0.05(1)	-0.01(1)	0.017(9)	-0.01(1)
C(2)	0.26(3)	0.10(2)	0.18(2)	-0.06(2)	-0.09(2)	0.06(1)
C(3)	0.13(2)	0.19(2)	0.13(2)	0.03(1)	-0.01(1)	0.02(2)
C(4)	0.049(8)	0.10(1)	0.15(2)	-0.009(8)	0.03(1)	0.05(1)
C(5)	0.14(2)	0.13(2)	0.14(2)	0.01(1)	0.01(1)	0.02(1)
C(6)	0.13(2)	0.18(2)	0.19(2)	0.02(2)	0.01(2)	0.12(2)
C(7)	0.055(8)	0.059(9)	0.08(1)	0.007(7)	0.003(7)	-0.004(8)
C(8)	0.09(1)	0.07(1)	0.08(1)	-0.007(9)	-0.022(9)	-0.022(8)
C(9)	0.046(8)	0.09(1)	0.10(1)	-0.013(8)	-0.013(8)	-0.02(1)
C(10)	0.032(7)	0.09(1)	0.10(1)	-0.001(7)	-0.004(7)	-0.005(9)
C(11)	0.032(6)	0.067(9)	0.055(8)	-0.002(6)	-0.001(6)	0.016(7)
C(12)	0.042(5)	0.062(7)	0.057(7)	0.01(1)	0.012(5)	-0.02(1)
C(13)	0.042(6)	0.09(1)	0.058(8)	-0.001(7)	0.004(6)	0.004(8)
C(14)	0.044(8)	0.11(1)	0.08(1)	0.020(9)	0.013(8)	0.02(1)
C(15)	0.063(9)	0.09(1)	0.08(1)	0.019(9)	0.012(8)	-0.005(9)
C(16)	0.060(9)	0.060(9)	0.09(1)	-0.005(8)	-0.003(8)	-0.008(8)

Fractional atomic coordinates and *B*eq values (Å^2) for the hydrogen atoms in [^{i}Pr$_2$SnCl$_2$(2,2'-bipyridyl)].

Atom	*x*	*y*	*z*	*B*eq
H(1a)	-0.3345	0.3317	0.4933	7.5
H(2a)	-0.0868	0.4292	0.5017	14.8
H(2b)	-0.2346	0.4585	0.4520	14.8
H(2c)	-0.2170	0.4504	0.5724	14.8
H(3a)	-0.2053	0.2333	0.4105	14.2
H(3b)	-0.2295	0.3261	0.3556	14.2
H(3c)	-0.0822	0.3051	0.4114	14.2
H(4a)	-0.1252	0.2267	0.8217	9.1
H(5a)	-0.3536	0.2029	0.8334	13.3
H(5b)	-0.3304	0.1049	0.7928	13.3
H(5c)	-0.2593	0.1351	0.8981	13.3
H(6a)	-0.0429	0.1014	0.8524	17.3
H(6b)	-0.0968	0.0652	0.7447	17.3
H(6c)	0.0239	0.1385	0.7509	17.3
H(7a)	-0.1330	0.4317	0.7734	5.5
H(8a)	0.0495	0.5278	0.8397	7.4
H(9a)	0.2875	0.4921	0.8022	7.5
H(10a)	0.3329	0.3738	0.6946	6.6
H(13a)	0.3689	0.2567	0.6057	6.3
H(14a)	0.3947	0.1305	0.5039	7.6
H(15a)	0.1965	0.0572	0.4459	7.1
H(16a)	-0.0311	0.1024	0.4948	6.2

Bond distances (Å) for [$^{i}Pr_2SnCl_2$(2,2'-bipyridyl)].

Atom - Atom	Distance	Atom - Atom	Distance
Sn - Cl(1)	2.569(4)	C(4) - C(5)	1.43(2)
Sn - Cl(2)	2.546(3)	C(4) - C(6)	1.49(2)
Sn - N(1)	2.400(9)	C(7) - C(8)	1.38(2)
Sn - N(2)	2.377(9)	C(8) - C(9)	1.36(2)
Sn - C(1)	2.13(1)	C(9) - C(10)	1.38(2)
Sn - C(4)	2.18(1)	C(10) - C(11)	1.39(2)
N(1) - C(7)	1.34(1)	C(11) - C(12)	1.49(2)
N(1) - C(11)	1.35(1)	C(12) - C(13)	1.35(1)
N(2) - C(12)	1.31(1)	C(13) - C(14)	1.36(2)
N(2) - C(16)	1.34(1)	C(14) - C(15)	1.32(2)
C(1) - C(2)	1.53(2)	C(15) - C(16)	1.38(2)
C(1) - C(3)	1.38(2)		

Bond angles (°) for [$^{i}Pr_2SnCl_2$(2,2'-bipyridyl)].

Atom - Atom - Atom	Angle	Atom - Atom - Atom	Angle
Cl(1) - Sn - Cl(2)	106.1(1)	Sn - C(1) - C(2)	116(1)
Cl(1) - Sn - N(1)	160.7(2)	Sn - C(1) - C(3)	120(1)
Cl(1) - Sn - N(2)	93.6(2)	C(2) - C(1) - C(3)	111(2)
Cl(1) - Sn - C(1)	90.3(4)	Sn - C(4) - C(5)	119(1)
Cl(1) - Sn - C(4)	91.2(4)	Sn - C(4) - C(6)	115(1)
Cl(2) - Sn - N(1)	92.9(2)	C(5) - C(4) - C(6)	111(1)
Cl(2) - Sn - N(2)	160.2(2)	N(1) - C(7) - C(8)	123(1)
Cl(2) - Sn - C(1)	88.8(4)	C(7) - C(8) - C(9)	118(1)
Cl(2) - Sn - C(4)	88.8(4)	C(8) - C(9) - C(10)	119(1)
N(1) - Sn - N(2)	67.4(3)	C(9) - C(10) - C(11)	122(1)
N(1) - Sn - C(1)	93.1(5)	N(1) - C(11) - C(10)	117(1)
N(1) - Sn - C(4)	86.2(4)	N(1) - C(11) - C(12)	117(1)
N(2) - Sn - C(1)	89.4(5)	C(10) - C(11) - C(12)	125(1)
N(2) - Sn - C(4)	92.8(4)	N(2) - C(12) - C(11)	114.9(9)
C(1) - Sn - C(4)	177.2(6)	N(2) - C(12) - C(13)	123(1)
Sn - N(1) - C(7)	121.2(8)	C(11) - C(12) - C(13)	122(1)
Sn - N(1) - C(11)	118.0(8)	C(12) - C(13) - C(14)	120(1)
C(7) - N(1) - C(11)	121(1)	C(13) - C(14) - C(15)	118(1)
Sn - N(2) - C(12)	121.6(8)	C(14) - C(15) - C(16)	120(1)
Sn - N(2) - C(16)	121.6(8)	N(2) - C(16) - C(15)	122(1)
C(12) - N(2) - C(16)	117(1)		

Observed and calculated structure factors for [$^{i}Pr_2SnCl_2$(2,2'-bipyridyl)].

h	k	l	Fo	Fc	sigF
0	0	2	372	491	7
0	0	4	71	173	49*
0	0	6	294	306	9
0	0	8	634	603	14
0	0	10	0	132	57*
0	0	12	210	211	15
0	0	14	202	196	15
0	0	16	0	68	49*
0	1	2	2591	2593	9
0	1	3	770	752	8
0	1	4	114	53	18
0	1	5	243	212	10
0	1	6	622	605	12
0	1	7	0	15	49*
0	1	8	289	291	11
0	1	9	71	92	39*
0	1	10	427	420	9
0	1	11	0	33	48*
0	1	12	222	217	15
0	1	13	6	16	41*
0	1	14	85	118	53*
0	1	15	0	8	51*
0	1	16	87	109	28*
0	1	17	60	5	47*
0	2	1	460	524	6
0	2	2	143	140	10
0	2	3	1273	1279	8
0	2	4	1876	1862	9
0	2	5	298	288	8
0	2	6	304	295	8
0	2	7	141	134	17
0	2	8	649	642	14
0	2	9	9	78	54*
0	2	10	247	233	14
0	2	11	84	95	57*
0	2	12	193	182	17
0	2	13	0	23	55*
0	2	14	124	159	25*
0	2	15	0	15	53*
0	2	16	0	53	51*
0	3	1	100	56	15
0	3	2	1648	1643	8
0	3	3	1576	1576	9
0	3	4	384	392	9
0	3	5	729	689	10
0	3	6	1211	1234	10
0	3	7	249	237	11
0	3	8	249	243	12
0	3	9	256	231	13
0	3	10	387	399	10
0	3	11	0	15	59*
0	3	12	193	222	18
0	3	13	87	15	45*
0	3	14	83	77	54*
0	3	15	69	23	37*
0	3	16	58	94	53*
0	4	0	0	114	44*
0	4	1	164	177	13
0	4	2	227	207	9
0	4	3	215	200	10
0	4	4	2212	2163	10
0	4	5	324	314	8
0	4	6	104	67	21*
0	4	7	0	4	49*
0	4	8	672	681	14
0	4	9	0	19	55*
0	4	10	309	299	12
0	4	11	0	28	57*
0	4	12	175	182	20
0	4	13	69	47	56*
0	4	14	64	138	57*
0	4	15	0	33	54*
0	4	16	67	41	45*
0	5	1	539	521	11
0	5	2	1093	1132	9
0	5	3	149	225	14
0	5	4	107	70	19*
0	5	5	0	33	46*
0	5	6	1420	1452	11
0	5	7	165	209	16
0	5	8	381	362	10
0	5	9	77	7	39*
0	5	10	289	261	12
0	5	11	0	59	59*
0	5	12	180	211	19
0	5	13	64	12	56*
0	5	14	109	94	29*
0	5	15	0	2	53*
0	5	16	13	85	47*
0	6	0	955	957	10
0	6	1	0	51	45*
0	6	2	256	256	9
0	6	3	196	221	11
0	6	4	1288	1279	10
0	6	5	91	102	48*
0	6	6	0	44	49*
0	6	7	52	67	52*
0	6	8	649	625	14
0	6	9	234	243	14
0	6	10	295	328	13
0	6	11	80	29	55*
0	6	12	103	163	58*
0	6	13	0	23	58*
0	6	14	0	120	61*
0	6	15	104	37	55*
0	6	16	75	51	56*
0	7	1	275	248	9
0	7	2	1422	1387	10
0	7	3	454	441	10
0	7	4	50	53	50*
0	7	5	187	173	14
0	7	6	584	638	14
0	7	7	390	371	9
0	7	8	237	214	14
0	7	9	0	18	57*
0	7	10	265	288	14
0	7	11	0	84	56*
0	7	12	229	194	15
0	7	13	78	57	54*
0	7	14	107	131	58*
0	7	15	55	3	55*
0	8	0	1328	1340	11
0	8	1	345	334	8
0	8	2	0	78	51*
0	8	3	166	170	16
0	8	4	822	824	12
0	8	5	234	233	13
0	8	6	300	297	11
0	8	7	0	70	54*
0	8	8	313	328	12
0	8	9	278	267	13
0	8	10	182	176	18
0	8	11	88	62	56*
0	8	12	211	245	17
0	8	13	61	8	40*
0	8	14	109	117	57*
0	8	15	0	19	58*
0	9	1	297	304	10
0	9	2	1030	1012	12
0	9	3	183	211	16
0	9	4	201	191	15
0	9	5	202	181	15
0	9	6	414	410	9
0	9	7	243	182	14
0	9	8	251	237	14
0	9	9	100	109	55*
0	9	10	319	334	12
0	9	11	0	78	57*
0	9	12	112	120	56*
0	9	13	8	60	58*
0	9	14	0	83	59*
0	9	15	93	9	33*
0	10	0	955	963	13
0	10	1	0	32	53*
0	10	2	290	266	11
0	10	3	39	74	47*
0	10	4	536	543	12
0	10	5	294	278	12
0	10	6	366	341	10
0	10	7	104	125	31*
0	10	8	365	353	10
0	10	9	35	26	46*
0	10	10	156	113	20
0	10	11	0	108	59*
0	10	12	148	171	23
0	10	13	75	53	55*
0	10	14	125	67	24*
0	11	1	0	41	55*
0	11	2	643	643	15
0	11	3	256	263	14
0	11	4	400	389	10
0	11	5	156	118	21
0	11	6	371	385	11
0	11	7	0	36	56*
0	11	8	84	133	44*
0	11	9	26	84	57*
0	11	10	273	262	13
0	11	11	69	42	52*
0	11	12	0	67	58*
0	11	13	0	44	53*
0	11	14	107	55	55*
0	12	0	522	524	12
0	12	1	218	209	16
0	12	2	229	250	16
0	12	3	0	59	59*
0	12	4	419	440	10
0	12	5	51	50	43*
0	12	6	195	184	18
0	12	7	0	104	57*
0	12	8	350	363	11
0	12	9	0	15	55*
0	12	10	119	122	27*
0	12	11	100	33	29*
0	12	12	0	65	56*
0	12	13	46	52	55*
0	13	1	211	221	18
0	13	2	415	420	10
0	13	3	140	110	23
0	13	4	73	159	45*
0	13	5	0	27	57*
0	13	6	382	407	11
0	13	7	0	18	59*
0	13	8	0	122	59*
0	13	9	77	36	54*
0	13	10	90	115	48*
0	13	11	106	32	30*
0	13	12	122	89	25*
0	14	0	369	389	12
0	14	1	146	196	25*
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4	5	8	337	330	13	4	7	1	33	28	50*	4	9	-2	95	116	36*	4	11	-1	115	110	32*	4	13	5	152	102	27*
4	5	9	0	99	64*	4	7	2	107	113	27*	4	9	-1	99	117	57*	4	11	0	615	626	13	4	13	6	166	134	26
4	5	10	219	239	20	4	7	3	129	80	23*	4	9	0	650	641	15	4	11	1	0	89	62*	4	13	7	126	134	64*
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4	5	12	191	229	24	4	7	5	270	264	14	4	9	2	178	163	20	4	11	3	165	116	23	4	13	9	0	61	66*
4	5	13	0	8	66*	4	7	6	347	326	12	4	9	3	253	238	14	4	11	4	301	314	15	4	13	10	123	81	35*
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4	6	-3	0	109	54*	4	8	-8	287	243	15	4	10	-9	100	43	54*	4	12	-6	0	193	69*	4	14	3	50	72	64*
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4	6	14	134	94	33*	4	8	9	154	84	24	4	10	8	0	144	66*	4	12	11	51	55	67*	4	15	0	191	170	22
4	6	15	14	6	67*	4	8	10	249	251	18	4	10	9	0	11	66*	4	12	12	117	82	68*	4	15	1	0	83	65*
4	15	2	79	107	63*	5	0	7	537	537	13	5	2	4	52	56	40*	5	4	-3	489	459	11	5	6	-7	751	717	16
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4	15	5	0	50	67*	5	0	13	150	103	28*	5	2	7	610	617	12	5	4	0	219	209	12	5	6	-4	100	40	33*
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4	15	8	181	159	24	5	1	-14	90	5	62*	5	2	10	60	142	62*	5	4	3	590	581	14	5	6	-1	517	553	11
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4	16	4	0	102	67*	5	1	0	617	571	12	5	3	-7	263	296	15	5	5	-13	160	171	27	5	6	13	0	46	68*
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4	17	-5	0	23	65*	5	1	5	843	857	13	5	3	-2	182	165	15	5	5	-8	273	230	15	5	7	-11	148	92	27*
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4	17	-2	20	27	54*	5	1	8	0	38	63*	5	3	1	801	778	11	5	5	-5	521	500	12	5	7	-8	267	217	16
4	17	-1	70	80	54*	5	1	9	415	427	11	5	3	2	0	26	49*	5	5	-4	66	33	39*	5	7	-7	164	180	24
4	17	0	193	177	23	5	1	10	24	44	61*	5	3	3	606	587	13	5	5	-3	875	870	13	5	7	-6	40	53	52*
4	17	1	109	46	67*	5	1	11	0	58	62*	5	3	4	355	343	10	5	5	-2	96	47	30*	5	7	-5	808	808	16
4	17	2	108	27	66*	5	1	12	0	9	62*	5	3	5	753	803	14	5	5	-1	503	504	10	5	7	-4	217	238	17
4	17	3	119	79	67*	5	1	13	186	193	24	5	3	6	96	26	58*	5	5	0	70	21	51*	5	7	-3	541	574	12
4	17	4	192	169	25	5	1	14	102	8	65*	5	3	7	123	63	29*	5	5	1	546	542	10	5	7	-2	0	60	57*
4	17	5	91	5	68*	5	1	15	0	63	66*	5	3	8	109	69	62*	5	5	2	104	57	53*	5	7	-1	216	220	16
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4	18	-1	68	51	65*	5	2	-12	103	62	60*	5	3	12	82	52	64*	5	5	6	81	45	59*	5	7	3	113	172	59*
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4	18	2	132	157	68*	5	2	-9	255	259	16	5	3	15	91	58	63*	5	5	9	447	451	12	5	7	6	0	58	61*

| | | |

6	13	1	209	205	22	7	0	-11	196	192	19	7	2	0	75	119	57*	7	4	1	192	204	18	7	6	2	112	112	61*
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6	13	5	0	77	69*	7	0	-3	79	134	55*	7	2	4	144	16	24*	7	4	5	357	386	13	7	6	6	130	181	33*
6	13	6	239	224	22	7	0	-1	807	710	15	7	2	5	462	496	11	7	4	6	89	21	43*	7	6	7	334	342	15
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6	13	8	0	84	71*	7	0	3	667	651	16	7	2	7	296	313	14	7	4	8	6	74	54*	7	6	9	268	259	18
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6	14	5	0	18	68*	7	1	-5	74	55	41*	7	3	-5	205	161	18	7	5	-4	94	93	51*	7	7	-1	138	158	29*
6	14	6	0	123	72*	7	1	-4	0	3	57*	7	3	-4	0	28	60*	7	5	-3	611	598	13	7	7	0	108	88	61*
6	14	7	30	40	70*	7	1	-3	609	600	11	7	3	-3	754	740	15	7	5	-2	203	184	19	7	7	1	632	647	13
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6	15	-6	0	39	66*	7	1	0	181	153	19	7	3	0	0	57	57*	7	5	1	681	685	17	7	7	4	0	118	63*
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6	15	-4	197	180	22	7	1	2	85	9	58*	7	3	2	0	57	59*	7	5	3	372	382	12	7	7	6	0	3	65*
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6	15	1	101	79	52*	7	1	7	277	314	16	7	3	7	408	423	12	7	5	8	0	38	67*	7	7	11	0	186	73*
6	15	2	131	140	69*	7	1	8	0	5	62*	7	3	8	0	29	65*	7	5	9	234	277	21	7	7	12	0	13	67*
6	15	3	0	9	68*	7	1	9	6	203	65*	7	3	9	257	298	18	7	5	10	94	26	66*	7	8	-12	0	26	69*
6	15	4	89	192	72*	7	1	10	61	9	61*	7	3	10	119	3	63*	7	5	11	182	167	26	7	8	-11	71	100	69*
6	15	5	128	84	38*	7	1	11	141	192	30*	7	3	11	164	193	27	7	5	12	0	2	71*	7	8	-10	0	7	68*
6	15	6	194	163	27	7	1	12	75	40	64*	7	3	12	0	29	64*	7	5	13	0	51	69*	7	8	-9	116	203	70*
6	16	-5	61	69	55*	7	1	13	128	121	33*	7	3	13	108	74	55*	7	6	-13	99	122	66*	7	8	-8	130	93	33*
6	16	-4	0	71	71*	7	2	-14	0	18	58*	7	4	-13	127	138	64*	7	6	-12	0	31	64*	7	8	-7	93	117	49*
6	16	-3	0	3	66*	7	2	-13	108	120	64*	7	4	-12	105	2	62*	7	6	-11	0	93	66*	7	8	-6	48	50	62*
6	16	-2	140	139	32*	7	2	-12	0	44	61*	7	4	-11	108	94	54*	7	6	-10	0	24	64*	7	8	-5	263	293	17
6	16	-1	68	50	68*	7	2	-11	100	152	53*	7	4	-10	0	49	63*	7	6	-9	224	244	21	7	8	-4	86	56	48*
6	16	0	0	136	72*	7	2	-10	109	29	61*	7	4	-9	237	240	19	7	6	-8	0	53	64*	7	8	-3	140	71	27*
6	16	1	100	43	57*	7	2	-9	349	352	13	7	4	-8	0	20	62*	7	6	-7	0	91	62*	7	8	-2	219	262	19
6	16	2	0	123	71*	7	2	-8	73	90	59*	7	4	-7	89	129	52*	7	6	-6	70	34	61*	7	8	-1	509	501	12
6	16	3	99	68	69*	7	2	-7	174	168	21	7	4	-6	55	81	62*	7	6	-5	290	320	14	7	8	0	196	213	20
6	16	4	97	111	54*	7	2	-6	133	91	28*	7	4	-5	628	651	13	7	6	-4	100	158	61*	7	8	1	137	186	29*
6	16	5	0	3	71*	7	2	-5	629	618	12	7	4	-4	245	264	15	7	6	-3	118	123	60*	7	8	2	91	48	43*
6	17	-1	0	21	67*	7	2	-4	97	185	63*	7	4	-3	123	106	30*	7	6	-2	0	43	63*	7	8	3	546	548	12
6	17	0	23	122	69*	7	2	-3	45	17	57*	7	4	-2	219	197	17	7	6	-1	691	703	17	7	8	4	0	22	67*
6	17	1	120	26	67*	7	2	-2	83	82	46*	7	4	-1	597	618	12	7	6	0	190	210	20	7	8	5	34	181	66*
7	0	-13	144	97	24	7	2	-1	660	658	15	7	4	0	0	27	58*	7	6	1	361	368	12	7	8	6	0	44	65*
7	8	7	206	229	23	7	11	-5	95	15	64*	7	14	-3	72	35	66*	8	1	6	460	502	11	8	3	10	168	208	27
7	8	8	81	52	66*	7	11	-4	72	52	54*	7	14	-2	116	7	64*	8	1	7	122	118	63*	8	3	11	0	25	67*
7	8	9	208	184	24	7	11	-3	361	350	14	7	14	-1	268	224	18	8	1	8	153	207	27*	8	3	12	0	94	66*
7	8	10	0	11	70*	7	11	-2	58	17	65*	7	14	0	0	74	71*	8	1	9	36	12	63*	8	4	-12	0	109	65*
7	8	11	115	91	68*	7	11	-1	0	66	66*	7	14	1	70	115	70*	8	1	10	214	206	19	8	4	-11	60	20	53*
7	9	-11	0	124	70*	7	11	0	117	82	63*	7	14	2	0	82	70*	8	1	11	0	5	68*	8	4	-10	84	130	64*
7	9	-10	0	51	68*	7	11	1	219	236	21	7	14	3	0	211	77*	8	1	12	0	133	64*	8	4	-9	117	7	64*
7	9	-9	140	103	32*	7	11	2	46	94	66*	7	14	4	0	21	71*	8	2	-13	0	4	63*	8	4	-8	310	298	15
7	9	-8	0	84	67*	7	11	3	53	112	67*	7	14	5	90	86	73*	8	2	-12	82	116	63*	8	4	-7	0	65	64*
7	9	-7	281	258	17	7	11	4	7	77	66*	7	14	6	0	37	74*	8	2	-11	22	3	61*	8	4	-6	267	236	15
7	9	-6	0	61	66*	7	11	5	228	246	23	7	15	-5	0	30	67*	8	2	-10	39	176	66*	8	4	-5	90	106	51*
7	9	-5	0	2	64*	7	11	6	111	69	43*	7	15	-4	125	32	70*	8	2	-9	88	30	46*	8	4	-4	431	452	11
7	9	-4	123	189	35*	7	11	7	237	186	21	7	15	-3	203	160	23	8	2	-8	297	306	14	8	4	-3	84	170	43*
7	9	-3	329	349	14	7	11	8	127	48	38*	7	15	-2	74	61	67*	8	2	-7	0	10	65*	8	4	-2	549	573	11
7	9	-2	0	48	63*	7	11	9	110	122	46*	7	15	-1	90	71	68*	8	2	-6	293	285	15	8	4	-1	160	194	24
7	9	-1	20	57	62*	7	12	-9	129	128	38*	7	15	0	0	70	75*	8	2	-5	229	217	18	8	4	0	666	639	12
7	9	0	12	107	65*	7	12	-8	106	49	58*	7	15	1	194	216	28	8	2	-4	680	640	12	8	4	1	0	65	61*
7	9	1	480	503	11	7	12	-7	0	32	67*	7	15	2	61	34	55*	8	2	-3	106	101	61*	8	4	2	173	178	22
7	9	2	107	61	63*	7	12	-6	0	25	66*	7	15	3	53	79	73*	8	2	-2	218	225	17	8	4	3	95	83	63*
7	9	3	189	193	23	7	12	-5	299	278	16	7	15	4	0	21	75*	8	2	-1	373	376	11	8	4	4	499	541	12
7	9	4	0	25	70*	7	12	-4	84	52	54*	7	16	-1	223	191	22	8	2	0	569	562	13	8	4	5	81	31	44*
7	9	5	262	302	19	7	12	-3	0	16	67*	7	16	0	71	20	69*	8	2	1	114	191	63*	8	4	6	144	93	27*
7	9	6	21	57	56*	7	12	-2	131	30	33*	7	16	1	104	59	69*	8	2	2	236	238	17	8	4	7	128	165	67*
7	9	7	201	175	24	7	12	-1	282	265	18	8	0	-12	85	97	46*	8	2	3	65	30	50*	8	4	8	183	186	25
7	9	8	40	48	69*	7	12	0	83	78	67*	8	0	-10	218	230	18	8	2	4	489	497	12	8	4	9	92	55	67*
7	9	9	96	129	70*	7	12	1	130	100	67*	8	0	-8	251	331	16	8	2	5	0	94	62*	8	4	10	25	46	56*
7	9	10	0	58	70*	7	12	2	0	85	65*	8	0	-6	269	255	13	8	2	6	60	40	48*	8	4	11	0	9	66*
7	9	11	183	142	28	7	12	3	251	234	19	8	0	-4	649	639	16	8	2	7	0	184	65*	8	4	12	188	147	24
7	10	-11	0	115	71*	7	12	4	0	75	66*	8	0	-2	0	6	58*	8	2	8	303	336	15	8	5	-12	182	147	23
7	10	-10	72	2	57*	7	12	5	202	172	25	8	0	0	794	699	15	8	2	9	0	61	66*	8	5	-11	0	47	66*
7	10	-9	175	156	26	7	12	6	0	80	72*	8	0	2	500	520	11	8	2	10	176	161	25	8	5	-10	21	168	69*
7	10	-8	148	82	30*	7	12	7	158	162	32*	8	0	4	434	423	11	8	2	11	76	16	45*	8	5	-9	95	3	54*
7	10	-7	98	69	54*	7	12	8	109	33	73*	8	0	6	95	43	58*	8	2	12	80	118	64*	8	5	-8	99	114	65*
7	10	-6	93	18	55*	7	12	9	59	92	74*	8	0	8	286	357	16	8	3	-12	120	117	62*	8	5	-7	0	2	65*
7	10	-5	402	384	13	7	13	-8	122	104	39*	8	0	10	127	179	66*	8	3	-11	122	11	32*	8	5	-6	336	348	14
7	10	-4	63	30	65*	7	13	-7	82	156	67*	8	0	12	0	127	66*	8	3	-10	206	197	21	8	5	-5	0	4	60*
7	10	-3	95	98	43*	7	13	-6	89	62	46*	8	1	-13	0	2	61*	8	3	-9	70	20	44*	8	5	-4	441	468	11
7	10	-2	109	157	38*	7	13	-5	0	14	69*	8	1	-12	145	113	27*	8	3	-8	186	192	22	8	5	-3	99	75	59*
7	10	-1	318	317	15	7	13	-4	0	14	67*	8	1	-11	0	0	57*	8	3	-7	100	97	62*	8	5	-2	485	500	11
7	10	0	83	46	62*	7	13	-3	228	253	22	8	1	-10	193	193	20	8	3	-6	450	451	11	8	5	-1	112	107	61*
7	10	1	0	37	56*	7	13	-2	0	94	70*	8	1	-9	0	13	50*	8	3	-5	80	116	61*	8	5	0	193	176	21
7	10	2	50	53	64*	7	13	-1	0	71	68*	8	1	-8	311	334	14	8	3	-4	406	405	12	8	5	1	87	167	63*
7	10	3	319	343	16	7	13	0	0	32	68*	8	1	-7	117	70	30*	8	3	-3	102	33	60*	8	5	2	691	677	13
7	10	4	0	76	67*	7	13	1	219	225	23	8	1	-6	416	465	11	8	3	-2	506	521	12	8	5	3	0	29	60*
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7	10	6	0	51	65*	7	13	3	52	145	74*	8	1	-4	73	130	62*	8	3	0	309	296	13	8	5	5	0	64	65*
7	10	7	191	203	26	7	13	4	140	127	71*	8	1	-3	101	46	60*	8	3	1	249	210	15	8	5	6	303	304	16
7	10	8	74	82	67*	7	13	5	211	189	24	8	1	-2	857	826	15	8	3	2	705	667	16	8	5	7	0	20	65*
7	10	9	122	147	62*	7	13	6	104	40	54*	8	1	-1	0	69	61*	8	3	3	24	34	60*	8	5	8	0	53	66*
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7	11	-8	0	29	67*	7	14	-6	133	64	67*	8	1	3	98	89	62*	8	3	7	0	64	66*	8	6	-12	88	67	66*
7	11	-7	271	269	19	7	14	-5	127	151	69*	8	1	4	301	320	14	8	3	8	59	56	66*	8	6	-11	0	27	66*
7	11	-6	113	84	65*	7	14	-4	126	76	34*	8	1	5	248	256	16	8	3	9	76	39	65*	8	6	-10	150	158	31*
8	6	-9	46	32	64*	8	8	0	490	487	11	8	11	-4	181	150	25	9	0	1	504	498	12	9	3	-8	110	35	64*
8	6	-8	253	246	18	8	8	1	127	133	64*	8	11	-3	132	38	32*	9	0	3	327	352	14	9	3	-7	348	313	14
8	6	-7	0	54	63*	8	8	2	174	144	25	8	11	-2	256	259	19	9	0	5	416	447	12	9	3	-6	60	8	63*
8	6	-6	175	227	24	8	8	3	81	5	65*	8	11	-1	140	37	30*	9	0	7	0	39	63*	9	3	-5	240	223	18
8	6	-5	133	106	29*	8	8	4	305	301	17	8	11	0	0	32	66*	9	0	9	272	291	16	9	3	-4	106	52	61*
8	6	-4	333	376	13	8	8	5	0	89	69*	8	11	1	107	7	41*	9	0	11	54	45	62*	9	3	-3	309	296	13
8	6	-3	109	6	35*	8	8	6	0	62	70*	8	11	2	224	213	23	9	1	-11	194	167	21	9	3	-2	122	65	31*
8	6	-2	295	305	15	8	8	7	0	29	68*	8	11	3	98	77	49*	9	1	-10	123	37	62*	9	3	-1	400	461	12
8	6	-1	234	217	18	8	8	8	231	238	22	8	11	4	83	25	72*	9	1	-9	55	64	44*	9	3	0	0	5	62*
8	6	0	649	662	13	8	8	9	0	24	70*	8	11	5	155	140	32*	9	1	-8	0	11	63*	9	3	1	225	219	18
8	6	1	95	163	65*	8	8	10	0	107	74*	8	11	6	296	281	19	9	1	-7	168	189	24	9	3	2	84	42	62*
8	6	2	23	25	53*	8	9	-10	144	101	33*	8	11	7	0	24	73*	9	1	-6	0	27	63*	9	3	3	505	500	11

8	6	3	0	51	64*	8	9	-9	0	16	70*	8	11	8	95	49	72*	9	1	-5	263	244	15	9	3	4	121	4	33*				
8	6	4	447	441	12	8	9	-8	225	242	23	8	12	-7	0	46	72*	9	1	-4	0	56	64*	9	3	5	0	173	67*				
8	6	5	102	37	62*	8	9	-7	0	60	67*	8	12	-6	203	147	22	9	1	-3	455	463	10	9	3	6	98	134	66*				
8	6	6	121	69	65*	8	9	-6	296	288	16	8	12	-5	57	67	56*	9	1	-2	79	14	56*	9	3	7	334	372	15				
8	6	7	0	19	67*	8	9	-5	0	15	64*	8	12	-4	181	204	26	-9	1	-1	629	601	13	9	3	8	82	60	66*				
8	6	8	183	179	27	8	9	-4	91	60	63*	8	12	-3	0	62	68*	9	1	0	107	10	62*	9	3	9	116	43	37*				
8	6	9	0	20	70*	8	9	-3	0	81	67*	8	12	-2	31	81	68*	9	1	1	289	248	14	9	3	10	67	27	55*				
8	6	10	65	77	58*	8	9	-2	346	354	15	8	12	-1	0	4	65*	9	1	2	0	16	64*	9	4	-11	0	37	67*				
8	6	11	0	84	59*	8	9	-1	0	14	66*	8	12	0	196	175	24	9	1	3	459	462	11	9	4	-10	99	28	66*				
8	7	-11	60	80	51*	8	9	0	64	120	65*	8	12	1	0	35	71*	9	1	4	0	84	62*	9	4	-9	262	246	19				
8	7	-10	119	115	38*	8	9	1	0	42	69*	8	12	2	79	23	70*	9	1	5	123	215	66*	9	4	-8	0	10	67*				
8	7	-9	81	39	57*	8	9	2	334	314	16	8	12	3	109	129	70*	9	1	6	0	47	64*	9	4	-7	190	166	23				
8	7	-8	191	188	24	8	9	3	0	181	71*	8	12	4	290	268	19	9	1	7	331	361	14	9	4	-6	0	47	64*				
8	7	-7	68	58	46*	8	9	4	0	50	70*	8	12	5	0	25	72*	9	1	8	0	24	65*	9	4	-5	247	276	17				
8	7	-6	258	297	18	8	9	5	47	16	51*	8	12	6	0	11	74*	9	1	9	0	17	66*	9	4	-4	90	81	41*				
8	7	-5	0	115	65*	8	9	6	270	293	20	8	12	7	0	72	76*	9	1	10	0	2	66*	9	4	-3	273	303	15				
8	7	-4	170	186	24	8	9	7	0	38	73*	8	13	-6	0	112	68*	9	1	11	0	169	67*	9	4	-2	0	42	63*				
8	7	-3	0	80	64*	8	9	8	84	118	70*	8	13	-5	97	49	44*	9	2	-11	27	31	53*	9	4	-1	254	253	16				
8	7	-2	457	463	12	8	9	9	131	82	71*	8	13	-4	82	131	52*	9	2	-10	0	60	68*	9	4	0	119	112	32*				
8	7	-1	176	149	23	8	9	10	100	160	52*	8	13	-3	123	38	66*	9	2	-9	175	219	24	9	4	1	498	471	11				
8	7	0	176	187	23	8	10	-9	133	70	34*	8	13	-2	174	190	29	9	2	-8	94	2	65*	9	4	2	0	20	63*				
8	7	1	202	182	21	8	10	-8	112	152	67*	8	13	-1	0	76	71*	9	2	-7	154	149	26*	9	4	3	0	156	66*				
8	7	2	580	599	12	8	10	-7	0	48	67*	8	13	0	0	3	66*	9	2	-6	26	143	65*	9	4	4	0	24	67*				
8	7	3	76	92	56*	8	10	-6	113	193	71*	8	13	1	0	72	69*	9	2	-5	302	287	16	9	4	5	443	462	13				
8	7	4	77	31	49*	8	10	-5	79	76	65*	8	13	2	178	220	31*	9	2	-4	0	49	65*	9	4	6	67	20	64*				
8	7	5	125	74	34*	8	10	-4	293	320	17	8	13	3	109	13	74*	9	2	-3	362	351	13	9	4	7	142	118	31*				
8	7	6	205	227	23	8	10	-3	0	47	66*	8	13	4	0	6	76*	9	2	-2	138	39	24*	9	4	8	130	44	67*				
8	7	7	110	29	65*	8	10	-2	100	58	67*	8	13	5	66	98	75*	9	2	-1	380	362	11	9	4	9	111	203	70*				
8	7	8	119	84	69*	8	10	-1	0	33	67*	8	14	-4	0	107	67*	9	2	0	80	33	50*	9	4	10	130	51	68*				
8	7	9	0	85	70*	8	10	0	79	232	70*	8	14	-3	0	61	69*	9	2	1	573	563	14	9	5	-10	114	17	38*				
8	7	10	193	144	26	8	10	1	0	104	69*	8	14	-2	133	79	67*	9	2	2	0	16	61*	9	5	-9	82	93	67*				
8	7	11	0	10	71*	8	10	2	103	81	44*	8	14	-1	155	60	30*	9	2	3	193	176	21	9	5	-8	0	2	67*				
8	8	-11	131	17	66*	8	10	3	0	40	68*	8	14	0	196	219	28	9	2	4	0	34	65*	9	5	-7	284	280	17				
8	8	-10	202	176	24	8	10	4	317	298	17	8	14	1	0	14	76*	9	2	5	411	445	13	9	5	-6	0	34	66*				
8	8	-9	0	67	70*	8	10	5	79	95	54*	8	14	2	73	15	70*	9	2	6	0	32	68*	9	5	-5	216	246	20				
8	8	-8	170	172	27	8	10	6	32	82	70*	8	14	3	129	78	72*	9	2	7	107	113	65*	9	5	-4	120	9	60*				
8	8	-7	122	8	34*	8	10	7	0	89	72*	8	14	4	119	187	76*	9	2	8	51	64	64*	9	5	-3	226	193	20				
8	8	-6	100	231	66*	8	10	8	226	235	25	9	0	-11	0	32	60*	9	2	9	169	254	29*	9	5	-2	0	118	67*				
8	8	-5	0	4	66*	8	10	9	79	4	72*	9	0	-9	129	167	29*	9	2	10	0	12	66*	9	5	-1	352	342	13				
8	8	-4	342	384	15	8	11	-8	35	149	58*	9	0	-7	25	111	59*	9	2	11	0	19	67*	9	5	0	0	35	64*				
8	8	-3	0	61	65*	8	11	-7	0	105	70*	9	0	-5	314	327	13	9	3	-11	159	141	28*	9	5	1	293	316	16				
8	8	-2	0	44	66*	8	11	-6	139	178	70*	9	0	-3	483	484	11	9	3	-10	100	38	64*	9	5	2	101	49	64*				
8	8	-1	23	145	66*	8	11	-5	110	51	65*	9	0	-1	382	329	13	9	3	-9	101	82	63*	9	5	3	526	519	13				
9	5	4	83	51	47*	9	8	-2	119	68	66*	9	11	6	0	57	77*	10	2	-1	113	23	59*	10	5	-2	202	165	22				
9	5	5	87	52	56*	9	8	-1	221	237	22	9	12	-5	180	184	27	10	2	0	413	365	12	10	5	-1	0	47	64*				
9	5	6	114	10	67*	9	8	0	107	44	66*	9	12	-4	51	86	69*	10	2	1	175	169	24	10	5	0	131	124	34*				
9	5	7	231	244	22	9	8	1	311	321	17	9	12	-3	0	131	71*	10	2	2	337	290	14	10	5	1	0	90	65*				
9	5	8	85	58	51*	9	8	2	0	23	70*	9	12	-2	149	35	31*	10	2	3	0	104	67*	10	5	2	324	354	16				
9	5	9	0	80	59*	9	8	3	145	161	33*	9	12	-1	67	132	54*	10	2	4	206	225	22	10	5	3	0	4	68*				
9	5	10	95	37	68*	9	8	4	99	43	68*	9	12	0	0	56	72*	10	2	5	59	63	65*	10	5	4	226	209	21				
9	6	-10	0	12	66*	9	8	5	214	232	25	9	12	1	203	199	28	10	2	6	195	248	25	10	5	5	87	26	71*				
9	6	-9	242	202	20	9	8	6	113	42	59*	9	12	2	109	29	48*	10	2	7	99	66	66*	10	5	6	0	199	74*				
9	6	-8	106	12	40*	9	8	7	23	11	71*	9	12	3	78	62	56*	10	2	8	68	105	69*	10	5	7	35	17	69*				
9	6	-7	193	167	22	9	8	8	53	26	72*	9	12	4	123	54	63*	10	2	9	0	4	66*	10	5	8	186	218	28				
9	6	-6	80	10	64*	9	9	-8	133	21	68*	9	13	-2	0	110	73*	10	3	-9	99	18	66*	10	6	-8	203	196	25				
9	6	-5	227	234	19	9	9	-7	204	200	24	9	13	-1	107	174	73*	10	3	-8	0	2	67*	10	6	-7	0	64	69*				
9	6	-4	0	128	66*	9	9	-6	74	107	56*	9	13	0	0	16	69*	10	3	-7	0	0	68*	10	6	-6	62	37	65*				
9	6	-3	315	314	15	9	9	-5	184	198	25	9	13	1	101	80	63*	10	3	-6	262	293	19	10	6	-5	80	46	50*				
9	6	-2	94	26	62*	9	9	-4	0	20	68*	9	13	2	127	35	75*	10	3	-5	81	21	65*	10	6	-4	309	303	15				
9	6	-1	300	247	14	9	9	-3	216	209	22	10	0	-10	82	12	62*	10	3	-4	0	43	65*	10	6	-3	132	64	67*				
9	6	0	149	71	27*	9	9	-2	0	6	68*	10	0	-8	174	211	22	10	3	-3	0	93	66*	10	6	-2	0	157	72*				
9	6	1	438	424	13	9	9	-1	264	244	19	10	0	-6	0	8	61*	10	3	-2	273	276	18	10	6	-1	0	112	69*				
9	6	2	0	70	65*	9	9	0	0	13	68*	10	0	-4	428	423	11	10	3	-1	45	111	63*	10	6	0	135	242	71*				
9	6	3	148	202	32*	9	9	1	116	162	68*	10	0	-2	99	176	62*	10	3	0	266	244	17	10	6	1	140	5	31*				
9	6	4	22	16	65*	9	9	2	99	41	47*	10	0	0	478	467	10	10	3	1	64	85	64*	10	6	2	144	107	30*				
9	6	5	295	309	17	9	9	3	243	265	22	10	0	2	313	306	14	10	3	2	347	349	14	10	6	3	71	10	69*				
9	6	6	104	16	67*	9	9	4	136	63	35*	10	0	4	106	84	53*	10	3	3	107	44	56*	10	6	4	258	271	21				
9	6	7	94	16	67*	9	9	5	126	51	68*	10	0	6	181	214	24	10	3	4	294	284	16	10	6	5	0	37	70*				
9	6	8	70	16	69*	9	9	6	0	60	72*	10	0	8	59	128	65*	10	3	5	79	5	66*	10	6	6	141	231	75*				
9	6	9	157	176	33*	9	9	7	195	216	30	10	1	-10	176	194	24	10	3	6	106	178	68*	10	6	7	81	14	68*				
9	6	10	99	48	49*	9	9	8	0	32	71*	10	1	-9	0	10	65*	10	3	7	106	53	68*	10	6	8	110	67	68*				
9	7	-10	72	43	68*	9	10	-7	106	71	56*	10	1	-8	0	5	66*	10	3	8	209	192	22	10	7	-8	82	29	70*				
9	7	-9	127	62	68*	9	10	-6	107	26	57*	10	1	-7	21	23	47*	10	3	9	0	36	69*	10	7	-7	0	33	69*				
9	7	-8	48	39	47*	9	10	-5	239	260	21	10	1	-6	232	234	19	10	4	-9	91	3	67*	10	7	-6	259	273	19				
9	7	-7	220	215	22	9	10	-4	139	38	32*	10	1	-5	69	16	51*	10	4	-8	288	277	18	10	7	-5	79	113	48*				
9	7	-6	121	81	65*	9	10	-3	182	216	26	10	1	-4	0	38	62*	10	4	-7	100	7	65*	10	7	-4	177	135	24				
9	7	-5	282	291	17	9	10	-2	95	8	51*	10	1	-3	0	39	60*	10	4	-6	86	67	55*	10	7	-3	0	47	66*				
9	7	-4	74	10	49*	9	10	-1	176	138	27	10	1	-2	562	556	13	10	4	-5	47	5	54*	10	7	-2	301	283	18				
9	7	-3	175	183	26	9	10	0	92	14	66*	10	1	-1	59	44	61*	10	4	-4	236	248	18	10	7	-1	0	28	67*				
9	7	-2	100	38	64*	9	10	1	220	214	23	10	1	0	277	290	17	10	4	-3	102	53	53*	10	7	0	0	78	68*				
9	7	-1	314	300	15	9	10	2	87	15	69*	10	1	1	92	87	56*	10	4	-2	41	112	68*	10	7	1	0	97	70*				
9	7	0	120	73	67*	9	10	3	54	75	73*	10	1	2	257	210	18	10	4	-1	66	95	63*	10	7	2	216	230	24				
9	7	1	314	290	16	9	10	4	134	81	71*	10	1	3	43	33	64*	10	4	0	295	274	16	10	7	3	0	24	71*				
9	7	2	0	76	67*	9	10	5	264	245	21	10	1	4	261	286	18	10	4	1	108	98	55*	10	7	4	150	177	34*				
9	7	3	320	337	17	9	10	6	61	3	72*	10	1	5	143	28	27*	10	4	2	273	251	17	10	7	5	25	5	72*				
9	7	4	0	37	71*	9	10	7	94	53	61*	10	1	6	167	132	25	10	4	3	76	69	66*	10	7	6	0	125	74*				
9	7	5	0	78	70*	9	11	-6	36	77	66*	10	1	7	0	14	64*	10	4	4	271	324	19	10	7	7	60	72	74*				
9	7	6	0	20	71*	9	11	-5	150	86	31*	10	1	8	162	185	27	10	4	5	0	30	57*	10	8	-7	29	44	67*				
9	7	7	244	228	22	9	11	-4	0	16	59*	10	1	9	0	12	65*	10	4	6	211	231	24	10	8	-6	0	2	71*				
9	7	8	54	21	70*	9	11	-3	138	209	71*	10	2	-10	0	38	68*	10	4	7	86	26	66*	10	8	-5	0	37	57*				
9	7	9	0	6	73*	9	11	-2	110	47	56*	10	2	-9	0	26	68*	10	4	8	0	92	73*	10	8	-4	259	303	21				
9	8	-9	206	159	23	9	11	-1	181	201	28	10	2	-8	243	253	19	10	5	-9	72	41	57*	10	8	-3	83	58	48*				
9	8	-8	115	104	41*	9	11	0	0	8	69*	10	2	-7	49	42	64*	10	5	-8	0	36	68*	10	8	-2	101	114	59*				
9	8	-7	207	148	22	9	11	1	108	62	46*	10	2	-6	92	25	55*	10	5	-7	0	16	58*	10	8	-1	0	57	72*				
9	8	-6	0	22	66*	9	11	2	72	61	70*	10	2	-5	78	89	65*	10	5	-6	304	343	16	10	8	0	281	261	18				
9	8	-5	189	214	24	9	11	3	244	220	23	10	2	-4	352	341	14	10	5	-5	0	67	65*	10	8	1	0	29	70*				
9	8	-4	128	38	32*	9	11	4	0	3	72*	10	2	-3	0	5	62*	10	5	-4	0	144	65*	10	8	2	83	131	62*				
9	8	-3	258	271	19	9	11	5	101	82	72*	10	2	-2	137	146	27*	10	5	-3	92	25	55*	10	8	3	92	103	74*				
10	8	4	93	124	75*	11	2	-4	0	114	70*	11	6	0	0	3	71*																
10	8	5	52	105	71*	11	2	-3	281	295	18	11	6	1	223	275	25																
10	8	6	145	180	38*	11	2	-2	104	39	62*	11	6	2	0	43	72*																
10	9	-6	120	176	69*	11	2	-1	0	21	65*	11	6	3	0	28	73*																
10	9	-5	162	43	27*	11	2	0	56	141	68*	11	6	4	77	45	51*																
10	9	-4	0	29	72*	11	2	1	349	333	15	11	6	5	155	199	36*																
10	9	-3	123	14	39*	11	2	2	0	121	69*	11	7	-4	163	107	27																
10	9	-2	258	286	22	11	2	3	102	136	46*	11	7	-3	128	24	70*																
10	9	-1	111	15	43*	11	2	4	0	4	72*	11	7	-2	0	6	72*																
10	9	0	45	129	73*	11	2	5	253	255	19	11	7	-1	278	269	20																
10	9	1	36	13	73*	11	2	6	106	57	55*	11	7	0	61	22	51*																
10	9	2	160	156	35*	11	3	-7	108	117	59*	11	7	1	130	23	71*																
10	9	3	0	72	75*	11	3	-6	0	48	75*	11	7	2	0	30	75*																
10	9	4	189	167	30	11	3	-5	257	243	19	11	7	3	0	216	78*																
10	9	5	0	58	74*	11	3	-4	24	6	53*	11	7	4	177	23	28																
10	10	-4	109	198	72*	11	3	-3	92	10	63*	11	8	-3	247	243	22																
10	10	-3	0	33	67*	11	3	-2	64	19	68*	11	8	-2	166	64	31*																
10	10	-2	27	44	72*	11	3	-1	326	340	15	11	8	-1	0	36	73*																
10	10	-1	0	34	72*	11	3	0	114	45	65*	11	8	0	0	2	73*																
10	10	0	69	239	77*	11	3	1	103	99	55*	11	8	1	230	257	25																
10	10	1	0	68	63*	11	3	2	32	96	67*	11	8	2	133	15	72*																
10	10	2	235	208	25	11	3	3	307	285	16	12	0	-2	182	234	28																
10	10	3	0	59	78*	11	3	4	0	25	70*	12	0	0	173	157	25																
10	10	4	166	96	34*	11	3	5	98	55	67*	12	0	2	270	270	17																
10	11	-2	206	192	27	11	3	6	0	17	57*	12	1	-3	120	4	61*																

10	11	-1	0	89	76*	11	4	-6	126	42	66*	12	1	-2	64	150	68*
10	11	0	113	144	76*	11	4	-5	0	84	69*	12	1	-1	0	12	67*
10	11	1	74	7	74*	11	4	-4	125	38	63*	12	1	0	235	241	21
10	11	2	130	164	45*	11	4	-3	285	321	17	12	1	1	0	22	70*
11	0	-7	226	245	19	11	4	-2	86	18	65*	12	1	2	106	75	68*
11	0	-5	155	52	22	11	4	-1	158	124	28*	12	2	-3	53	47	70*
11	0	-3	273	285	16	11	4	0	85	122	56*	12	2	-2	239	274	21
11	0	-1	133	129	68*	11	4	1	288	281	18	12	2	-1	90	26	70*
11	0	1	361	350	14	11	4	2	118	48	37*	12	2	0	165	97	31*
11	0	3	235	195	18	11	4	3	0	13	70*	12	2	1	42	82	72*
11	0	5	227	238	19	11	4	4	124	10	70*	12	2	2	265	239	20
11	0	7	138	119	29*	11	4	5	273	271	19	12	3	-2	16	95	71*
11	1	-7	70	14	64*	11	4	6	107	28	68*	12	3	-1	67	5	57*
11	1	-6	76	41	55*	11	5	-6	0	27	70*	12	3	0	284	263	18
11	1	-5	249	249	20	11	5	-5	247	280	19	12	3	1	0	6	70*
11	1	-4	45	14	64*	11	5	-4	58	62	63*						
11	1	-3	139	139	28*	11	5	-3	0	55	69*						
11	1	-2	0	8	63*	11	5	-2	104	39	57*						
11	1	-1	330	323	14	11	5	-1	297	301	18						
11	1	0	0	22	67*	11	5	0	0	2	69*						
11	1	1	0	36	65*	11	5	1	0	42	69*						
11	1	2	81	74	50*	11	5	2	0	26	70*						
11	1	3	323	328	16	11	5	3	229	262	23						
11	1	4	0	46	69*	11	5	4	0	25	71*						
11	1	5	137	204	69*	11	5	5	136	56	71*						
11	1	6	0	27	68*	11	6	-5	0	82	68*						
11	1	7	189	169	24	11	6	-4	48	75	70*						
11	2	-7	0	226	70*	11	6	-3	310	289	17						
11	2	-6	0	5	68*	11	6	-2	0	42	69*						
11	2	-5	99	58	57*	11	6	-1	76	53	54*						

D. [Bz_2SnCl_2(2,2'-bipyridyl)]

Crystallographic Data and Refinement details for $[Bz_2SnCl_2(2,2'\text{-bipyridyl})]$.

Formula	$C_{24}H_{22}Cl_2N_2Sn$
Formula weight	528.1
Crystal morphology	yellow block
Crystal dimensions (mm)	0.13 x 0.35 x 0.48
Crystal system	triclinic
Space group	$P\bar{1}$, (C_i^1, No. 2)
Temperature (°C)	20.0
a (Å)	10.547(3)
b (Å)	13.152(3)
c (Å)	9.363(2)
α (°)	98.66(2)
β (°)	111.74(2)
γ (°)	67.71(2)
V (Å^3)	1116.1(5)
Z	2
D_{calc} (g cm^{-3})	1.571
F(000)	528
Radiation	MoKα (λ = 0.7107Å)
μ (cm^{-1})	14.02
θ limits, data (°)	3.0 to 27.5
hkl range	0 to 14 , -17 to 17, -12 to 12
Range of transmission factors	0.969 to 1
Scan technique	ω:2θ
Scan width (°)	1.05
No. of data measured	5415
No. of unique data	5137
R_{amal}	0.040
Program for structure solution	Direct Methods (SHELXS86)
No. of unique data used	4403
No. of parameters	262
R	0.028
R_w	0.031
G.O.F.	1.97
Min./Max. residual electron density (e Å^{-3})	-0.69 to +0.55

Fractional atomic coordinates ($Å^2$) for the non-hydrogen atoms in $[Bz_2SnCl_2(2,2'\text{-bipyridyl})]$.

Atom	*x*	*y*	*z*
Sn	0.08500(2)	0.18564(2)	0.42152(2)
Cl(1)	0.3022(1)	0.0313(1)	0.5704(1)
Cl(2)	-0.0832(1)	0.2422(1)	0.5762(1)
N(1)	-0.0716(3)	0.3274(2)	0.2382(3)
N(2)	0.1812(3)	0.1759(2)	0.2254(3)
C(1)	-0.0135(3)	0.0693(3)	0.2851(4)
C(2)	-0.1523(3)	0.1197(2)	0.1575(3)
C(3)	-0.1535(4)	0.1311(3)	0.0121(4)
C(4)	-0.2823(5)	0.1835(3)	-0.1037(4)
C(5)	-0.4113(4)	0.2243(3)	-0.0749(5)
C(6)	-0.4125(4)	0.2122(3)	0.0671(2)
C(7)	-0.2847(4)	0.1603(3)	0.1841(4)
C(8)	0.1789(3)	0.3057(3)	0.5534(3)
C(9)	0.2762(3)	0.3320(3)	0.4959(3)
C(10)	0.4179(3)	0.2594(3)	0.5137(4)
C(11)	0.5088(4)	0.2843(3)	0.4639(5)
C(12)	0.4616(5)	0.3828(4)	0.3919(5)
C(13)	0.3223(5)	0.4563(3)	0.3727(4)
C(14)	0.2210(4)	0.4304(3)	0.4219(4)
C(15)	-0.1942(6)	0.4028(3)	0.2548(4)
C(16)	-0.2808(4)	0.4893(3)	0.1551(5)
C(17)	-0.2385(5)	0.4980(4)	0.0371(5)
C(18)	-0.1135(5)	0.4204(3)	0.0191(5)
C(19)	-0.0322(3)	0.3343(3)	0.1216(4)
C(20)	0.1002(3)	0.2448(3)	0.1056(3)
C(21)	0.1363(4)	0.2276(3)	-0.0250(4)
C(22)	0.2576(4)	0.1391(4)	-0.0335(4)
C(23)	0.3412(4)	0.0729(3)	0.0904(4)
C(24)	0.3002(3)	0.0931(3)	0.2176(4)

Anisotropic thermal parameters ($Å^2$) for the non-hydrogen atoms in $[Bz_2SnCl_2(2,2'\text{-bipyridyl})]$.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Sn	0.0406(1)	0.0415(1)	0.0382(1)	-0.0138(8)	0.0123(7)	0.0008(7)
Cl(1)	0.057(1)	0.059(1)	0.062(1)	-0.005(1)	0.013(1)	0.019(1)
Cl(2)	0.057(1)	0.080(1)	0.057(1)	-0.027(1)	0.028(1)	-0.004(1)
N(1)	0.048(1)	0.038(1)	0.047(1)	-0.016(1)	0.011(1)	0.001(1)
N(2)	0.049(1)	0.044(1)	0.042(1)	-0.018(1)	0.015(1)	-0.001(1)
C(1)	0.063(2)	0.042(2)	0.053(2)	-0.024(2)	0.02(1)	-0.01(1)
C(2)	0.052(2)	0.039(2)	0.055(2)	-0.03(1)	0.02(1)	-0.01(1)
C(3)	0.063(2)	0.050(2)	0.052(2)	-0.029(2)	0.016(2)	-0.01(1)
C(4)	0.095(3)	0.063(2)	0.055(2)	-0.034(2)	0.004(2)	-0.001(2)
C(5)	0.067(2)	0.066(3)	0.076(3)	-0.011(2)	-0.007(2)	-0.007(2)
C(6)	0.052(2)	0.073(3)	0.105(3)	-0.022(2)	0.018(2)	-0.023(2)
C(7)	0.064(2)	0.064(2)	0.070(2)	-0.036(2)	0.026(2)	-0.017(2)
C(8)	0.050(2)	0.053(2)	0.048(2)	-0.022(2)	0.02(1)	-0.01(1)
C(9)	0.046(2)	0.049(2)	0.048(2)	-0.02(1)	0.01(1)	-0.01(1)
C(10)	0.046(2)	0.057(2)	0.063(2)	-0.018(2)	0.017(2)	-0.007(2)
C(11)	0.052(2)	0.080(3)	0.084(3)	-0.027(2)	0.030(2)	-0.017(2)
C(12)	0.084(3)	0.099(3)	0.093(3)	-0.057(3)	0.047(2)	-0.024(3)
C(13)	0.101(3)	0.064(2)	0.073(2)	-0.045(2)	0.032(2)	-0.005(2)
C(14)	0.056(2)	0.053(2)	0.062(2)	-0.022(2)	0.016(2)	-0.011(2)
C(15)	0.057(2)	0.046(2)	0.065(2)	-0.012(2)	0.018(2)	-0.004(2)
C(16)	0.071(2)	0.049(2)	0.090(3)	0.003(2)	0.017(2)	0.007(2)
C(17)	0.095(3)	0.064(3)	0.094(3)	0.001(2)	0.021(3)	0.035(2)
C(18)	0.088(3)	0.068(3)	0.076(3)	-0.018(2)	0.019(2)	0.028(2)
C(19)	0.057(2)	0.044(2)	0.050(2)	-0.02(1)	0.01(1)	0.01(1)
C(20)	0.055(2)	0.051(2)	0.04(1)	-0.03(1)	0.01(1)	-0.01(1)
C(21)	0.076(2)	0.083(3)	0.045(2)	-0.037(2)	0.018(2)	0.008(2)
C(22)	0.089(3)	0.094(3)	0.055(2)	-0.045(2)	0.041(2)	-0.013(2)
C(23)	0.069(2)	0.067(2)	0.072(2)	-0.025(2)	0.040(2)	-0.011(2)
C(24)	0.053(2)	0.052(2)	0.053(2)	-0.02(1)	0.03(1)	-0.01(1)

Fractional atomic coordinates and *B*eq values ($Å^2$) for the hydrogen atoms in $[Bz_2SnCl_2(2,2'\text{-bipyridyl})]$.

Atom	x	y	z	B_{eq}
H(1a)	0.0556	0.0158	0.2408	4.8
H(1b)	-0.0330	0.0323	0.3522	5.1
H(3a)	-0.0626	0.1020	-0.0088	5.1
H(4a)	-0.2813	0.1911	-0.2049	6.8
H(5a)	-0.5017	0.2619	-0.1550	7.3
H(6a)	-0.5042	0.2403	0.0857	7.2
H(7a)	-0.2872	0.1522	0.2843	5.9
H(8a)	0.0991	0.3734	0.5558	4.6
H(8b)	0.2348	0.2782	0.6570	5.3
H(10a)	0.4524	0.1894	0.5630	4.8
H(11a)	0.6070	0.2325	0.4787	6.3
H(12a)	0.5257	0.4001	0.3549	7.2
H(13a)	0.2890	0.5264	0.3243	6.8
H(14a)	0.1312	0.4818	0.4048	5.5
H(15a)	-0.2225	0.3962	0.3398	5.5
H(16a)	-0.3693	0.5428	0.1685	7.3
H(17a)	-0.2965	0.5585	-0.0342	8.3
H(18a)	-0.0828	0.4261	-0.0640	7.4
H(21a)	0.0769	0.2773	-0.1108	5.9
H(22a)	0.2824	0.1246	-0.1263	6.6
H(23a)	0.4289	0.0122	0.0890	5.9
H(24a)	0.3602	0.0451	0.3052	4.8

Bond distances (Å) for [Bz_2SnCl_2(2,2'-bipyridyl)].

Atom - Atom	Distance	Atom - Atom	Distance
Sn - Cl(1)	2.504(1)	C(8) - C(9)	1.483(4)
Sn - Cl(2)	2.525(1)	C(9) - C(10)	1.398(4)
Sn - N(1)	2.383(2)	C(9) - C(14)	1.390(4)
Sn - N(2)	2.372(2)	C(10) - C(11)	1.364(5)
Sn - C(1)	2.165(3)	C(11) - C(12)	1.380(6)
Sn - C(8)	2.166(3)	C(12) - C(13)	1.381(6)
N(1) - C(15)	1.345(4)	C(13) - C(14)	1.382(5)
N(1) - C(19)	1.330(4)	C(15) - C(16)	1.378(5)
N(2) - C(20)	1.349(4)	C(16) - C(17)	1.369(6)
N(2) - C(24)	1.332(4)	C(17) - C(18)	1.379(6)
C(1) - C(2)	1.489(4)	C(18) - C(19)	1.386(4)
C(2) - C(3)	1.387(4)	C(19) - C(20)	1.487(4)
C(2) - C(7)	1.396(4)	C(20) - C(21)	1.374(4)
C(3) - C(4)	1.385(5)	C(21) - C(22)	1.384(5)
C(4) - C(5)	1.373(6)	C(22) - C(23)	1.358(5)
C(5) - C(6)	1.366(6)	C(23) - C(24)	1.370(4)
C(6) - C(7)	1.385(5)		

Bond angles (°) for [Bz_2SnCl_2(2,2'-bipyridyl)].

Atom - Atom - Atom	Angle	Atom - Atom - Atom	Angle
Cl(1) - Sn - Cl(2)	104.37(3)	C(3) - C(4) - C(5)	119.7(4)
Cl(1) - Sn - N(1)	162.05(6)	C(4) - C(5) - C(6)	120.0(3)
Cl(1) - Sn - N(2)	93.54(6)	C(5) - C(6) - C(7)	121.0(4)
Cl(1) - Sn - C(1)	90.33(8)	C(2) - C(7) - C(6)	119.7(4)
Cl(1) - Sn - C(8)	91.27(8)	Sn - C(8) - C(9)	116.5(2)
Cl(2) - Sn - N(1)	93.29(6)	C(8) - C(9) - C(10)	121.6(3)
Cl(2) - Sn - N(2)	162.08(6)	C(8) - C(9) - C(14)	121.2(3)
Cl(2) - Sn - C(1)	92.24(9)	C(10) - C(9) - C(14)	117.3(3)
Cl(2) - Sn - C(8)	87.70(8)	C(9) - C(10) - C(11)	121.7(3)
N(1) - Sn - N(2)	68.88(8)	C(10) - C(11) - C(12)	120.3(3)
N(1) - Sn - C(1)	92.2(1)	C(11) - C(12) - C(13)	119.3(4)
N(1) - Sn - C(8)	86.2(1)	C(12) - C(13) - C(14)	120.3(4)
N(2) - Sn - C(1)	86.9(1)	C(9) - C(14) - C(13)	121.1(3)
N(2) - Sn - C(8)	92.6(1)	N(1) - C(15) - C(16)	122.0(3)
C(1) - Sn - C(8)	178.4(1)	C(15) - C(16) - C(17)	118.2(3)
Sn - N(1) - C(15)	121.4(2)	C(16) - C(17) - C(18)	120.0(4)
Sn - N(1) - C(19)	118.7(2)	C(17) - C(18) - C(19)	119.1(4)
C(15) - N(1) - C(19)	119.9(3)	N(1) - C(19) - C(18)	120.8(3)
Sn - N(2) - C(20)	118.7(2)	N(1) - C(19) - C(20)	116.9(3)
Sn - N(2) - C(24)	121.4(2)	C(18) - C(19) - C(20)	122.2(3)
C(20) - N(2) - C(24)	118.9(3)	N(2) - C(20) - C(19)	115.9(3)
Sn - C(1) - C(2)	114.2(2)	N(2) - C(20) - C(21)	120.7(3)
C(1) - C(2) - C(3)	121.4(3)	C(19) - C(20) - C(21)	123.3(3)
C(1) - C(2) - C(7)	120.1(3)	C(20) - C(21) - C(22)	119.8(3)
C(3) - C(2) - C(7)	118.5(3)	C(21) - C(22) - C(23)	118.8(3)
C(2) - C(3) - C(4)	121.0(3)	C(22) - C(23) - C(24)	119.2(3)
N(2) - C(24) - C(23)	122.5(3)		

Observed and calculated structure factors for $[Bz_2SnCl_2(2,2'\text{-bipyridyl})]$.

h	k	l	Fo	Fc	sigF
0	0	2	1227	1236	7
0	0	3	309	308	3
0	0	4	161	173	3
0	0	5	621	626	4
0	0	6	663	680	5
0	0	7	485	479	4
0	0	8	223	226	4
0	0	9	141	139	3
0	0	10	51	47	4
0	0	11	109	105	3
0	1	-11	100	96	3
0	1	-10	160	154	3
0	1	-9	85	83	3
0	1	-8	43	46	5
0	1	-7	36	27	5
0	1	-6	282	279	3
0	1	-5	392	392	3
0	1	-4	540	535	4
0	1	-3	107	113	2
0	1	-2	125	137	2
0	1	2	379	402	3
0	1	3	330	352	3
0	1	4	388	396	3
0	1	5	0	11	12*
0	1	6	220	232	4
0	1	7	358	355	4
0	1	8	271	278	4
0	1	9	202	206	4
0	1	10	100	99	3
0	1	11	21	38	12*
0	2	-11	0	5	14*
0	2	-10	46	43	5
0	2	-9	246	243	4
0	2	-8	215	214	4
0	2	-7	192	188	4
0	2	-6	287	285	3
0	2	-5	10	23	13*
0	2	-4	333	330	3
0	2	-3	517	523	3
0	2	-2	817	815	5
0	2	-1	773	780	4
0	2	0	1041	1031	6
0	2	1	231	243	2
0	2	2	422	426	3
0	2	3	133	121	3
0	2	4	504	505	4
0	2	5	314	334	3
0	2	6	387	385	4
0	2	7	180	172	4
0	2	8	10	6	15*
0	2	9	101	98	3
0	2	10	134	133	3
0	2	11	136	134	3
0	3	-11	102	104	3
0	3	-10	93	91	3
0	3	-9	101	84	3
0	3	-8	159	157	3
0	3	-7	218	208	4
0	3	-6	339	337	4
0	3	-5	507	493	4
0	3	-4	380	381	3
0	3	-3	205	206	3
0	3	-2	270	280	3
0	3	-1	265	277	2
0	3	0	996	975	6
0	3	1	568	559	4
0	3	2	350	359	3
0	3	3	16	16	12*
0	3	4	133	150	3
0	3	5	463	458	4
0	3	6	227	232	4
0	3	7	274	277	4
0	3	8	185	177	4
0	3	9	90	87	3
0	3	10	0	5	15*
0	3	11	45	46	5
0	4	-10	175	173	4
0	4	-9	231	233	4
0	4	-8	301	300	4
0	4	-7	133	130	3
0	4	-6	89	93	3
0	4	-5	353	353	3
0	4	-4	581	582	4
0	4	-3	814	814	5
0	4	-2	1350	1311	8
0	4	-1	686	672	4
0	4	0	287	283	3
0	4	1	35	33	4
0	4	2	451	468	3
0	4	3	645	654	4
0	4	4	832	840	5
0	4	5	265	283	4
0	4	6	145	144	3
0	4	7	0	5	14*
0	4	8	123	121	3
0	4	9	181	175	4
0	4	10	152	152	3
0	5	-10	85	84	3
0	5	-9	179	178	4
0	5	-8	301	294	4
0	5	-7	324	316	4
0	5	-6	406	404	4
0	5	-5	138	131	3
0	5	-4	277	276	3
0	5	-3	276	290	3
0	5	-2	741	754	5
0	5	-1	921	916	5
0	5	0	652	655	4
0	5	1	276	282	3
0	5	2	13	9	13*
0	5	3	405	405	4
0	5	4	748	741	5
0	5	5	567	581	4
0	5	6	468	475	4
0	5	7	240	234	4
0	5	8	57	66	4
0	5	9	23	41	15*
0	5	10	149	138	3
0	6	-10	49	51	5
0	6	-9	36	38	7*
0	6	-8	34	33	7*
0	6	-7	79	83	3
0	6	-6	208	222	4
0	6	-5	329	332	4
0	6	-4	199	201	3
0	6	-3	40	31	4
0	6	-2	119	108	3
0	6	-1	213	210	3
0	6	0	370	374	3
0	6	1	373	388	3
0	6	2	331	334	3
0	6	3	312	318	4
0	6	4	13	13	15*
0	6	5	83	90	3
0	6	6	127	124	3
0	6	7	199	202	5
0	6	8	134	146	3
0	6	9	129	131	3
0	6	10	60	58	4
0	7	-10	94	92	3
0	7	-9	125	117	3
0	7	-8	176	168	5
0	7	-7	132	123	3
0	7	-6	144	144	3
0	7	-5	191	185	4
0	7	-4	228	236	4
0	7	-3	347	353	4
0	7	-2	411	413	4
0	7	-1	289	292	3
0	7	0	224	214	3
0	7	1	246	247	4
0	7	2	371	359	4
0	7	3	358	356	4
0	7	4	458	464	4
0	7	5	214	206	4
0	7	6	150	147	4
0	7	7	23	37	17*
0	7	8	91	97	4
0	7	9	124	132	3
0	7	10	138	145	4
0	8	-9	45	45	6
0	8	-8	125	124	3
0	8	-7	146	147	4
0	8	-6	332	346	4
0	8	-5	185	190	4
0	8	-4	138	142	3
0	8	-3	32	27	7*
0	8	-2	131	130	3
0	8	-1	386	375	4
0	8	0	421	418	4
0	8	1	472	461	4
0	8	2	69	68	4
0	8	3	86	94	4
0	8	4	95	99	3
0	8	5	188	187	4
0	8	6	266	264	5
0	8	7	160	156	4
0	8	8	76	84	4
0	8	9	18	34	17*
0	9	-9	130	127	3
0	9	-8	61	57	5
0	9	-7	43	39	6
0	9	-6	161	153	3
0	9	-5	374	396	4
0	9	-4	381	393	4
0	9	-3	367	357	4
0	9	-2	385	375	4
0	9	-1	81	68	4
0	9	0	137	142	3
0	9	1	436	454	4
0	9	2	416	409	4
0	9	3	370	360	4
0	9	4	280	277	5
0	9	5	198	193	4
0	9	6	72	68	5
0	9	7	132	137	3
0	9	8	180	176	4
0	9	9	140	135	4
0	10	-8	146	145	3
0	10	-7	96	92	3
0	10	-6	53	56	5
0	10	-5	83	80	4
0	10	-4	234	243	5
0	10	-3	305	298	5
0	10	-2	358	349	5
0	10	-1	271	262	4
0	10	0	149	141	4
0	10	1	83	75	4
0	10	2	257	251	5
0	10	3	255	256	5
0	10	4	274	263	5
0	10	5	274	259	5
0	10	6	126	127	3
0	10	7	52	46	6
0	10	8	0	19	18*
0	11	-8	47	39	6
0	11	-7	73	77	4
0	11	-6	119	120	3
0	11	-5	101	97	3
0	11	-4	149	148	4
0	11	-3	0	11	19*
0	11	-2	0	5	19*
0	11	-1	283	274	5
0	11	0	148	141	4
0	11	1	252	243	5
0	11	2	129	127	4
0	11	3	94	98	4
0	11	4	0	49	19*
0	11	5	122	119	4
0	11	6	156	160	4
0	11	7	70	72	5
0	11	8	104	111	4
0	12	-7	0	33	17*
0	12	-6	24	16	15*
0	12	-5	82	90	4
0	12	-4	148	145	3
0	12	-3	184	167	4
0	12	-2	205	204	4
0	12	-1	85	84	5
0	12	0	119	110	4
0	12	1	86	88	5
0	12	2	168	164	4
0	12	3	277	270	5
0	12	4	217	213	4
0	12	5	113	117	4
0	12	6	24	38	19*
0	12	7	20	14	19*
0	13	-6	108	112	4
0	13	-5	85	79	5
0	13	-4	26	1	15*
0	13	-3	31	60	20*
0	13	-2	144	131	4
0	13	-1	230	226	4
0	13	0	201	191	5
0	13	1	68	63	6
0	13	2	90	94	5
0	13	3	0	30	20*
0	13	4	111	112	4
0	13	5	123	128	4
0	13	6	67	67	6
0	14	-5	155	149	4
0	14	-4	148	139	4
0	14	-3	49	53	9*
0	14	-2	15	15	20*
0	14	-1	102	96	5
0	14	0	178	180	4
0	14	1	226	228	5
0	14	2	125	123	4
0	14	3	151	155	4
0	14	4	24	36	20*
0	14	5	25	23	15*
0	15	-3	101	97	6
0	15	-2	81	80	6
0	15	-1	72	60	7
0	15	0	0	16	22*
0	15	1	3	60	22*
0	15	2	96	95	6
0	15	3	101	105	5
1	-15	-2	99	113	5
1	-15	-1	84	90	6
1	-15	0	0	22	22*
1	-15	1	0	16	21*
1	-15	2	43	48	11*
1	-14	-4	26	12	20*
1	-14	-3	64	53	7
1	-14	-2	111	114	5
1	-14	-1	150	152	4
1	-14	0	108	110	5
1	-14	1	81	92	6
1	-14	2	28	29	17*
1	-14	3	0	5	20*
1	-14	4	94	100	5
1	-13	-6	82	79	5
1	-13	-5	130	141	4
1	-13	-4	159	171	4
1	-13	-3	117	115	4
1	-13	-2	88	87	5
1	-13	-1	62	48	6
1	-13	0	65	59	6
1	-13	1	82	79	5
1	-13	2	114	111	4
1	-13	3	77	79	5
1	-13	4	58	48	6
1	-13	5	0	20	18*
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12	6	-1	23	7	16*	12	12	-2	92	85	5	13	9	-2	112	111	4												
12	6	0	81	74	4	12	12	-1	20	20	15*	13	10	-6	52	59	6												
12	6	1	108	109	4	12	13	-5	43	47	10*	13	10	-5	39	42	9*												
12	7	-9	133	139	3	12	13	-4	25	16	18*	13	10	-4	0	6	19*												
12	7	-8	134	139	3	12	13	-3	0	45	22*	13	10	-3	98	97	5												
12	7	-7	88	94	4	13	2	-6	94	95	4	13	10	-2	109	102	4												

Chapter 4 (Section II)

Examination of the Effect of Crystal Packing Forces on Geometric Parameters: A Crystallographic and Theoretical Study of 1,10-Phenanthroline Adducts of R_2SnCl_2

4.6 Introduction

In section I of this chapter we have shown that R_2SnCl_2(2,2'-bipyridyl) adducts are suitable candidates for systematic investigation. The structural motif is constant (i.e. *trans*-C_2, distorted octahedral), and the Lewis acidity of the tin center can be moderated by changing the nature of the tin-bound substituents. It was possible to determine the effect of crystal packing on molecular geometry and the influence of Lewis acidity on the geometric parameters [1]. It was established that crystal packing effects do indeed influence both the molecular geometry about the tin atom as, invariably, in the gas phase more symmetric structures are found and the derived interatomic parameters about the tin atom are lengthened. Given that the coordination potential of 2,2'-bipyridyl is approximately the same as that for 1,10-phenanthroline [2], it was thought worthwhile to conduct a similar crystallographic and theoretical study on a number of R_2SnCl_2(1,10-Phenanthroline) compounds.

In this section the crystal and molecular structures of R_2SnCl_2(1,10-Phenanthroline) are reported where R = ^{i}Pr, Cy, Bz and R_2 = Me, Ph (i.e. a mixed diorganotin system) and their derived interatomic parameters compared with the literature structures, i.e. R = Me [3], ^{n}Bu [4] and Ph [5]. Geometry optimisations have been conducted for all seven compounds (that for R = Me from [3, chapter 3] at the Hartree-Fock (HF) level of theory using the LanL2DZ basis set. As indicated in Chapter3 and earlier work [1,3] this procedure has proved appropriate for examining systems of the type reported herein. The results of this study will enable an examination of the influence of crystal packing on the molecular geometry as well as on the derived geometric parameters. In addition, it will be possible to correlate the variation of the Sn-ligand distances with systematic variations in the Lewis acidity of the R_2Sn moieties. This section expands the range of R_2Sn centers that have been examined using a combined crystallographic/theoretical approach and finally, it will provide a check of the consistency of the results obtained in section I of this chapter of the 2,2'-bipyridyl systems [1].

4.7 Results

Details of the experimental procedure employed in the synthesis of the compounds reported in this chapter are provided in Chapter 2. Spectroscopic characterizations are also provided in Chapter 2.

4.7.1 Crystallographic Studies

A series of structurally similar molecules R_2SnCl_2(1,10-phenanthroline) as determined by X-Ray crystallography are described and then compared to analogous literature structures. The experimental procedure employed in the data collection and the structure determinations are summarised in Chapter 2. Presented below are the experimental details unique to the R_2SnCl_2(1,10-phenanthroline), R= ^{i}Pr, Cy, CH_2Ph and R_2 = Me, Ph structure determinations. Details specific to each structure determination are summarised in Table 4.5. Crystal data and refinement details specific for these molecular structure determinations are provided in Appendix B of this chapter. All diagrams are drawn with ORTEP [6] at the 35% probability level.

In this section, a description of the four crystal and molecular structures of R_2SnCl_2(1,10-phenathroline) R = ^{i}Pr, Cy, CH_2Ph and R_2 = Me, Ph will be given as well as a summary of three related literature structures R = Me, [3] ^{n}Bu [4] and Ph[5]. Table 4.6 lists selected interatomic parameters for all seven structures. It is important to mention here that a correction for secondary extinction was applied in the refinement of [Ph(Me)$SnCl_2$(1,10-phenanthroline)] such that the extinction coefficient was 4.86714×10^{-8}.

TABLE 4.5: Crystallographic Data for R_2SnCl_2(1,10-phenanthroline) for R= ^{i}Pr, Cy Ph(Me) and Bz

	R_2SnCl_2(1,10-phenanthroline)			
Crystallographic Data	**R = ^{i}Pr**	**R = Cy**	**R = Ph(Me)**	**R = Bz**
Formula	$C_{18}H_{22}Cl_2N_2Sn$	$C_{24}H_{30}Cl_2N_2Sn$	$C_{19}H_{16}Cl_2N_2Sn$	$C_{26}H_{22}Cl_2N_2Sn$
Formula weight	454.1	536.1	461.9	552.1
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic
Space group	$P2_1/c$	$P2_1/n$	$P2_1/n$	$P2_1/n$
a, Å	8.261(2)	10.477(1)	9.118(2)	10.356(3)
b, Å	15.804(2)	16.167(2)	11.023(2)	17.540(2)
c, Å	15.804(2)	14.341(3)	18.712(2)	13.817(9)
α, (°)	90	90	90	90
β, (°)	104.82(1)	101.46(1)	93.03(1)	105.93(5)
γ, (°)	90	90	90	90
V, Å^3	1908.9(7)	2379.9(6)	1878.1(4)	2413(1)
Z	4	4	4	4
D_{calcd}, g cm^{-3}	1.579	1.496	1.634	1.519
Radiation, Å	Mo, 0.7107	Cu, 1.5418	Mo, 0.7107	Mo, 0.7107
μ, cm^{-1}	16.25	107.03	16.47	12.95
Trans coeff	0.978 - 1	0.972 - 1	0.987 - 1	0.938 - 1
2θ range, (°)	6.0 - 55.0	6.0 - 120.0	6.0 - 55.0	6.0 - 55.0
No. reflns meas	4891	3924	4842	6083
No. unique reflns	4590	3700	4565	5778
No of reflns used	2200	2644	2538	2576
No. of variables	208	262	218	271
R	0.045	0.043	0.036	0.045
R_W	0.046	0.054	0.036	0.044
Residual e$^-$/Å^3	0.50	1.03	0.41	1.07

[a] $I \geq 3.0\sigma(I)$

TABLE 4.6: Crystallographically Determined Interatomic Parameters (Å, deg.) for R_2SnCl_2(1,10-phenanthroline) for R= Me [3], ^{n}Bu [4], ^{i}Pr, Cy, Bz, Ph [5], and the mixed species Ph(Me)

	R_2SnCl_2(1,10-phenanthroline)						
Bond Distance	R = Me [a] (y = 1')	R = ^{n}Bu [b] (y = 5)	R = ^{i}Pr (y = 4)	R= Cy (y = 7)	R= Ph/Me (y = C(Ph))	R= Bz (y = 8)	R= Ph [c] (y = 7)
Sn-Cl(1)	2.521(3)	2.55(1)	2.569(2)	2.544(2)	2.500(2)	2.510(2)	2.449(1)
Sn-Cl(2)	2.521(3)	2.55(1)	2.536(2)	2.538(2)	2.487(1)	2.511(2)	2.456(1)
Sn-N(1)	2.385(9)	2.35(3)	2.396(6)	2.394(7)	2.386(4)	2.356(5)	2.341(3)
Sn-N(2)	2.385(9)	2.43(3)	2.399(6)	2.408(6)	2.410(4)	2.365(5)	2.378(3)
Sn-C(1)	2.075(8)	2.09(4)	2.155(9)	2.152(9)	2.130(6)	2.161(8)	2.143(4)
Sn-C(y)	2.075(8)	2.22(5)	2.171(8)	2.161(8)	2.146(5)	2.146(9)	2.133(4)
Bond Angle							
Cl(1)-Sn-Cl(2)	106.1(1)	104.7(4)	107.79(7)	105.70(8)	104.91(7)	104.46(7)	101.94(4)
Cl(1)-Sn-N(1)	161.3(3)	159.9(9)	160.9(1)	159.3(2)	163.4(1)	163.8(1)	162.89(8)
Cl(1)-Sn-N(2)	92.6(3)	92.4(7)	91.9(1)	89.6(2)	94.3(1)	93.8(1)	93.11(8)
Cl(1)-Sn-C(1)	90.7(1)	89(1)	91.8(3)	89.7(2)	89.1(2)	91.4(2)	94.6(1)
Cl(1)-Sn-C(y)	90.7(1)	91(1)	88.0(2)	90.9(2)	93.8(2)	87.2(2)	93.1(1)
Cl(2)-Sn-N(1)	92.6(3)	95.2(9)	91.2(2)	95.0(2)	91.4(1)	91.6(1)	95.17(8)
Cl(2)-Sn-N(2)	161.3(3)	162.6(2)	160.2(1)	164.6(2)	160.8(1)	161.7(1)	164.68(8)
Cl(2)-Sn-C(1)	90.7(1)	90(1)	88.9(3)	89.3(2)	92.1(2)	87.9(2)	92.24(9)
Cl(2)-Sn-C(y)	90.7(1)	87(1)	89.8(2)	87.4(2)	91.9(1)	92.3(2)	92.09(9)
N(1)-Sn-N(2)	68.7(5)	68(1)	69.1(2)	69.8(2)	69.4(1)	70.2(2)	69.8(1)
N(1)-Sn-C(1)	89.1(1)	88(1)	89.9(3)	91.0(3)	87.1(2)	90.9(2)	85.1(1)
N(1)-Sn-C(y)	89.1(1)	92(1)	90.8(3)	89.5(3)	88.8(2)	90.5(3)	85.8(1)
N(2)-Sn-C(1)	89.1(1)	93(1)	89.0(3)	92.5(3)	89.0(2)	90.0(2)	83.6(1)
N(2)-Sn-C(y)	89.1(1)	90(2)	92.6(2)	90.7(3)	86.0(2)	90.2(3)	90.0(1)
C(1)-Sn-C(y)	177.8(4)	177(2)	178.5(3)	176.7(3)	174.4(2)	178.5(3)	170.3(1)

a molecule has crystallographic *m2m* symmetry and ref: [3]; *b* [4]; *c* [5]

4.7.1a. [$^{i}Pr_2SnCl_2$(1,10-phenanthroline)]

White crystals were obtained from the slow evaporation of an acetonitrile/benzene solution (9/1 *v/v*) of the compound [$^{i}Pr_2SnCl_2$(1,10-phenanthroline)]; melting point: 228 - 230 °C.

The molecular structure of [$^{i}Pr_2SnCl_2$(1,10-phenanthroline)] is shown in Figure 4.13 from which it can be seen that the tin atoms exists in a *trans*-C_2, distorted octahedral geometry with two chloride atoms and two nitrogen atoms, derived from a bidentate 1,10-phenanthroline ligand, defining the basal plane. This motif is common to all of the structures described herein. The conformation of the ^{i}Pr groups is such that one has the methine hydrogen directed towards one side of the molecule approaching the Cl(1) atom and the other (containing the C(4) atom) with the methine hydrogen orientated between the two chloride atoms. This arrangement leads to a number of *intra*molecular Cl...H contacts, i.e. Cl(1)...H(1a), H(2a) and H(5b) of 2.90 Å, 2.76 Å and 2.89 Å, respectively and Cl(2)...H(6b) of 2.94 Å. Close Cl(1)...H(18) and Cl(2)...H(7) contacts of 2.87 Å and 2.85 Å, respectively are also noted. There are also several intermolecular Cl...H interactions of note (i.e. < 3.1 Å) involving Cl(1) with H(12a)^{i} and H(9a)^{i} of 2.92 Å and 3.04 Å, respectively and Cl(2) with H(17a)^{ii} and H(18a)^{ii} of 2.91 Å and 2.93 Å, respectively [symmetry operation *i*: -1 + *x*, 0.5 - *y*, -0.5 + *z*; *ii*: - *x*, 0.5 + *y*, 0.5 - *z*]; no evidence for base stacking was found in the crystal lattice. With this pattern of Cl...H interactions, it is not surprising that the Sn-Cl(1) distance of 2.569(2) Å is significantly longer than the Sn-Cl(2) distance of 2.536(2) Å in [$^{i}Pr_2SnCl_2$(1,10-phenanthroline)]; the significance of a consideration of *intra*- and inter-molecular Cl...H interactions and their importance in influencing geometric parameters have been noted [3]. The disparity in the Sn-Cl distances in this structure is not reflected in any difference between the Sn-N bond distances.

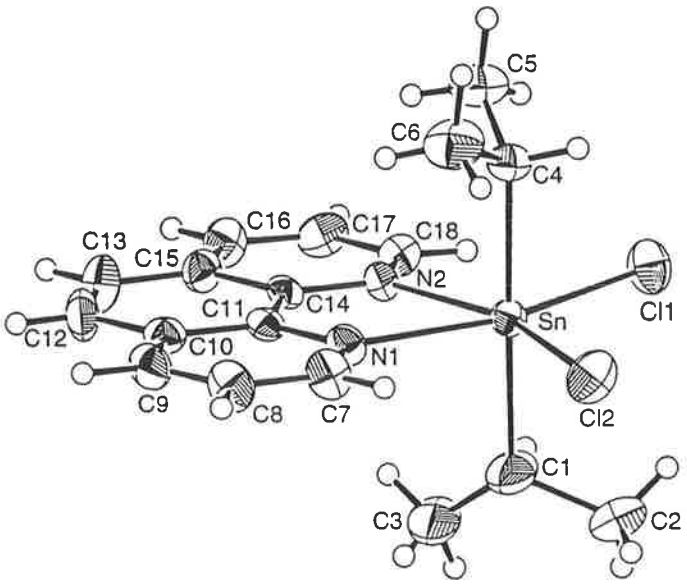


Figure 4.13

The molecular structure of [$^{i}Pr_2SnCl_2$(1,10-phenanthroline)]

4.7.1b. [Cy_2SnCl_2(1,10-phenanthroline)]

Yellow crystals were then obtained from the slow evaporation of an acetonitrile solution of [Cy_2SnCl_2(1,10-phenanthroline)]; melting point: 271 - 272°C.

The structure of [Cy_2SnCl_2(1,10-phenanthroline)] is illustrated in Figure 4.14. The cyclohexyl groups in this structure are orientated so that the both methine hydrogen atoms lie in positions between the two chloride atoms. In this conformation, several Cl...H interactions are present: Cl(1)...H(6b), H(8a) and H(24) are 2.98 Å, 2.95 Å and 2.76 Å, respectively and Cl(2)...H(2a), H(12b) and H(13) are 2.89 Å, 2.91 Å and 3.02 Å, respectively. Intermolecular Cl...H interactions are also present with Cl(1)...H(19a)^{i} and H(14a)^{ii} of 2.69 Å and 2.95 Å, respectively and Cl(2)...H(18a)^{i} and H(9a)^{iii} of 2.92 Å and 3.02 Å, respectively [symmetry operation *i*: -1 + *x*, *y*, *z*; *ii*: -0.5 + *x*, 0.5 - *y*, 0.5 + *z*; *iii*: -0.5 + *x*, 0.5 - *y*, -0.5 + *z*]. No base stacking was found in the lattice and no significant differences were found in the Sn-Cl bond distances or in the Sn-N distances.

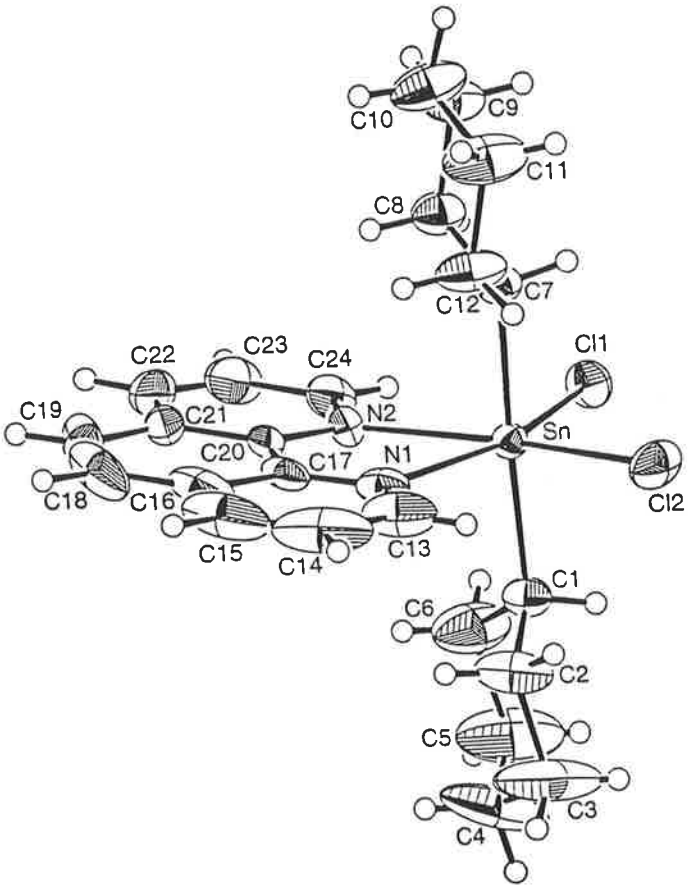


Figure 4.14

The molecular structure of [Cy_2SnCl_2(1,10-phenanthroline)]

4.7.1c. [Bz_2SnCl_2(1,10-phenanthroline)]

Orange crystals were then obtained from the slow evaporation of an acetonitrile/benzene solution (9/1 *v/v*) of [Bz_2SnCl_2(1,10-phenanthroline)], melting point: 220 - 221°C.

Figure 4.15 shows the molecular structure of [Bz_2SnCl_2(1,10-phenanthroline)] in which the benzyl groups lie to either side of the molecule. Except for the Cl...H(1,10-phenanthroline) *intra*molecular contacts (Cl(1)...H(26) 2.87 Å and Cl(2)...H(15) 2.77 Å), there are no such contacts involving the hydrogen atoms of the benzyl groups. Intermolecular Cl(1)...H(16)^{i} and H(24)^{ii} contacts of 2.70 Å and 2.96 Å and Cl(2)...H(20)^{iii} and H(25)^{ii} of 2.82 Å and 2.85 Å, respectively are found [symmetry operation *i*: 0.5 - *x*, -0.5 + *y*, -0.5 + *z*; *ii*: -0.5 - *x*, -0.5 + *y*, -0.5 + *z*; *iii*: -1 + *x*, *y*, *z*]; again, there is no base stacking in the lattice. Each of the pairs of Sn-Cl and Sn-N bond distances are equal within experimental error.

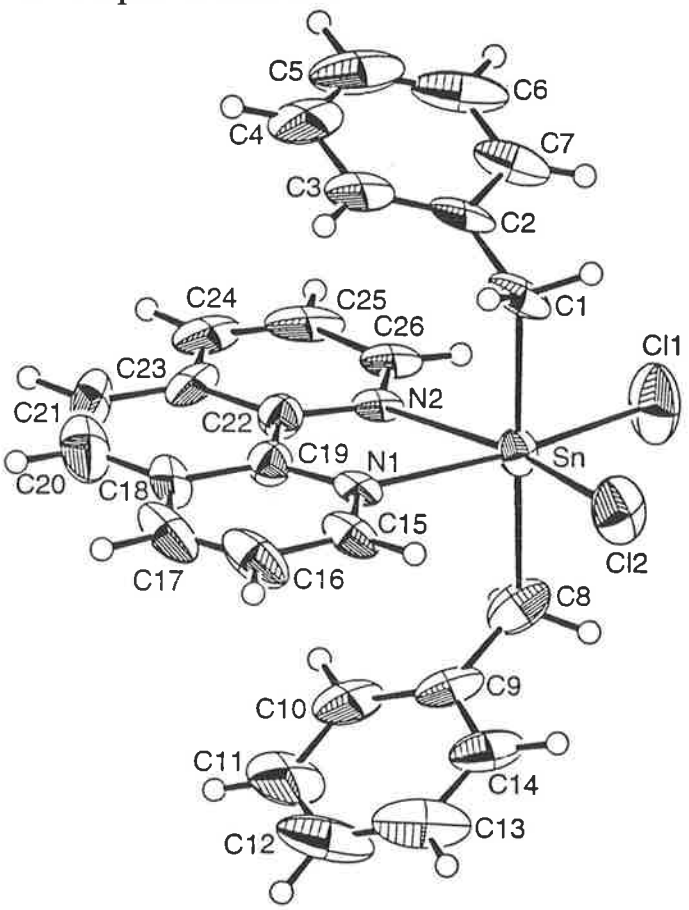


Figure 4.15

The molecular structure of [Bz_2SnCl_2(1,10-phenanthroline)]

4.7.1d. [Ph(Me)$SnCl_2$(1,10-phenanthroline)]

Transparent crystals were then obtained from the slow evaporation of an acetonitrile/chloroform solution of [Ph(Me)$SnCl_2$(1,10-phenanthroline)]; melting point: 207 - 209 °C.

The molecular structure of the mixed diorganotin compound, [Ph(Me)$SnCl_2$(1,10-phenanthroline)], is shown in Figure 4.16. The phenyl group is not symmetrically disposed in the molecule as seen in the C(1)/Sn/C(2)/C(3) torsion angle of -79(2)°. This has the result that the Cl(1) atom forms a contact of 2.70 Å with H(7) but except for Cl...H(1,10-phenanthroline) contacts (i.e. Cl(1)...H(19) is 2.98 Å and Cl(2)...H(8) 2.82 Å) there are no other Cl...H *intra*molecular interactions of note. In the lattice there are Cl(1)...H(18)^{i} and Cl(2)...H(17)^{ii} contacts of 2.86 Å and 2.79 Å, respectively [symmetry operation *i*: 1 - *x*, 2 - *y*, 1- *z*; *ii*: -0.5 + *x*, 1.5 - *y*, 0.5 + *z*]; no evidence was found for base stacking in the lattice. As for the R = Cy and Bz structures, there was no significant disparity in the Sn-Cl and Sn-N bond distances.

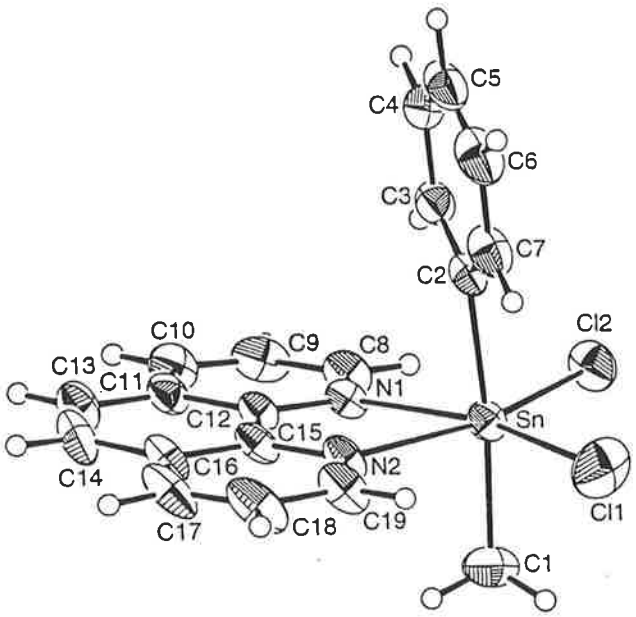


Figure 4.16

The molecular structure of [Ph(Me)$SnCl_2$(1,10-phenanthroline)]

4.7.1d. Other R_2SnCl_2(1,10-phenanthroline) structures: [Me_2SnCl_2(1,10-phenanthroline)] [3], [$^nBu_2SnCl_2$(1,10-phenanthroline)] [4] and [Ph_2SnCl_2(1,10-phenanthroline)] [5].

In addition to the four structures reported above, there are three other R_2SnCl_2(1,10-phenanthroline) structures that have been examined crystallographically. The three structures each feature the common motif and selected geometric parameters involving tin are collected in Table 4.6. In the R = Me compound [3] the tin atom lies on a site of symmetry *m2m*, implying a high degree of molecular symmetry and equivalence between chemically related pairs of geometric parameters. The R = ^{n}Bu structure [4] shows symmetrical Sn-Cl and Sn-N distances within experimental error, however, no molecular symmetry is evident; the rather low level of precision precludes a detailed discussion of geometric parameters. The R = Ph structure [5] shows that the phenyl rings are twisted so that the dihedral angle between them is 90.4°. This arrangement has the consequence that the *ortho*-hydrogen atoms of one phenyl group interact with the chloride atoms while those of the second phenyl group do not. Interestingly, the Sn-Cl bond distances are equal in this structure, but the Sn-N distances are not, even at the 5σ level. The chloride atoms form equivalent Cl...H *intra*- and inter-molecular interactions and no other feature in the crystal structure gives a clue for the apparent disparity in the Sn-N distances.

4.7.2 Geometry Optimisations

Experimental details pertaining to the geometry optimisation calculations presented below are discussed in Chapter 2. The results of the optimisations are discussed below.

In order to ascertain the influence of crystal packing effects on the molecular geometries and, therefore, the geometric parameters describing the tin atoms, all seven R_2SnCl_2(1,10-phenanthroline) structures have been subjected to geometry optimisation calculations at the HF level of theory employing the LanL2DZ basis set. This protocol has been demonstrated to be effective for the R_2SnCl_2(2,2'-bipyridyl) systems, (section one of this chapter and earlier work [3]).

The results of the geometry optimisation calculations for R_2SnCl_2(1,10-phenanthroline) will be described in the same order as the data presented in Table 4.7, which lists selected interatomic parameters calculated in the theoretical study.

4.7.2a. [Me_2SnCl_2(1,10-phenanthroline)] [3]

The geometry optimised structure of [Me_2SnCl_2(1,10-phenanthroline)] has been reported previously [3]. The crystallographically determined structure was shown to possess *m2m* symmetry and the same result was found in the optimised structure. Hence, this system provided an example where the influence of crystal packing effects on geometric parameters can be monitored in the absence of a significant change in molecular geometry. The key result of this study was that the Sn-Cl, Sn-N and Sn-C bond distances expanded by 0.029 Å, 0.034 Å and 0.038 Å, respectively in the isolated gas phase (i.e. theoretical) structure compared with the solid state. Hence, it may be concluded that at this level of theory, the removal of crystal packing effects allows for an expansion in the Sn-ligand bond distances. Similar observations were noted in related systems.

TABLE 4.7: Interatomic Parameters (Å, deg.) for R_2SnCl_2(1,10-phenanthroline) for R= Me[3], ^{n}Bu, ^{i}Pr, Cy, Bz, Ph, and the mixed species Ph(Me) as Derived from Geometry Optimisation Calculations

	R_2SnCl_2(2,2'-bipyridyl)						
Bond Distance	R = Me [3] (y = 2)	R = ^{n}Bu (y = 5)	R = ^{i}Pr (y = 4)	R= Cy (y = 7)	R= Ph/Me (y = C(Ph))	R= Bz (y = 8)	R= Ph (y = 7)
Sn-Cl(1)	2.550	2.566	2.632	2.595	2.538	2.573	2.522
Sn-Cl(2)	2.550	2.566	2.583	2.594	2.538	2.573	2.522
Sn-N(1)	2.419	2.439	2.413	2.388	2.407	2.354	2.373
Sn-N(2)	2.419	2.439	2.419	2.388	2.406	2.354	2.373
Sn-C(1)	2.113	2.136	2.166	2.171	2.115	2.155	2.137
Sn-C(y)	2.113	2.136	2.166	2.171	2.140	2.155	2.146
Bond Angle							
Cl(1)-Sn-Cl(2)	111.9	114.3	117.2	110.3	111.3	109.4	108.0
Cl(1)-Sn-N(1)	158.6	157.1	155.8	159.8	159.1	160.7	161.2
Cl(1)-Sn-N(2)	89.5	88.6	86.8	89.8	89.5	89.7	90.8
Cl(1)-Sn-C(1)	91.1	91.8	92.5	88.6	90.2	90.8	91.4
Cl(1)-Sn-C(y)	91.1	91.8	92.5	88.6	93.5	87.0	92.7
Cl(2)-Sn-N(1)	89.5	88.6	87.0	89.8	89.5	89.7	90.8
Cl(2)-Sn-N(2)	158.6	157.1	156.1	159.8	159.2	160.7	161.2
Cl(2)-Sn-C(1)	91.1	91.8	86.4	88.6	90.3	87.0	91.4
Cl(2)-Sn-C(y)	91.1	91.8	86.4	88.6	93.5	90.8	92.7
N(1)-Sn-N(2)	69.2	68.5	69.0	70.0	69.7	70.9	70.4
N(1)-Sn-C(1)	88.4	87.3	88.9	92.1	88.2	89.3	89.0
N(1)-Sn-C(y)	88.4	87.3	88.9	92.1	86.4	93.8	85.3
N(2)-Sn-C(1)	88.4	87.3	92.9	92.1	88.2	89.3	89.0
N(2)-Sn-C(y)	88.4	87.3	92.9	92.1	86.4	93.8	85.3
C(1)-Sn-C(y)	176.0	173.4	172.6	174.9	173.4	176.2	173.0

4.7.2b [$^nBu_2SnCl_2$(1,10-phenanthroline)] [4]

A symmetric structure was found in the gas phase for [$^nBu_2SnCl_2$(1,10-phenanthroline)] as shown in Figure 4.17. The structure in the gas phase has effective *m2m* symmetry and there appears to be a small elongation in the Sn-Cl distances but a more significant expansion of the Sn-N distances compared with the solid state structure. The optimised geometry is 1196.2 kJ mol^{-1} more stable than the solid state structure.

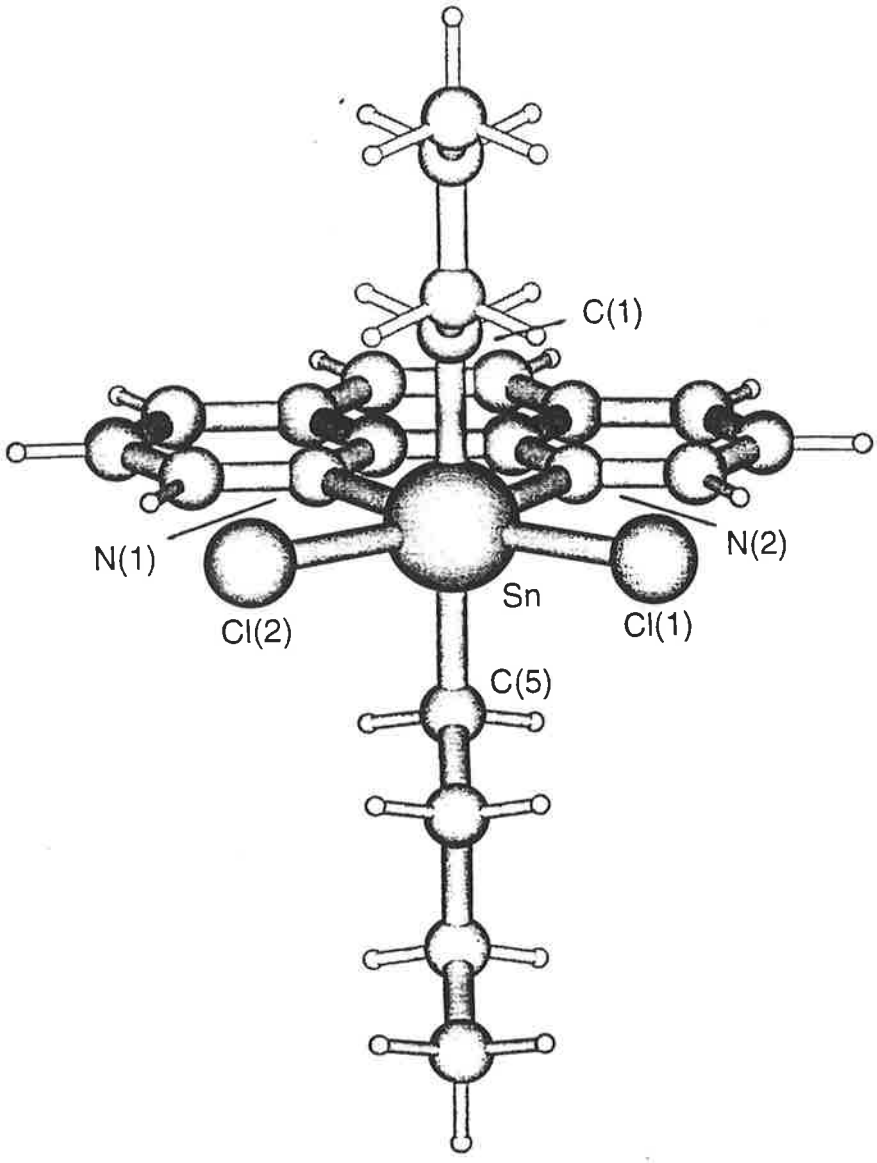


Figure 4.17

The optimised structure of [$^nBu_2SnCl_2$(1,10-phenanthroline)]

4.7.2c. [$^iPr_2SnCl_2$(1,10-phenanthroline)]

Consistent with the results of the previous study [1], the geometry optimisation of [$^iPr_2SnCl_2$(1,10-phenanthroline)] converges to a non-symmetrical structure with regard to the disposition of the isopropyl groups. As shown in Figure 4.18, the methyl groups of the tin-bound isopropyl substituents tend to lie over to one side of the molecule. More symmetric structures for [$^iPr_2SnCl_2$(1,10-phenanthroline)] were found to be of higher energy and it is suggested that the stability of the conformation shown in Figure 4.17 arises as a result of significant *intra*molecular Cl...H interactions. Thus, while both the Cl(1) and Cl(2) atoms form close *intra*molecular Cl...H(methyl) interactions of 2.85 Å (x 2) and 2.90 Å (x2), respectively, there are also two Cl(1)...H(methine) contacts of 3.07 Å but no equivalent Cl(2)...H(methine) distances. The consequence of the different *intra*molecular contacts is that the Sn-Cl(1) bond distance of 2.632 Å is significantly longer than the Sn-Cl(2) distance of 2.583 Å. It is noteworthy that the disparity in the Sn-Cl distances is not reflected in the Sn-N distances that are very similar, i.e. 2.413 Å and 2.419 Å. The most stable structure was 1200.1 kJ mol^{-1} lower in energy compared with the crystallographic determined structure.

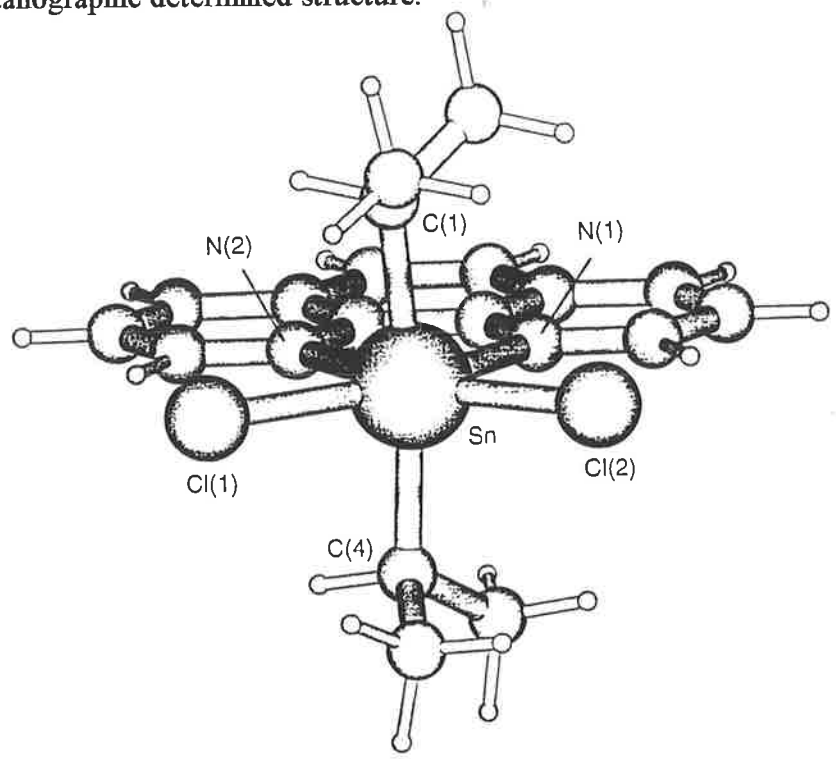


Figure 4.18

The optimised structure of [$^iPr_2SnCl_2$(1,10-phenanthroline)]

4.7.2d. [Cy_2SnCl_2(1,10-phenanthroline)]

The optimised structure of [Cy_2SnCl_2(1,10-phenanthroline)] is shown in Fig. 4.19. The gas phase (theoretical) structure is similar to the solid state structure (Figure 4.14), however, is more symmetrical, having very nearly *m2m* symmetry as found for [Me_2SnCl_2(1,10-phenanthroline)]. The Sn-Cl distances in the gas phase have expanded by approximately 0.05 Å compared with the crystal structure and the Sn-N distances have contracted marginally. The optimised structure was calculated to be 1396.2 kJ mol^{-1} more stable than the crystallographically determined structure.

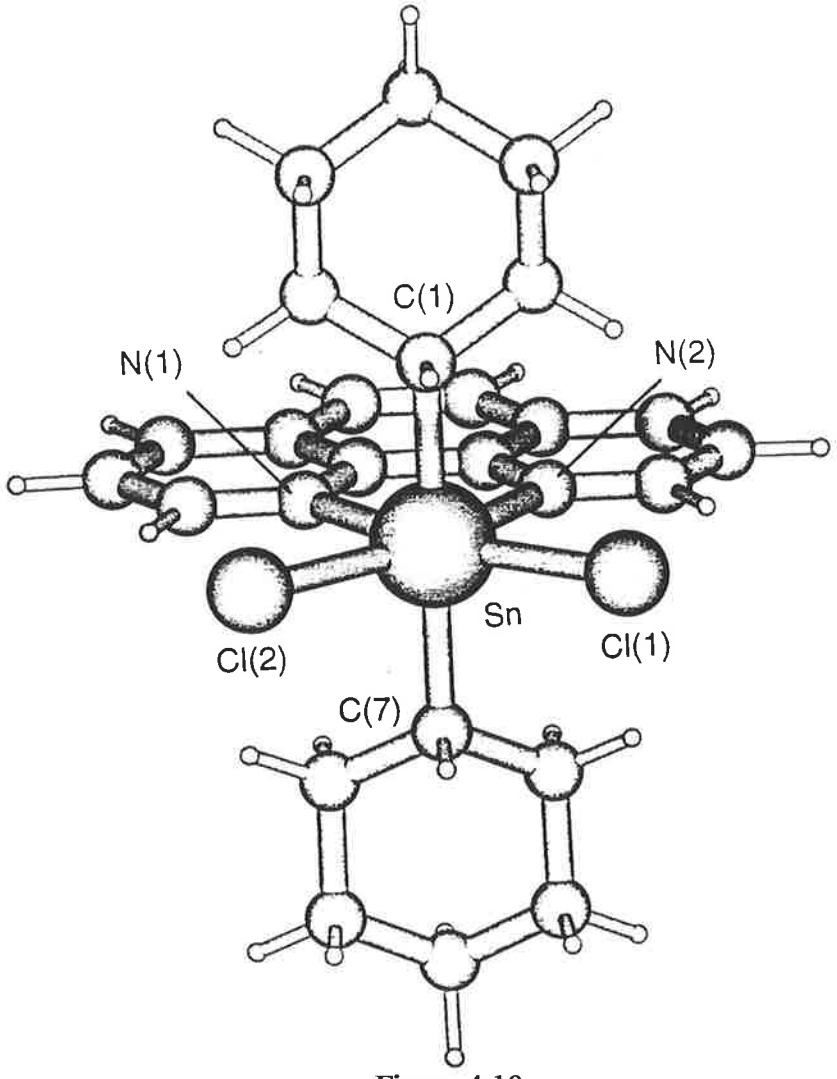


Figure 4.19

The optimised structure of [Cy_2SnCl_2(1,10-phenanthroline)]

4.7.2e. [Ph(Me)$SnCl_2$(1,10-phenanthroline)]

In the gas phase a more symmetrical structure is also found for [Ph(Me)$SnCl_2$(1,10-phenanthroline)] as shown in Figure 4.20; the different tin-bound substituents preclude *m2m* symmetry, however, the molecule is very close to *2m* symmetry. An expansion in the Sn-Cl distances is evident (*ca* 0.045 Å) as is a small increase in the Sn-N distance. The optimised geometry is 428.7 kJ mol^{-1} more stable than the solid state structure.

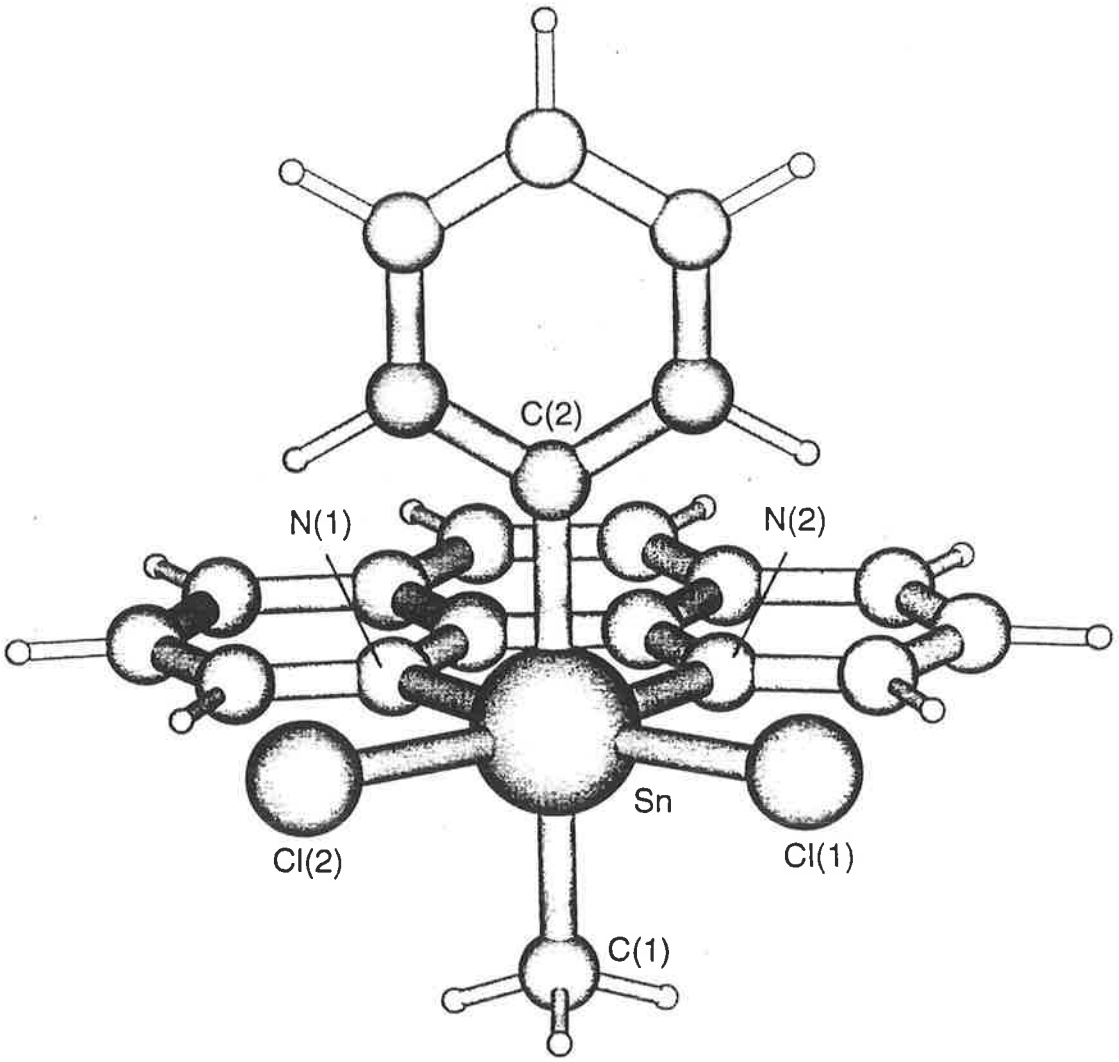


Figure 4.20
The optimised structure of [Ph(Me)$SnCl_2$(1,10-phenanthroline)]

4.7.2f [Bz_2SnCl_2(1,10-phenanthroline)]

Symmetrisation of the [Bz_2SnCl_2(1,10-phenanthroline)] molecule is also evident in the gas phase structure, see Figure 4.21, which has two-fold symmetry in which the axis bisects the $SnCl_2$ atoms. An expansion of approximately 0.06 Å is noted in the Sn-Cl distances with no significant change in Sn-N. The optimised structure was calculated to be 646.9 kJ mol^{-1} more stable than the solid state structure.

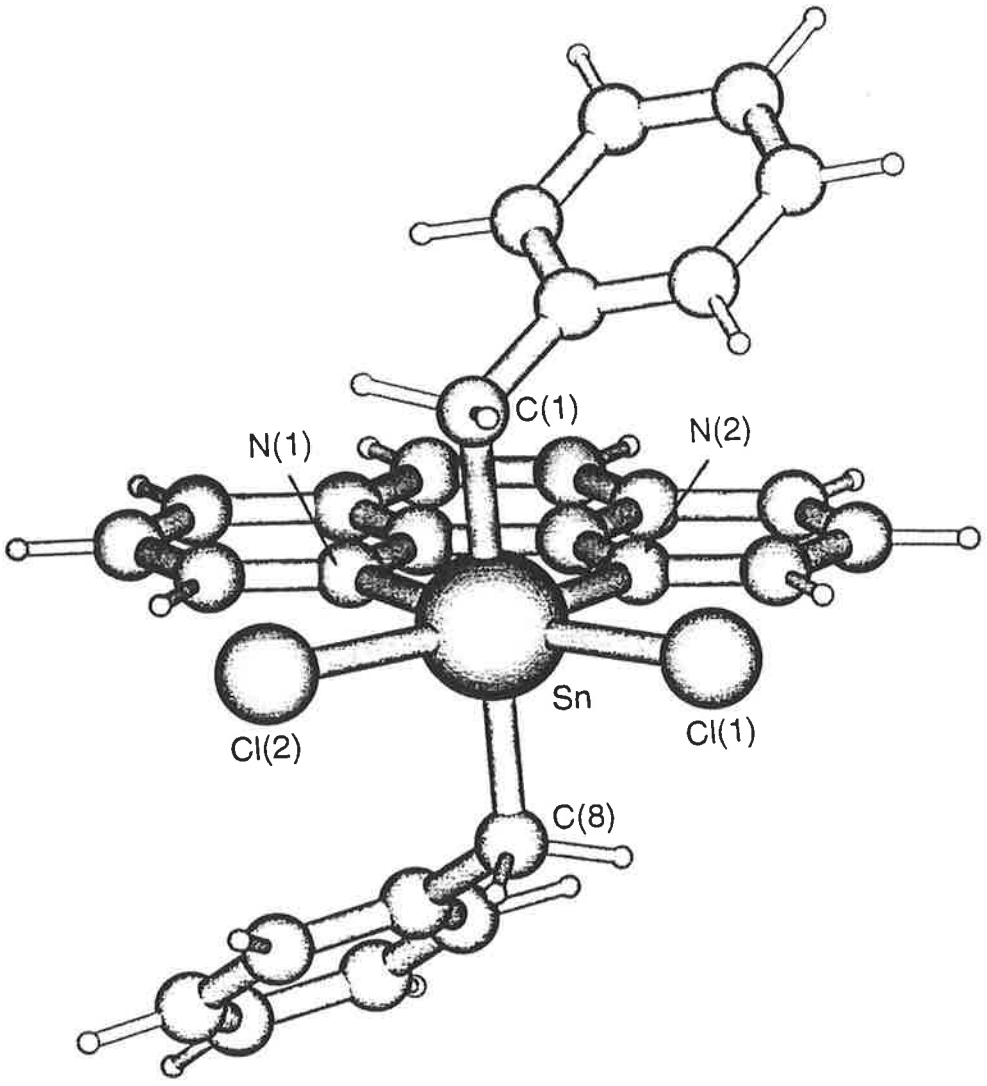


Figure 4.21

The optimised structure of [Bz_2SnCl_2(1,10-phenanthroline)]

4.7.2g [Ph_2SnCl_2(1,10-phenanthroline)]

The last structure to be subjected to a geometry optimisation is that of [Ph_2SnCl_2(1,10-phenanthroline)] as shown in Figure 4.22. In the gas phase structure the phenyl groups are rotated 90° with respect to each other and hence, there are *intra*molecular Cl...H(phenyl) interactions present for one phenyl group but not the for the other which accounts for the small disparity in the Sn-C distances. The molecule approximates 2*m* symmetry and an expansion in the Sn-Cl distances is noted. The optimised structure was calculated to be 518.0 kJ mol^{-1} more stable than the crystallographically determined structure.

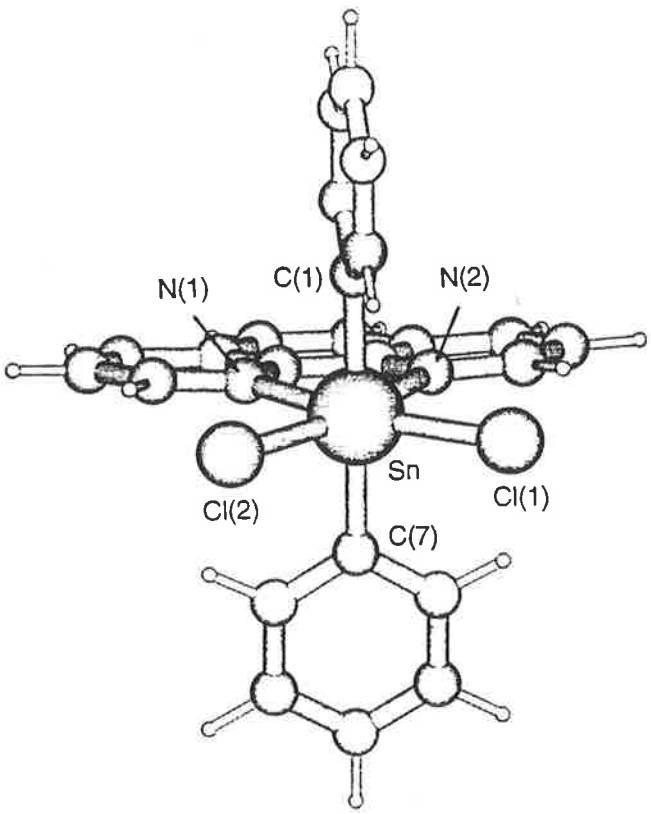


Figure 4.22

The optimised structure of [Ph_2SnCl_2(1,10-phenanthroline)]

4.7.3 Energy considerations

In previous contributions in this area, it has been argued that the energy differences calculated between the crystallographically determined structure and the optimised geometry are overestimated owing to a number of factors [1, 3]. A particularly important factor is the treatment of hydrogen atoms in the refinement. Another possible source of error in the calculated energies could be associated with the ECP approximation used to treat the tin atom. This has been eliminated as a significant source of error by comparing the energy difference between the crystal structure and optimised (isolated) geometry for [Bz_2SnCl_2(1,10-phenanthroline)] at both the LanL2DZ basis set (incorporating the ECP treatment) and the 3-21G** basis set (incorporating an all-electron treatment). The difference in energies using the LanL2DZ basis set is 646.9 kJ mol^{-1}, compared with 606.7 kJ mol^{-1} calculated using the 3-21G** basis set. The energy differences vary by only 6.2 %, a relatively minor amount compared to differences associated with hydrogen-atom location [3]. This result indicates that energy uncertainties do not arise from basis set approximations. For completeness the energy differences calculated for the seven compounds studied are collected in Table 4.8. It is noted from this table that the smallest energy differences are found for the structures that underwent the smallest changes upon geometry optimisation, e.g. the R = Me and R_2 = Ph(Me) systems. Conversely, the greatest energy differences are found for the larger systems (e.g. R = Cy) and those that changed most upon geometry optimisation, e.g. R = ^{i}Pr and ^{n}Bu.

TABLE 4.8: Calculated Energies (hartrees, kJ mol^{-1}) Employing the LanL2DZ Basis Set for R_2SnCl_2(1,10-phenanthroline).

	Calculated Energies		
R_2SnCl_2(1,10-phenanthroline)	**Single point (hartrees)**	**Optimised geometry (hartrees)**	**Δ (kJ mol^{-1})**
[Me_2SnCl_2(1,10-phenanthroline)] [3]	-679.6752	-679.8329	414.0
[$^nBu_2SnCl_2$(1,10-phenanthroline)]	-913.5012	-913.9568	1196.2
[$^iPr_2SnCl_2$(1,10-phenanthroline)]	-835.4416	-835.8987	1200.1
[Cy_2SnCl_2(1,10-phenanthroline)]	-1067.1783	-1067.7101	1396.2
[Ph(Me)$SnCl_2$(1,10-phenanthroline)]	-870.1183	-870.2816	428.7
[Bz_2SnCl_2(1,10-phenanthroline)]	-1138.5508	-1138.7972	646.9
[Ph_2SnCl_2(1,10-phenanthroline)]	-1060.5325	-1060.7298	518.0

4.8 Discussion

The optimised structure of each of the seven R_2SnCl_2(1,10-phenanthroline) adducts are compared with the crystallographically determined structures. Significant differences that are found between the solid state and gas phase structures are correlated with crystal packing effects.

The geometry optimisation calculations show, in general, that more symmetrical structures are found in the gas phase. This result indicates that crystal packing effects do indeed influence the molecular geometry of the R_2SnCl_2(1,10-phenanthroline) compounds. Further, a comparison of the calculated geometric parameters with those derived from the crystallographic studies reveals two important observations; see Tables 4.6 and 4.7. The first conclusion is that there is, generally, an elongation in the Sn-Cl

and Sn-N parameters (see below for further discussion on this point). Also, and significantly, the disparity in the Sn-Cl and Sn-N parameters that are sometimes found in a solid state structure no longer pertains in the absence of crystal packing effects. Finally, the geometry optimised structures reported herein are consistent with the results obtained for the related 2,2'-bipyridyl structures [1].

The availability of a series of crystal structures of the general formula R_2SnCl_2(1,10-phenanthroline) enables an evaluation of the derived interatomic parameters in order to ascertain whether any systematic variations exist. The obvious correlation to make is one between the Sn-ligand distances and the Lewis acidity of the tin center which is moderated as the nature of the tin-bound substituent is altered. The Sn-Cl and Sn-N bond distances have been selected as the most appropriate parameters for examination as they are the most accurately determined and are most likely to be influenced by changes in the Lewis acidity of the tin center. As an approximate measure of the Lewis acidity of the tin atoms in the R_2Sn moieties, the tin-119 NMR chemical shifts, recorded in non-coordinating (i.e. $CHCl_3$) solvent, for the R_2SnCl_2 precursors has been chosen [1].

4.8.1 Structural Correlations Based on Crystal Structures.

Figure 4.23 shows a plot of the crystallographically determined Sn-Cl and Sn-N bond distances for R_2SnCl_2(1,10-phenanthroline) versus $\delta(^{119}Sn)$ for each of R_2SnCl_2. It is immediately apparent from this graph that as the Lewis acidity of the tin atom decreases, i.e. as the $\delta(^{119}Sn)$ is shifted downfield, there is a general increase in both the Sn-Cl and Sn-N distances. In support of the findings in section I of this chapter, this result indicates that using $\delta(^{119}Sn)$ for R_2SnCl_2 is a reliable first approximation for Lewis acidity in these systems. It is also noteworthy that there is a spread of Sn-Cl and Sn-N distances, which reflects the disparity of these parameters within individual structures. The variation in the Sn-Cl distances has been correlated with the influence of *inter-* and *intra-*molecular Cl...H interactions, however, no reasons were found for differences in the Sn-N distances.

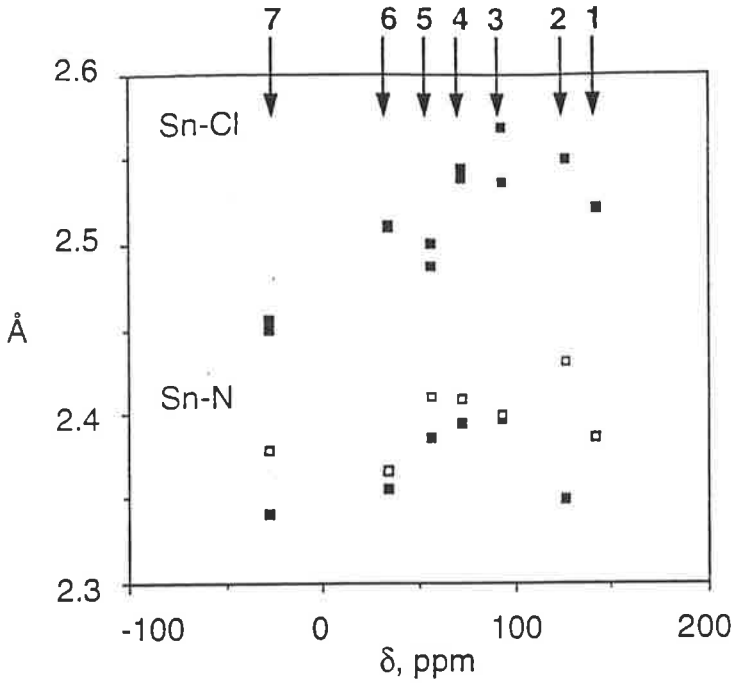


Figure 4.23

Variation of the experimental Sn-Cl and Sn-N (Å) bond lengths of [R_2SnCl_2(1,10-phenanthroline)] where R = Me (**1**), R = ^{n}Bu(**2**), R = ^{i}Pr(**3**), R = Cy(**4**), R_2 = Ph(Me)(**5**), R = Bz(**6**) and R = Ph(**7**) versus the experimental chemical shift δ(^{119}Sn) for R_2SnCl_2 (ppm)

In order to ascertain the influence of intermolecular forces i.e. crystal packing effects, on the Sn-Cl and Sn-N bond distances an analogous graph has been plotted using the results derived from the geometry optimisation studies.

4.8.2 Structural Correlations Based on Geometry Optimisations.

From 4.24 it is clear that the general trend to increasing Sn-Cl and Sn-N bond distances with decreasing Lewis acidity of tin, as for the solid state results, is found. Also apparent is that there is a reduced spread of Sn-Cl and Sn-N values reflecting the increased symmetry found in the gas phase structures, i.e. in the absence of crystal packing effects. A close examination of Figure 4.24 suggests that the Sn-Cl distances in the R = Bz, Cy and ^{i}Pr structures are perhaps longer than expected and further, the Sn-N distance in the [Bz_2SnCl_2(1,10-phenanthroline)] structure is shorter than expected. These deviations from the incremental trend of longer distances fro reduced Lewis acidicty at the tin centre may be explained in terms of *intra*molecular Cl...H interactions in the gas phase structures.

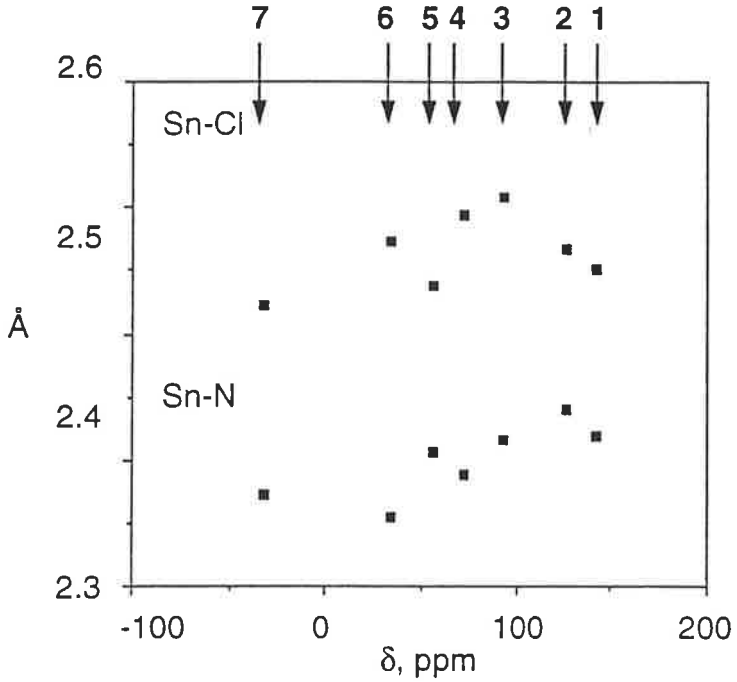


Figure 4.24

Variation of the calculated Sn-Cl and Sn-N (Å) bond lengths of [R_2SnCl_2(1,10-phenanthroline)] where R = Me (1), R = ^{n}Bu(2), R = ^{i}Pr(3), R = Cy(4), R_2 = Ph(Me)(5), R = Bz(6) and R = Ph(7) versus the experimental chemical shift δ(^{119}Sn) for R_2SnCl_2 (ppm)

Consistent with the previous study on R_2SnCl_2(2,2'-bipyridyl) [1], the Sn-N distance in the [Bz_2SnCl_2(1,10-phenanthroline)] structure is marginally shorter than those found in the solid state, i.e. against the general trend of bond elongation for both Sn-N and Sn-Cl. This result is correlated with the presence of significant *intra*molecular Cl...H interactions which results in significant elongation of the associated Sn-Cl distances. Thus, in [Bz_2SnCl_2(1,10-phenanthroline)] each chloride atoms forms a contact of 2.62 Å with H(1,10-phenanthroline) as well as a contact of 3.04 Å with an *ortho*-H from the phenyl group of one benzyl residue and a contact of 3.07 Å with a methylene-*H* atom of the other benzyl substituent. This behaviour contrasts that found in the solid state structure (see above). The small shortening of the Sn-N distances compensates for the greater than usual elongation of the Sn-Cl distances that occur owing to the effects of the *intra*molecular Cl...H interactions. Similar arguments are evoked for the R = Cy structure where a marginal contraction in Sn-N is also observed. Close *intra*molecular Cl...H interactions are also noted in this structure with 2.86 Å (x2) contacts formed

between the chloride atoms and methylene-*H* atoms as well as 2.64 Å between each chloride atom and a H(1,10-phenanthroline) atom. In the R = ^{i}Pr structure, where significant elongation of the Sn-Cl(1) distance arises owing to a Cl...H pattern involving the Cl(1) atom in preference to the Cl(2) atom ensures that the average Sn-Cl distance is greater than would otherwise be expected. Thus, over and above the effect of moderating the Lewis acidity of the tin center, the R groups may also influence the geometric parameters about the tin center by participating in *intra*molecular Cl...H interactions.

4.9 Conclusion

The combined crystallographic/theoretical study reported herein on a series of R_2SnCl_2(1,10-phenanthroline) compounds demonstrates a number of important results. A comparison of molecular geometries determined by crystallography with those derived from geometry optimisations shows that in the absence of crystal packing effects, symmetrical structures are usually found. This result indicates that there is no inherent chemical reason that explains the lack of symmetry in the solid state for these systems and that crystal packing effects are responsible for deviations from molecular symmetry. Further, generally in the gas phase there is an elongation in Sn-ligand bond distances; deviations from this generalisation may be rationalised in terms of *intra*molecular Cl...H interactions. This effect may be ascribed, in part, to the influence of crystal packing on the geometric parameters, however, it is known that at the HF level elongation of bond distances involving heavy-metal centres is often observed owing to the theoretical approximations involoved [3]. At present, we are unable to quantify the relative influences of crystal packing effects and the theoretical approximations on bond elongation. Differences in bond angles in the R_2SnCl_2(1,10-phenanthroline) compounds are associated with the symmetrisation of the structures. Finally, the validity of the combined crystallographic/theoretical approach in the study of crystal packing effects is vindicated by the consistency of the results obtained herein with those found in the 2,2'-bipyridyl series [1].

4.10 References

(1) Tiekink, E.R.T.; Hall, V.J.; Hook, J.; Buntine, M.A. *J. Phys. Chem. A*, **1998**, submitted.

(2) Bessel, C.A.; Margarucci, J.A.; Acquaye, J.H.; Rubino, R.S.; Crandall, J. *Inorg. Chem.* **1993**, *32*, 5779.

(3) Buntine, M.A.; Hall, V.J.; Kosovel, F.J.; Tiekink, E.R.T. *J. Phys. Chem. A*, **1998**, *102*, 2472.

(4) Ganis, P.; Peruzzo, V.; Valle, G. *J. Organomet.* Chem. **256** (1983) 245.

(5) Cox, M.J.; Tiekink, E.R.T. *Z. Kristallogr.* **209** (1994) 190.

(6) Johnson, C.K.: ORTEP. Report ORNL-5138, Oak Ridge National Laboratory, Tennessee 1976.

Appendix - Chapter 4, Section II

Crystal data and refinement details for:

A. [$^{i}Pr_2SnCl_2$(1,10-phenanthroline)]

B [Cy_2SnCl_2(1,10-phenanthroline)]

C [Bz_2SnCl_2(1,10-phenanthroline)].

D [Ph(Me)$SnCl_2$(1,10-phenanthroline)].

A. [$^{i}Pr_2SnCl_2$(1,10-phenanthroline)]

Crystallographic Data and Refinement details for [$^{i}Pr_2SnCl_2$(1,10-phenanthroline)].

Formula	$C_{18}H_{22}Cl_2N_2Sn$
Formula weight	456.0
Crystal morphology	colourless block
Crystal dimensions (mm)	0.06 x 0.15 x 0.40
Crystal system	monoclinic
Space group	$P2_1/c$ (C_{2h}^5, No. 14)
Temperature (°C)	20.0
a (Å)	8.261(2)
b (Å)	15.125(3)
c (Å)	15.804(2)
β (°)	104.82(1)
V (Å^3)	1908.9(7)
Z	4
D_{calc} (g cm^{-3})	1.586
F(000)	912
Radiation	MoKα (λ = 0.7107Å)
μ (cm^{-1})	16.18
θ limits, data (°)	3.0 to 27.5
hkl range	0 to 11, 0 to 20, -21 to 21
Range of transmission factors	0.978 to 1.000
Scan technique	ω:2θ
Scan width (°)	0.89
No. of data measured	4891
No. of unique data	4590
R_{amal}	0.055
Program for structure solution	Direct Methods (SHELXS86)
No. of unique data used	2200
No. of parameters	208
R	0.045
R_w	0.042
G.O.F.	1.37
Min./Max. residual electron density (e Å^{-3})	-0.62 to +0.50

Fractional atomic coordinates ($Å^2$) for the non-hydrogen atoms in [$^iPr_2SnCl_2$.(1,10-phenanthroline)].

Atom	*x*	*y*	*z*
Sn	0.06574(6)	0.19927(3)	0.25941(3)
Cl(1)	-0.1536(3)	0.0789(1)	0.2009(1)
Cl(2)	0.0284(3)	0.3197(1)	0.1443(1)
N(1)	0.2877(7)	0.2801(4)	0.3556(4)
N(2)	0.1808(7)	0.1175(4)	0.3912(4)
C(1)	0.245(1)	0.1364(8)	0.2009(6)
C(2)	0.175(1)	0.1133(7)	0.1040(6)
C(3)	0.396(1)	0.114(1)	0.2435(8)
C(4)	-0.118(1)	0.2641(5)	0.3149(5)
C(5)	-0.168(1)	0.2096(6)	0.3840(6)
C(6)	-0.078(1)	0.3581(6)	0.3455(7)
C(7)	0.338(1)	0.3611(5)	0.3387(6)
C(8)	0.465(1)	0.4063(5)	0.3975(6)
C(9)	0.539(1)	0.3693(6)	0.4753(6)
C(10)	0.490(1)	0.2849(5)	0.4961(5)
C(11)	0.3615(9)	0.2427(5)	0.4339(5)
C(12)	0.565(1)	0.2407(6)	0.5760(5)
C(13)	0.511(1)	0.1599(6)	0.5930(6)
C(14)	0.3058(9)	0.1549(5)	0.4520(5)
C(15)	0.382(1)	0.1151(5)	0.5328(5)
C(16)	0.326(1)	0.0310(5)	0.5458(5)
C(17)	0.204(1)	-0.0084(5)	0.4835(5)
C(18)	0.133(1)	0.0371(5)	0.4059(5)

Anisotropic thermal parameters ($Å^2$) for the non-hydrogen atoms in [$^iPr_2SnCl_2$(1,10-phenanthroline)].

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Sn	0.0344(2)	0.0368(2)	0.0352(3)	0.0017(3)	0.0084(2)	0.0039(3)
Cl(1)	0.057(1)	0.045(1)	0.065(1)	-0.005(1)	0.001(1)	-0.006(1)
Cl(2)	0.087(2)	0.058(1)	0.050(1)	0.004(1)	0.017(1)	0.017(1)
N(1)	0.038(4)	0.042(4)	0.047(4)	-0.005(3)	0.010(3)	0.007(3)
N(2)	0.031(3)	0.038(3)	0.038(4)	-0.001(3)	0.004(3)	0.002(3)
C(1)	0.072(7)	0.13(1)	0.058(6)	0.043(7)	0.020(6)	-0.011(6)
C(2)	0.091(8)	0.083(7)	0.059(6)	0.002(6)	0.040(6)	-0.004(6)
C(3)	0.074(9)	0.368(2)	0.087(9)	0.10(1)	0.008(7)	-0.08(1)
C(4)	0.045(5)	0.046(4)	0.048(5)	0.007(4)	0.019(4)	0.004(4)
C(5)	0.075(7)	0.076(7)	0.080(7)	0.013(6)	0.041(6)	0.005(6)
C(6)	0.091(8)	0.048(5)	0.097(8)	0.005(5)	0.040(7)	-0.019(5)
C(7)	0.055(6)	0.046(5)	0.061(6)	-0.001(4)	0.008(5)	0.012(4)
C(8)	0.055(6)	0.039(5)	0.075(7)	-0.013(4)	0.010(5)	-0.009(5)
C(9)	0.045(5)	0.047(5)	0.065(6)	-0.012(4)	0.009(5)	-0.023(5)
C(10)	0.039(4)	0.040(5)	0.049(5)	0.001(4)	0.016(4)	-0.007(4)
C(11)	0.029(4)	0.035(4)	0.041(5)	0.010(3)	0.011(3)	0.000(4)
C(12)	0.047(6)	0.071(6)	0.045(6)	0.004(5)	-0.010(4)	-0.009(5)
C(13)	0.068(7)	0.066(6)	0.044(5)	0.000(5)	-0.007(5)	0.004(5)
C(14)	0.025(4)	0.040(4)	0.042(5)	0.008(3)	0.008(3)	-0.004(4)
C(15)	0.046(5)	0.051(5)	0.038(5)	0.010(4)	0.005(4)	0.004(4)
C(16)	0.059(6)	0.049(5)	0.044(5)	0.010(5)	0.004(4)	0.012(4)
C(17)	0.071(6)	0.042(5)	0.051(5)	-0.001(4)	0.026(5)	0.011(4)
C(18)	0.051(5)	0.038(4)	0.045(5)	0.005(4)	0.013(4)	0.002(4)

Fractional atomic coordinates and B_{eq} values ($Å^2$) for the hydrogen atoms in [$^iPr_2SnCl_2$(1,10-phenanthroline)].

Atom	*x*	*y*	*z*	B_{eq}
H(1a)	0.2032	0.0778	0.2141	7.2
H(2a)	0.0574	0.1033	0.0925	7.0
H(2b)	0.1948	0.1610	0.0688	7.0
H(2c)	0.2279	0.0615	0.0905	7.0
H(3a)	0.3976	0.1017	0.3028	16.8
H(3b)	0.4284	0.0624	0.2176	16.8
H(3c)	0.4708	0.1607	0.2413	16.8
H(4a)	-0.2162	0.2682	0.2681	4.2
H(5a)	-0.2563	0.2385	0.4016	6.9
H(5b)	-0.2050	0.1530	0.3609	6.9
H(5c)	-0.0747	0.2030	0.4332	6.9
H(6a)	0.0210	0.3588	0.3921	7.1
H(6b)	-0.0611	0.3928	0.2983	7.1
H(6c)	-0.1683	0.3818	0.3651	7.1
H(7a)	0.2861	0.3884	0.2845	5.2
H(8a)	0.4986	0.4631	0.3831	5.4
H(9a)	0.6240	0.4004	0.5161	5.0
H(12a)	0.6538	0.2683	0.6179	5.5
H(13a)	0.5623	0.1323	0.6473	6.0
H(16a)	0.3744	0.0006	0.5989	5.0
H(17a)	0.1667	-0.0662	0.4925	5.0
H(18a)	0.0483	0.0090	0.3622	4.2

Bond distances (Å) for [$^{i}Pr_2SnCl_2$(1,10-phenanthroline)].

Atom - Atom	Distance	Atom - Atom	Distance
Sn - Cl(1)	2.569(2)	C(4) - C(6)	1.51(1)
Sn - Cl(2)	2.536(2)	C(7) - C(8)	1.39(1)
Sn - N(1)	2.396(6)	C(8) - C(9)	1.35(1)
Sn - N(2)	2.399(6)	C(9) - C(10)	1.40(1)
Sn - C(1)	2.155(9)	C(10) - C(11)	1.40(1)
Sn - C(4)	2.171(8)	C(10) - C(12)	1.42(1)
N(1) - C(7)	1.343(9)	C(11) - C(14)	1.458(9)
N(1) - C(11)	1.356(8)	C(12) - C(13)	1.35(1)
N(2) - C(14)	1.343(8)	C(13) - C(15)	1.41(1)
N(2) - C(18)	1.318(9)	C(14) - C(15)	1.41(1)
C(1) - C(2)	1.53(1)	C(15) - C(16)	1.38(1)
C(1) - C(3)	1.30(1)	C(16) - C(17)	1.36(1)
C(4) - C(5)	1.51(1)	C(17) - C(18)	1.40(1)

Bond angles (°) for [$^{i}Pr_2SnCl_2$(1,10-phenanthroline)].

Atom - Atom - Atom	Angle	Atom - Atom - Atom	Angle
Cl(1) - Sn - Cl(2)	107.79(7)	Sn - C(4) - C(5)	113.3(5)
Cl(1) - Sn - N(1)	160.9(1)	Sn - C(4) - C(6)	115.9(6)
Cl(1) - Sn - N(2)	91.9(1)	C(5) - C(4) - C(6)	111.2(8)
Cl(1) - Sn - C(1)	91.8(3)	N(1) - C(7) - C(8)	122.4(8)
Cl(1) - Sn - C(4)	88.0(2)	C(7) - C(8) - C(9)	119.6(8)
Cl(2) - Sn - N(1)	91.2(2)	C(8) - C(9) - C(10)	120.1(7)
Cl(2) - Sn - N(2)	160.2(1)	C(9) - C(10) - C(11)	117.4(7)
Cl(2) - Sn - C(1)	88.9(3)	C(9) - C(10) - C(12)	123.3(8)
Cl(2) - Sn - C(4)	89.8(2)	C(11) - C(10) - C(12)	119.3(7)
N(1) - Sn - N(2)	69.1(2)	N(1) - C(11) - C(10)	122.3(7)
N(1) - Sn - C(1)	89.9(3)	N(1) - C(11) - C(14)	118.0(7)
N(1) - Sn - C(4)	90.8(3)	C(10) - C(11) - C(14)	119.8(7)
N(2) - Sn - C(1)	89.0(3)	C(10) - C(12) - C(13)	120.7(8)
N(2) - Sn - C(4)	92.6(2)	C(12) - C(13) - C(15)	122.1(8)
C(1) - Sn - C(4)	178.5(3)	N(2) - C(14) - C(11)	117.8(7)
Sn - N(1) - C(7)	124.5(5)	N(2) - C(14) - C(15)	123.5(7)
Sn - N(1) - C(11)	117.3(5)	C(11) - C(14) - C(15)	118.6(7)
C(7) - N(1) - C(11)	118.1(7)	C(13) - C(15) - C(14)	119.5(8)
Sn - N(2) - C(14)	117.8(5)	C(13) - C(15) - C(16)	124.3(8)
Sn - N(2) - C(18)	124.0(5)	C(14) - C(15) - C(16)	116.2(7)
C(14) - N(2) - C(18)	118.1(6)	C(15) - C(16) - C(17)	120.6(7)
Sn - C(1) - C(2)	113.8(7)	C(16) - C(17) - C(18)	119.2(7)
Sn - C(1) - C(3)	124.4(8)	N(2) - C(18) - C(17)	122.2(7)
C(2) - C(1) - C(3)	121.6(9)		

Observed and calculated structure factors for [$^{i}Pr_2SnCl_2$(1,10-phenanthroline)].

h	k	l	Fo	Fc	sigF
0	0	4	784	770	13
0	0	6	1125	1156	16
0	0	8	1112	1133	18
0	0	10	662	677	16
0	0	12	484	472	15
0	0	14	321	329	19
0	0	16	248	196	23
0	0	18	247	261	24
0	1	3	821	814	12
0	1	4	154	142	16
0	1	5	514	518	11
0	1	6	347	343	10
0	1	7	188	174	17
0	1	8	356	361	11
0	1	9	58	23	50*
0	1	10	475	465	13
0	1	11	312	305	17
0	1	12	390	391	17
0	1	13	203	198	27
0	1	14	401	413	17
0	1	15	233	237	25
0	1	16	499	508	16
0	1	17	120	103	78*
0	1	18	375	358	18
0	1	19	0	90	76*
0	2	2	1478	1390	15
0	2	3	1735	1692	18
0	2	4	518	552	11
0	2	5	1454	1468	17
0	2	6	797	853	15
0	2	7	1022	1012	17
0	2	8	926	939	17
0	2	9	117	47	59*
0	2	10	928	936	20
0	2	11	120	100	68*
0	2	12	585	582	15
0	2	13	234	235	25
0	2	14	0	126	74*
0	2	15	402	399	18
0	2	16	294	272	21
0	2	17	120	131	74*
0	2	18	80	154	58*
0	2	19	136	51	78*
0	3	1	117	101	17
0	3	2	437	421	10
0	3	3	550	536	13
0	3	4	697	727	14
0	3	5	249	242	12
0	3	6	1027	1015	16
0	3	7	352	350	11
0	3	8	331	367	13
0	3	9	331	324	14
0	3	10	313	329	17
0	3	11	609	612	14
0	3	12	197	207	27
0	3	13	337	371	19
0	3	14	109	97	72*
0	3	15	290	274	20
0	3	16	104	151	79*
0	3	17	256	202	21
0	3	18	158	165	37*
0	3	19	185	207	31*
0	4	0	318	312	9
0	4	1	480	474	11
0	4	2	57	21	41*
0	4	3	1288	1317	16
0	4	4	538	546	11
0	4	5	1850	1913	20
0	4	6	411	408	10
0	4	7	1024	1055	18
0	4	8	244	230	15
0	4	9	821	839	20
0	4	10	257	265	19
0	4	11	625	604	14
0	4	12	262	269	20
0	4	13	481	510	15
0	4	14	0	51	71*
0	4	15	453	490	17
0	4	16	201	189	27
0	4	17	0	123	77*
0	4	18	0	35	81*
0	4	19	124	23	74*
0	5	1	918	874	14
0	5	2	205	201	13
0	5	3	873	860	15
0	5	4	0	25	50*
0	5	5	357	359	10
0	5	6	395	388	11
0	5	7	624	592	14
0	5	8	0	96	61*
0	5	9	544	546	14
0	5	10	146	42	30*
0	5	11	522	514	14
0	5	12	86	77	50*
0	5	13	405	404	16
0	5	14	98	98	73*
0	5	15	319	294	19
0	5	16	70	38	75*
0	5	17	189	199	34*
0	5	18	103	6	65*
0	5	19	116	237	82*
0	6	0	244	259	12
0	6	1	1196	1183	16
0	6	2	131	126	20
0	6	3	1270	1263	17
0	6	4	178	177	16
0	6	5	1204	1206	18
0	6	6	0	80	57*
0	6	7	827	826	19
0	6	8	615	616	15
0	6	9	594	588	14
0	6	10	634	622	14
0	6	11	550	525	14
0	6	12	248	254	23
0	6	13	477	499	15
0	6	14	0	94	77*
0	6	15	260	219	23
0	6	16	0	16	76*
0	6	17	126	129	76*
0	6	18	0	68	75*
0	7	1	272	256	12
0	7	2	353	354	10
0	7	3	161	147	18
0	7	4	0	53	44*
0	7	5	31	46	56*
0	7	6	412	435	12
0	7	7	195	213	22
0	7	8	462	472	13
0	7	9	272	233	18
0	7	10	229	185	21
0	7	11	424	407	15
0	7	12	0	71	71*
0	7	13	410	397	16
0	7	14	204	189	29
0	7	15	341	309	19
0	7	16	249	198	24
0	7	17	297	262	23
0	7	18	0	162	79*
0	8	0	655	698	17
0	8	1	955	924	17
0	8	2	1322	1342	19
0	8	3	664	662	14
0	8	4	730	741	18
0	8	5	419	434	12
0	8	6	674	645	14
0	8	7	365	365	13
0	8	8	698	694	16
0	8	9	326	320	18
0	8	10	547	530	14
0	8	11	264	223	20
0	8	12	259	270	22
0	8	13	162	162	33*
0	8	14	0	108	78*
0	8	15	0	98	79*
0	8	16	0	191	83*
0	8	17	0	60	77*
0	8	18	114	170	82*
0	9	1	183	175	18
0	9	2	334	328	12
0	9	3	157	148	21
0	9	4	170	172	22
0	9	5	104	133	59*
0	9	6	220	222	19
0	9	7	281	298	17
0	9	8	369	386	16
0	9	9	265	232	19
0	9	10	348	345	18
0	9	11	0	87	74*
0	9	12	0	282	84*
0	9	13	119	6	43*
0	9	14	341	340	21
0	9	15	0	98	76*
0	9	16	309	329	24
0	9	17	0	123	84*
0	10	0	938	955	19
0	10	1	149	173	24
0	10	2	932	931	19
0	10	3	323	312	13
0	10	4	836	827	19
0	10	5	266	265	17
0	10	6	638	646	14
0	10	7	343	367	16
0	10	8	857	881	17
0	10	9	73	18	67*
0	10	10	365	377	17
0	10	11	114	68	41*
0	10	12	306	264	19
0	10	13	122	24	71*
0	10	14	270	263	21
0	10	15	113	60	66*
0	10	16	0	193	86*
0	10	17	97	64	57*
0	11	1	159	132	23
0	11	2	278	264	15
0	11	3	126	174	63*
0	11	4	385	367	13
0	11	5	128	180	68*
0	11	6	131	151	34*
0	11	7	364	382	15
0	11	8	472	474	14
0	11	9	0	7	68*
0	11	10	144	269	77*
0	11	11	178	180	30*
0	11	12	222	221	28
0	11	13	197	218	30
0	11	14	272	288	25
0	11	15	97	42	82*
0	11	16	213	166	29
0	12	0	455	460	12
0	12	1	398	427	14
0	12	2	372	372	14
0	12	3	460	479	13
0	12	4	484	477	13
0	12	5	305	302	16
0	12	6	469	484	14
0	12	7	433	424	14
0	12	8	571	562	15
0	12	9	217	196	22
0	12	10	325	317	17
0	12	11	289	281	19
0	12	12	274	216	21
0	13	1	0	176	68*
0	13	2	270	270	17
0	13	3	405	397	14
0	13	4	166	184	26
0	13	5	235	244	18
0	13	6	0	65	64*
0	13	7	111	133	39*
0	13	8	128	59	32*
0	13	9	241	240	22
0	13	10	192	214	26
0	13	11	229	205	24
0	13	12	16	180	76*
0	13	13	0	106	78*
0	14	0	156	164	24
0	14	1	507	545	13
0	14	2	248	238	17
0	14	3	434	456	14
0	14	4	102	298	74*
0	14	5	412	422	14
0	14	6	0	49	64*
0	14	7	514	534	14
0	14	8	0	74	67*
0	14	9	290	311	19
0	14	10	0	48	63*
0	14	11	276	282	20
0	14	12	0	32	67*
0	14	13	250	292	24
0	15	1	40	84	61*
0	15	2	103	76	38*
0	15	3	41	60	62*
0	15	4	0	18	66*
0	15	5	146	97	27*
0	15	6	181	159	23
0	15	7	84	109	67*
0	15	8	206	151	21
0	15	9	270	250	19
0	15	10	108	59	54*
0	15	11	152	161	32*
0	15	12	0	127	73*
0	16	0	188	155	22
0	16	1	506	515	13
0	16	2	120	182	66*
0	16	3	441	482	14
0	16	4	99	147	52*
0	16	5	141	316	77*
0	16	6	100	114	54*
0	16	7	249	222	19
0	16	8	0	152	66*
0	16	9	193	186	24
0	16	10	99	141	64*
0	16	11	204	179	23
0	17	1	68	85	64*
0	17	2	0	63	65*
0	17	3	75	35	63*
0	17	4	0	12	63*
0	17	5	0	59	61*
0	17	6	89	43	62*
0	17	7	170	179	26
0	17	8	81	30	65*
0	17	9	110	101	68*
0	17	10	0	24	60*
0	18	0	319	341	17
0	18	1	17	176	66*
0	18	2	284	334	17
0	18	3	0	123	67*
0	18	4	249	259	19
0	18	5	0	116	67*
0	18	6	172	232	28
0	18	7	0	69	63*
0	18	8	121	126	65*
0	19	1	69	10	52*
0	19	2	0	81	64*
0	19	3	0	53	59*
0	19	4	92	44	42*
0	19	5	116	130	63*
1	0	-20	216	205	33
1	0	-18	356	348	23
1	0	-16	371	328	21
1	0	-14	461	465	17
1	0	-12	631	619	16
1	0	-10	932	911	20
1	0	-8	1394	1357	19
1	0	-6	1061	1061	15
1	0	-4	734	711	13
1	0	-2	3111	3284	29
1	0	2	2252	2275	21
1	0	4	378	395	10
1	0	6	407	411	11
1	0	8	631	644	14
1	0	10	550	544	14
1	0	12	52	167	76*
1	0	14	79	89	73*
1	0	16	193	157	28
1	0	18	139	92	36*
1	1	-20	0	147	86*
1	1	-19	175	101	38*
1	1	-18	330	273	22
1	1	-17	0	79	85*
1	1	-16	400	402	19
1	1	-15	107	99	54*
1	1	-14	322	281	20
1	1	-13	0	41	79*
1	1	-12	0	45	75*
1	1	-11	41	93	71*
1	1	-10	193	206	24
1	1	-9	122	91	62*
1	1	-8	367	355	12
1	1	-7	823	792	16
1	1	-6	79	77	49*
1	1	-5	484	486	11
1	1	-4	362	355	10
1	1	-3	186	183	11
1	1	-2	512	432	11
1	1	1	443	431	10
1	1	2	372	371	8
1	1	3	0	81	50*
1	1	4	441	455	11
1	1	5	48	135	52*
1	1	6	1052	1059	16
1	1	7	251	239	13
1	1	8	1243	1201	19
1	1	9	358	369	14
1	1	10	816	805	16
1	1	11	250	245	20
1	1	12	444	441	15
1	1	13	422	433	16
1	1	14	518	524	14
1	1	15	105	175	57*
1	1	16	404	451	18
1	1	17	0	110	75*
1	1	18	301	307	21
1	1	19	0	50	72*
1	2	-20	0	162	87*
1	2	-19	0	117	73*
1	2	-18	267	250	27
1	2	-17	0	140	83*
1	2	-16	360	353	22
1	2	-15	297	320	23
1	2	-14	456	478	18
1	2	-13	431	426	17
1	2	-12	743	717	18
1	2	-11	227	220	23
1	2	-10	946	959	21
1	2	-9	239	227	18
1	2	-8	898	905	18
1	2	-7	1006	976	17
1	2	-6	848	841	15
1	2	-5	1600	1551	18
1	2	-4	378	405	9
1	2	-3	256	223	10
1	2	-2	1645	1674	17
1	2	-1	1469	1465	15
1	2	0	1141	1106	13
1	2	1	742	735	11
1	2	2	1723	1680	18
1	2	3	461	455	11
1	2	4	1066	1047	15
1	2	5	800	820	15
1	2	6	612	598	16
1	2	7	386	378	11
1	2	8	929	886	18
1	2	9	86	68	51*
1	2	10	707	696	15
1	2	11	80	127	69*
1	2	12	101	62	68*
1	2	13	434	432	15
1	2	14	200	189	25
1	2	15	28	130	69*
1	2	16	0	10	73*
1	2	17	46	29	54*
1	2	18	93	47	60*
1	2	19	103	24	68*
1	3	-20	0	96	83*
1	3	-19	155	136	44*
1	3	-18	181	83	35*
1	3	-17	0	191	90*
1	3	-16	138	100	46*
1	3	-15	0	23	75*
1	3	-14	336	314	20
1	3	-13	354	363	20
1	3	-12	72	35	63*
1	3	-11	428	422	15
1	3	-10	0	18	70*
1	3	-9	310	259	14
1	3	-8	487	494	13
1	3	-7	409	401	10
1	3	-6	635	617	16
1	3	-5	315	311	10
1	3	-4	158	178	17
1	3	-3	92	110	26*
1	3	-2	365	326	9
1	3	-1	381	382	10
1	3	0	0	24	43*
1	3	1	898	911	13
1	3	2	976	974	13
1	3	3	956	969	14
1	3	4	968	971	15
1	3	5	1227	1240	16
1	3	6	382	388	10
1	3	7	247	262	14
1	3	8	573	573	14
1	3	9	455	456	13
1	3	10	351	361	16
1	3	11	708	690	17
1	3	12	0	171	76*
1	3	13	456	495	15
1	3	14	161	83	28*
1	3	15	367	396	18
1	3	16	116	248	76*
1	3	17	227	222	25
1	3	18	223	225	24
1	3	19	168	210	33*
1	4	-19	0	148	84*
1	4	-18	192	130	33*
1	4	-17	379	355	20
1	4	-16	0	53	85*
1	4	-15	519	537	18
1	4	-14	428	415	17
1	4	-13	887	844	19
1	4	-12	242	239	24
1	4	-11	830	814	18
1	4	-10	313	283	16
1	4	-9	752	756	15
1	4	-8	329	313	13
1	4	-7	1126	1091	18
1	4	-6	364	351	11
1	4	-5	1531	1519	19
1	4	-4	488	492	11
1	4	-3	1171	1160	15
1	4	-2	445	430	11
1	4	-1	442	455	11
1	4	0	439	425	10
1	4	1	891	929	13
1	4	2	279	282	9
1	4	3	1679	1698	18
1	4	4	713	731	14
1	4	5	1383	1427	18
1	4	6	256	262	13
1	4	7	1011	999	18
1	4	8	331	313	12
1	4	9	535	529	13
1	4	10	71	67	64*
1	4	11	331	330	16
1	4	12	58	21	68*
1	4	13	270	300	21
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1	4	15	0	121	73*
1	4	16	0	52	74*
1	4	17	72	4	66*
1	4	18	63	2	61*
1	5	-19	0	192	86*
1	5	-18	0	1	82*
1	5	-17	0	81	80*
1	5	-16	155	1	79*
1	5	-15	75	148	79*
1	5	-14	0	108	75*
1	5	-13	295	268	21
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1	5	-6	199	165	17
1	5	-5	154	173	18
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1	5	17	284	305	21
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1	6	-19	184	158	36*
1	6	-18	88	152	72*
1	6	-17	287	255	24
1	6	-16	208	190	30
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1	6	-13	567	553	14
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1	7	-18	63	64	61*
1	7	-17	167	207	86*
1	7	-16	231	163	26
1	8	-1	606	670	13
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1	10	-16	133	268	85*
1	10	-15	159	24	37*
1	10	-14	303	303	25
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1	11	7	138	51	30*
1	11	8	396	415	15
1	13	-3	109	11	64*
1	13	-2	67	17	65*
1	13	-1	180	196	23
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6	8	-11	0	86	88*	6	10	-10	0	204	84*	6	12	-5	0	135	85*	6	15	-5	271	254	25	7	1	6	0	143	69*
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6	8	-9	0	159	78*	6	10	-8	198	133	26	6	12	-3	0	110	75*	6	15	-3	94	237	84*	7	1	8	0	92	70*
6	8	-8	163	194	36*	6	10	-7	201	174	27	6	12	-2	298	313	22	6	15	-2	0	90	82*	7	1	9	98	24	56*
6	8	-7	180	194	32*	6	10	-6	255	285	25	6	12	-1	235	194	23	6	15	-1	285	267	22	7	1	10	103	27	66*
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6	8	7	236	234	21	6	10	8	309	302	18	6	13	-8	0	193	85*	7	0	-14	35	215	94*	7	2	-6	373	397	21
6	8	8	342	360	18	6	10	9	0	29	71*	6	13	-7	270	245	25	7	0	-12	429	494	23	7	2	-5	242	206	27

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8	1	-3	0	74	83*	8	3	-1	0	58	78*	8	5	3	0	18	72*	8	8	-11	0	130	97*	8	11	-10	154	90	82*
8	1	-2	133	15	75*	8	3	0	60	27	75*	8	5	4	118	137	63*	8	8	-10	287	312	32	8	11	-9	0	22	86*
8	1	-1	106	64	56*	8	3	1	191	137	29	8	5	5	0	150	75*	8	8	-9	187	116	40*	8	11	-8	80	88	84*
8	1	0	111	42	75*	8	3	2	181	131	30	8	5	6	18	30	68*	8	8	-8	242	182	31	8	11	-7	113	30	68*
8	1	1	105	120	73*	8	3	3	40	67	76*	8	5	7	130	218	76*	8	8	-7	0	151	72*	8	11	-6	81	38	67*
8	1	2	173	166	33*	8	3	4	100	155	62*	8	5	8	0	24	71*	8	8	-6	243	262	30	8	11	-5	120	13	79*
8	1	3	100	101	71*	8	3	5	0	85	75*	8	6	-15	0	181	99*	8	8	-5	182	124	34*	8	11	-4	0	30	84*
8	1	4	215	207	27	8	3	6	118	108	70*	8	6	-14	173	100	88*	8	8	-4	328	362	23	8	11	-3	0	25	78*
8	1	5	166	63	31*	8	3	7	178	153	29	8	6	-13	171	199	97*	8	8	-3	231	238	30	8	11	-2	0	19	79*
8	1	6	189	179	28	8	3	8	148	128	76*	8	6	-12	180	95	96*	8	8	-2	355	349	20	8	11	-1	144	40	39*
8	1	7	78	9	68*	8	3	9	158	175	30*	8	6	-11	342	349	29	8	8	-1	276	248	23	8	11	0	0	3	77*
8	11	1	73	35	64*	9	2	-12	226	260	41*	9	4	1	239	206	28	9	7	0	123	83	79*	10	1	-3	0	78	88*
8	11	2	70	70	80*	9	2	-11	0	160	98*	9	4	2	201	94	26	9	7	1	147	101	76*	10	1	-2	163	237	90*
8	11	3	88	35	69*	9	2	-10	316	313	29	9	4	3	140	239	80*	9	7	2	166	62	32*	10	1	-1	0	126	87*
8	12	-9	0	162	89*	9	2	-9	0	190	98*	9	4	4	124	16	45*	9	7	3	105	177	62*	10	1	0	232	276	31
8	12	-8	238	217	31	9	2	-8	401	394	24	9	4	5	125	125	45*	9	8	-11	0	76	97*	10	1	1	76	37	81*
8	12	-7	49	226	87*	9	2	-7	239	281	36	9	5	-14	0	58	99*	9	8	-10	200	174	44*	10	1	2	183	186	35*
8	12	-6	229	270	34	9	2	-6	338	292	26	9	5	-13	43	37	78*	9	8	-9	0	175	91*	10	2	-11	95	122	80*
8	12	-5	97	184	86*	9	2	-5	239	182	31	9	5	-12	0	56	95*	9	8	-8	182	195	47*	10	2	-10	239	216	40*
8	12	-4	150	235	85*	9	2	-4	377	356	23	9	5	-11	0	11	98*	9	8	-7	129	175	89*	10	2	-9	104	112	93*
8	12	-3	95	143	84*	9	2	-3	176	210	41*	9	5	-10	199	33	41*	9	8	-6	234	174	30	10	2	-8	149	193	80*
8	12	-2	0	231	91*	9	2	-2	287	295	25	9	5	-9	105	69	89*	9	8	-5	99	133	69*	10	2	-7	137	157	77*
8	12	-1	123	172	75*	9	2	-1	299	291	25	9	5	-8	148	54	54*	9	8	-4	275	254	28	10	2	-6	249	235	34
8	12	0	219	210	28	9	2	0	252	264	30	9	5	-7	127	26	60*	9	8	-3	0	169	81*	10	2	-5	82	151	89*
8	12	1	234	216	25	9	2	1	289	237	23	9	5	-6	60	96	76*	9	8	-2	274	259	26	10	2	-4	206	200	37*
8	13	-6	102	75	75*	9	2	2	137	118	45*	9	5	-5	0	89	82*	9	8	-1	178	157	36*	10	2	-3	147	170	55*
8	13	-5	0	9	80*	9	2	3	185	189	32*	9	5	-4	117	29	61*	9	8	0	234	239	29	10	2	-2	167	166	43*
8	13	-4	77	4	73*	9	2	4	0	129	78*	9	5	-3	0	107	84*	9	8	1	158	182	40*	10	2	-1	0	132	72*
8	13	-3	86	32	70*	9	2	5	0	160	77*	9	5	-2	77	100	82*	9	8	2	207	227	31	10	2	0	0	94	92*
8	13	-2	63	9	74*	9	2	6	70	116	73*	9	5	-1	209	200	31	9	9	-10	104	40	87*	10	2	1	133	101	77*
9	0	-14	0	256	99*	9	3	-14	138	32	95*	9	5	0	112	40	82*	9	9	-9	0	17	74*	10	2	2	116	49	74*
9	0	-12	337	304	28	9	3	-13	0	17	96*	9	5	1	147	99	77*	9	9	-8	0	2	92*	10	3	-11	41	94	99*
9	0	-10	418	401	24	9	3	-12	188	15	94*	9	5	2	134	120	79*	9	9	-7	0	40	87*	10	3	-10	120	82	94*
9	0	-8	379	366	23	9	3	-11	95	27	96*	9	5	3	295	272	21	9	9	-6	0	106	81*	10	3	-9	101	75	72*
9	0	-6	378	399	25	9	3	-10	39	28	91*	9	5	4	53	58	81*	9	9	-5	0	25	83*	10	3	-8	0	17	98*
9	0	-4	409	382	22	9	3	-9	151	56	54*	9	5	5	238	237	23	9	9	-4	170	94	39*	10	3	-7	118	198	90*

9	0	-2	436	413	19	9	3	-8	0	50	87*	9	6	-13	222	238	45*	9	9	-3	139	15	45*	10	3	-6	0	29	85*			
9	0	0	418	409	19	9	3	-7	141	56	73*	9	6	-12	121	130	94*	9	9	-2	125	168	57*	10	3	-5	0	110	95*			
9	0	2	307	294	21	9	3	-6	0	22	83*	9	6	-11	167	253	99*	9	9	-1	0	32	79*	10	3	-4	0	133	95*			
9	0	4	258	247	24	9	3	-5	0	90	83*	9	6	-10	0	105	98*	9	9	0	121	151	81*	10	3	-3	236	156	29			
9	0	6	163	177	34*	9	3	-4	0	43	86*	9	6	-9	0	294	99*	9	9	1	0	32	76*	10	3	-2	0	125	85*			
9	1	-15	156	43	80*	9	3	-3	0	67	80*	9	6	-8	0	85	93*	9	10	-8	175	276	91*	10	3	-1	0	233	94*			
9	1	-14	19	9	95*	9	3	-2	16	71	81*	9	6	-7	307	270	29	9	10	-7	95	11	83*	10	3	0	157	186	43*			
9	1	-13	186	18	97*	9	3	-1	31	157	84*	9	6	-6	150	200	54*	9	10	-6	0	223	89*	10	3	1	0	184	85*			
9	1	-12	141	128	96*	9	3	0	66	46	75*	9	6	-5	430	406	21	9	10	-5	143	23	78*	10	4	-11	203	227	51*			
9	1	-11	100	35	71*	9	3	1	258	253	27	9	6	-4	0	69	84*	9	10	-4	165	252	86*	10	4	-10	85	105	99*			
9	1	-10	0	52	94*	9	3	2	131	202	82*	9	6	-3	281	254	26	9	10	-3	43	7	69*	10	4	-9	226	259	42*			
9	1	-9	0	31	89*	9	3	3	98	137	66*	9	6	-2	0	152	81*	9	10	-2	248	256	29	10	4	-8	0	23	96*			
9	1	-8	138	27	77*	9	3	4	96	124	77*	9	6	-1	228	221	31	9	10	-1	171	39	34*	10	4	-7	324	308	30			
9	1	-7	131	30	84*	9	3	5	0	179	81*	9	6	0	91	50	73*	10	0	-12	204	270	48*	10	4	-6	70	215	79*			
9	1	-6	107	169	77*	9	3	6	154	145	35*	9	6	1	263	271	26	10	0	-10	259	216	36	10	4	-5	0	183	90*			
9	1	-5	136	71	87*	9	4	-14	154	49	91*	9	6	2	0	23	81*	10	0	-8	233	225	40*	10	4	-4	151	50	46*			
9	1	-4	151	207	51*	9	4	-13	270	256	37	9	6	3	248	279	27	10	0	-6	0	269	98*	10	4	-3	95	161	85*			
9	1	-3	0	57	84*	9	4	-12	0	88	99*	9	6	4	143	39	37*	10	0	-4	285	258	29	10	4	-2	113	22	59*			
9	1	-2	204	191	35*	9	4	-11	268	277	37	9	7	-12	0	3	99*	10	0	-2	289	306	28	10	4	-1	24	113	83*			
9	1	-1	85	119	70*	9	4	-10	0	127	99*	9	7	-11	149	76	80*	10	0	0	208	186	33	10	4	0	0	38	78*			
9	1	0	201	200	33	9	4	-9	313	352	32	9	7	-10	121	13	69*	10	0	2	33	123	66*	10	4	1	32	131	70*			
9	1	1	146	131	78*	9	4	-8	155	155	56*	9	7	-9	0	42	91*	10	1	-12	0	90	99*	10	5	-10	0	50	99*			
9	1	2	250	242	26	9	4	-7	429	438	24	9	7	-8	183	13	40*	10	1	-11	83	46	92*	10	5	-9	0	101	95*			
9	1	3	95	54	76*	9	4	-6	0	14	69*	9	7	-7	0	28	99*	10	1	-10	0	81	72*	10	5	-8	143	31	91*			
9	1	4	188	205	34*	9	4	-5	390	412	25	9	7	-6	158	45	80*	10	1	-9	0	69	98*	10	5	-7	201	123	43*			
9	1	5	0	22	74*	9	4	-4	125	189	84*	9	7	-5	0	111	86*	10	1	-8	5	119	67*	10	5	-6	134	33	87*			
9	1	6	23	160	76*	9	4	-3	319	315	24	9	7	-4	138	91	71*	10	1	-7	0	91	75*	10	5	-5	137	177	90*			
9	2	-15	185	193	99*	9	4	-2	0	68	84*	9	7	-3	140	167	71*	10	1	-6	231	218	37	10	5	-4	0	65	86*			
9	2	-14	235	179	39	9	4	-1	327	290	22	9	7	-2	116	42	81*	10	1	-5	124	93	61*	10	5	-3	99	197	92*			
9	2	-13	182	174	98*	9	4	0	73	21	65*	9	7	-1	126	205	85*	10	1	-4	167	251	98*	10	5	-2	0	0	84*			

10	5	-1	0	161	85*
10	5	0	103	51	69*
10	6	-9	135	232	85*
10	6	-8	132	116	66*
10	6	-7	257	252	34
10	6	-6	0	16	91*
10	6	-5	0	206	99*
10	6	-4	103	51	84*
10	6	-3	160	135	45*
10	6	-2	0	53	77*
10	6	-1	167	117	39*
10	7	-6	0	75	90*
10	7	-5	0	174	89*
10	7	-4	0	122	86*
10	7	-3	0	225	89*

B. [Cy_2SnCl_2(1,10-phenanthroline)]

Crystallographic Data and Refinement details for [Cy_2SnCl_2(1,10-phenanthroline)].

Formula	$C_{24}H_{30}Cl_2N_2Sn$
Formula weight	536.1
Crystal morphology	yellow block
Crystal dimensions (mm)	0.15 x 0.21 x 0.26
Crystal system	monoclinic
Space group	$P2_1/n$ (C_{2h}^5, No. 14)
Temperature (°C)	20.0
a (Å)	10.477(1)
b (Å)	16.167(2)
c (Å)	14.341(3)
β (°)	101.46(1)
V (Å^3)	2379.9(6)
Z	4
D_{calc} (g cm^{-3})	1.496
F(000)	1088
Radiation	CuKα (λ = 1.5418Å)
μ (cm^{-1})	107.03
θ limits, data (°)	3.0 to 60.0
hkl range	0 to 12, 0 to 18, -16 to +16
Range of transmission factors	0.972 to 1.000
Scan width (°)	1.37
Scan technique	ω:2θ
No. of data measured	3924
No. of unique data	3700
R_{amal}	0.030
Program for structure solution	Direct Methods (SHELXS86)
No. of unique data used	2644
No. of parameters	262
R	0.043
R_w	0.054
G.O.F.	2.02
Min./Max. residual electron density (e Å^{-3})	-0.60 to +1.03

Fractional atomic coordinates ($Å^2$) for the non-hydrogen atoms in [Cy_2SnCl_2(1,10-phenanthroline)].

Atom	*x*	*y*	*z*
Sn	-0.00731(4)	0.16597(3)	0.30080(3)
Cl(1)	-0.1182(2)	0.1392(2)	0.4405(2)
Cl(2)	-0.1846(2)	0.2198(2)	0.1676(2)
N(1)	0.1624(7)	0.1747(4)	0.2113(5)
N(2)	0.1975(6)	0.1242(4)	0.3975(5)
C(1)	-0.0532(8)	0.0418(5)	0.2511(6)
C(2)	-0.038(1)	0.0244(7)	0.1532(9)
C(3)	-0.099(2)	-0.062(1)	0.119(1)
C(4)	-0.041(2)	-0.1251(8)	0.182(1)
C(5)	-0.060(2)	-0.1094(8)	0.276(1)
C(6)	0.006(1)	-0.0243(7)	0.312(1)
C(7)	0.0295(7)	0.2930(5)	0.3447(6)
C(8)	0.1102(9)	0.3061(6)	0.4428(7)
C(9)	0.108(1)	0.3983(7)	0.4726(7)
C(10)	0.152(1)	0.4532(7)	0.4039(9)
C(11)	0.077(2)	0.4398(7)	0.3045(9)
C(12)	0.078(1)	0.3479(6)	0.2751(7)
C(13)	0.147(1)	0.1993(7)	0.1220(7)
C(14)	0.250(2)	0.2108(9)	0.077(1)
C(15)	0.370(2)	0.198(1)	0.124(2)
C(16)	0.394(1)	0.1713(7)	0.216(1)
C(17)	0.284(8)	0.1595(5)	0.2594(8)
C(18)	0.521(2)	0.155(1)	0.275(2)
C(19)	0.536(1)	0.130(1)	0.364(2)
C(20)	0.3032(7)	0.1340(5)	0.3574(7)
C(21)	0.4296(9)	0.1188(7)	0.411(1)
C(22)	0.438(1)	0.0946(8)	0.507(1)
C(23)	0.332(1)	0.0847(7)	0.5426(8)
C(24)	0.2110(9)	0.1002(6)	0.4875(6)

Anisotropic thermal parameters ($Å^2$) for the non-hydrogen atoms in $[Cy_2SnCl_2(1,10\text{-phenanthroline})]$

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Sn	0.0344(3)	0.0333(3)	0.0333(3)	-0.0000(3)	0.0055(2)	-0.0002(3)
Cl(1)	0.055(1)	0.070(2)	0.060(1)	-0.007(1)	0.031(1)	-0.008(1)
Cl(2)	0.073(1)	0.062(2)	0.063(1)	0.007(1)	-0.025(1)	0.001(1)
N(1)	0.075(5)	0.036(4)	0.054(4)	-0.017(4)	0.033(4)	-0.008(4)
N(2)	0.034(3)	0.044(4)	0.051(4)	0.005(3)	0.012(3)	-0.004(3)
C(1)	0.062(5)	0.039(5)	0.057(5)	-0.003(4)	0.013(4)	-0.004(4)
C(2)	0.162(1)	0.063(8)	0.086(9)	-0.010(8)	0.043(8)	-0.024(7)
C(3)	0.338(3)	0.085(1)	0.118(1)	0.038(2)	-0.055(2)	-0.055(1)
C(4)	0.337(3)	0.052(8)	0.087(1)	0.064(1)	0.037(1)	-0.006(7)
C(5)	0.314(2)	0.045(8)	0.103(1)	-0.021(1)	0.029(1)	0.016(8)
C(6)	0.172(1)	0.053(8)	0.108(1)	-0.004(8)	-0.016(1)	-0.000(7)
C(7)	0.053(5)	0.035(5)	0.046(5)	-0.001(4)	0.002(4)	0.000(4)
C(8)	0.082(7)	0.045(6)	0.057(6)	-0.003(5)	0.005(5)	-0.001(4)
C(9)	0.108(8)	0.059(7)	0.055(6)	-0.003(6)	0.005(6)	-0.011(5)
C(10)	0.150(1)	0.057(7)	0.077(8)	-0.044(8)	0.002(8)	0.000(6)
C(11)	0.191(1)	0.046(7)	0.077(8)	-0.020(8)	-0.002(9)	0.011(6)
C(12)	0.131(9)	0.047(6)	0.053(6)	-0.025(6)	0.014(6)	-0.003(5)
C(13)	0.154(1)	0.063(7)	0.051(7)	-0.027(7)	0.053(7)	-0.006(5)
C(14)	0.256(2)	0.059(9)	0.096(1)	-0.067(1)	0.118(1)	-0.018(8)
C(15)	0.190(2)	0.071(1)	0.184(2)	-0.056(1)	0.161(2)	-0.049(1)
C(16)	0.109(1)	0.042(6)	0.168(1)	-0.030(7)	0.105(1)	-0.035(8)
C(17)	0.057(5)	0.034(5)	0.095(8)	-0.017(5)	0.051(5)	-0.025(5)
C(18)	0.080(1)	0.065(1)	0.347(4)	-0.033(1)	0.136(2)	-0.077(2)
C(19)	0.039(7)	0.056(1)	0.327(3)	-0.016(6)	0.044(1)	-0.055(1)
C(20)	0.036(4)	0.033(5)	0.090(7)	-0.000(4)	0.012(5)	-0.025(5)
C(21)	0.038(5)	0.048(7)	0.165(1)	-0.004(5)	0.010(7)	-0.047(8)
C(22)	0.064(7)	0.080(9)	0.125(1)	0.031(7)	-0.048(8)	-0.043(8)
C(23)	0.095(8)	0.077(8)	0.072(8)	0.035(7)	-0.029(7)	-0.019(6)
C(24)	0.070(6)	0.052(6)	0.047(5)	0.021(5)	-0.005(4)	0.002(4)

Fractional atomic coordinates and B_{eq} values ($Å^2$) for the hydrogen atoms in [Cy_2SnCl_2(1,10-phenanthroline)].

Atom	*x*	*y*	*z*	B_{eq}
H(1a)	-0.1440	0.0362	0.2492	5.0
H(2a)	-0.0804	0.0663	0.1120	8.5
H(2b)	0.0524	0.0241	0.1512	8.5
H(3a)	-0.1899	-0.0610	0.1181	12.9
H(3b)	-0.0846	-0.0735	0.0570	11.7
H(4a)	0.0497	-0.1270	0.1819	11.9
H(4b)	-0.0794	-0.1768	0.1604	11.9
H(5a)	-0.0218	-0.1526	0.3167	12.6
H(5b)	-0.1508	-0.1067	0.2755	12.6
H(6a)	0.0963	-0.0268	0.3105	11.0
H(6b)	-0.0050	-0.0144	0.3749	11.0
H(7a)	-0.0538	0.3147	0.3479	4.1
H(8a)	0.0762	0.2730	0.4868	5.7
H(8b)	0.1976	0.2902	0.4430	5.7
H(9a)	0.1631	0.4052	0.5332	7.4
H(9b)	0.0211	0.4130	0.4766	7.4
H(10a)	0.2419	0.4428	0.4051	7.4
H(10b)	0.1416	0.5091	0.4217	7.4
H(11a)	0.1145	0.4722	0.2617	9.4
H(11b)	-0.0109	0.4567	0.3013	9.4
H(12a)	0.1650	0.3325	0.2724	7.7
H(12b)	0.0241	0.3412	0.2140	7.7
H(13a)	0.0610	0.2094	0.0875	6.6
H(14a)	0.2345	0.2280	0.0121	7.7
H(15a)	0.4414	0.2071	0.0931	8.3
H(18a)	0.5963	0.1615	0.2483	7.8
H(19a)	0.6214	0.1191	0.3985	9.8
H(22a)	0.5215	0.0854	0.5465	7.7
H(23a)	0.3396	0.0668	0.6066	7.3
H(24a)	0.1358	0.0936	0.5145	5.5

Bond distances (Å) for [Cy_2SnCl_2.(1,10-phenanthroline)].

Atom - Atom	Distance	Atom - Atom	Distance
Sn - Cl(1)	2.544(2)	C(7) - C(12)	1.50(1)
Sn - Cl(2)	2.538(2)	C(8) - C(9)	1.55(1)
Sn - N(1)	2.394(7)	C(9) - C(10)	1.47(1)
Sn - N(2)	2.408(6)	C(10) - C(11)	1.50(1)
Sn - C(1)	2.152(9)	C(11) - C(12)	1.55(1)
Sn - C(7)	2.161(8)	C(13) - C(14)	1.38(2)
N(1) - C(13)	1.32(1)	C(14) - C(15)	1.33(2)
N(1) - C(17)	1.35(1)	C(15) - C(16)	1.36(2)
N(2) - C(20)	1.35(1)	C(16) - C(17)	1.43(1)
N(2) - C(24)	1.33(1)	C(16) - C(18)	1.45(3)
C(1) - C(2)	1.47(1)	C(17) - C(20)	1.44(1)
C(1) - C(6)	1.44(1)	C(18) - C(19)	1.32(3)
C(2) - C(3)	1.58(2)	C(19) - C(21)	1.42(2)
C(3) - C(4)	1.41(2)	C(20) - C(21)	1.41(1)
C(4) - C(5)	1.42(2)	C(21) - C(22)	1.42(2)
C(5) - C(6)	1.58(2)	C(22) - C(23)	1.32(2)
C(7) - C(8)	1.51(1)	C(23) - C(24)	1.38(1)

Bond angles (°) for [Cy_2SnCl_2(1,10-phenanthroline)].

Atom - Atom - Atom	Angle	Atom Atom Atom	Angle
Cl(1) - Sn - Cl(2)	105.70(8)	Sn - C(7) - C(8)	116.1(6)
Cl(1) - Sn - N(1)	159.3(2)	Sn - C(7) - C(12)	115.7(6)
Cl(1) - Sn - N(2)	89.6(2)	C(8) - C(7) - C(12)	109.7(7)
Cl(1) - Sn - C(1)	89.7(2)	C(7) C(8) - C(9)	110.8(7)
Cl(1) - Sn - C(7)	90.9(2)	C(8) - C(9) - C(10)	111.7(9)
Cl(2) - Sn - N(1)	95.0(2)	C(9) - C(10) - C(11)	111.8(9)
Cl(2) - Sn - N(2)	164.6(2)	C(10) - C(11) - C(12)	111.5(9)
Cl(2) - Sn - C(1)	89.3(2)	C(7) - C(12) - C(11)	111.3(9)
Cl(2) - Sn - C(7)	87.4(2)	N(1) - C(13) - C(14)	123(1)
N(1) - Sn - N(2)	69.8(2)	C(13) - C(14) - C(15)	120(2)
N(1) - Sn - C(1)	91.0(3)	C(14) - C(15) - C(16)	121(1)
N(1) - Sn - C(7)	89.5(3)	C(15) - C(16) - C(17)	117(1)
N(2) - Sn - C(1)	92.5(3)	C(15) - C(16) - C(18)	126(1)
N(2) - Sn - C(7)	90.7(3)	C(17) - C(16) - C(18)	117(1)
C(1) - Sn - C(7)	176.7(3)	N(1) - C(17) - C(16)	121(1)
Sn - N(1) - C(13)	125.1(8)	N(1) - C(17) - C(20)	118.9(7)
Sn - N(1) - C(17)	116.4(6)	C(16)- C(17) - C(20)	120(1)
C(13) - N(1) - C(17)	118.3(9)	C(16) - C(18) - C(19)	123(2)
Sn - N(2) - C(20)	115.6(6)	C(18) - C(19) - C(21)	123(2)
Sn - N(2) - C(24)	123.5(5)	N(2) - C(20) - C(17)	118.9(7)
C(20) - N(2) - C(24)	120.6(7)	N(2) - C(20) - C(21)	120(1)
Sn - C(1) - C(2)	115.8(7)	C(17) - C(20) - C(21)	121(1)
Sn - C(1) - C(6)	116.9(7)	C(19) - C(21) - C(20)	117(1)
C(2) - C(1) - C(6)	109(1)	C(19) - C(21) - C(22)	126(1)
C(1) - C(2) - C(3)	110(1)	C(20) - C(21) - C(22)	117(1)
C(2) - C(3) - C(4)	110(1)	C(21) - C(22) - C(23)	121(1)
C(3) - C(4) - C(5)	110(1)	C(22) - C(23) - C(24)	121(1)
C(4) - C(5) - C(6)	109(1)	N(2) - C(24) - C(23)	121(1)
C(1) - C(6) - C(5)	110(1)		

Observed and calculated structure factors for [Cy_2SnCl_2(1,10-phenanthroline)].

0	0	2	2112	2140	28	0	4	2	198	190	6	0	7	12	274	260	12	0	11	11	250	241	12	0	17	4	313	362	12
0	0	4	362	317	10	0	4	3	449	530	9	0	7	13	246	208	12	0	11	12	219	222	12	0	17	5	0	58	53*
0	0	6	421	480	10	0	4	4	820	811	13	0	7	14	386	366	11	0	12	0	430	407	12	0	18	0	473	471	12
0	0	8	1160	1209	19	0	4	5	23	79	32*	0	8	0	533	479	15	0	12	1	195	175	15	0	18	1	0	22	58*
0	0	10	725	728	17	0	4	6	181	219	9	0	8	1	1240	1256	19	0	12	2	781	768	18	0	18	2	462	466	12
0	0	12	489	482	14	0	4	7	680	763	14	0	8	2	673	730	13	0	12	3	87	53	46*	1	0	-15	414	437	11
0	0	14	74	121	37*	0	4	8	451	425	11	0	8	3	782	791	14	0	12	4	689	661	16	1	0	-13	538	543	14
0	1	1	667	733	10	0	4	9	972	955	18	0	8	4	172	202	9	0	12	5	72	93	48*	1	0	-11	143	140	26*
0	1	2	1334	1258	18	0	4	10	458	469	11	0	8	5	486	427	13	0	12	6	213	235	13	1	0	-9	142	171	21
0	1	3	192	132	6	0	4	11	692	703	18	0	8	6	122	131	14	0	12	7	213	211	15	1	0	-7	912	931	17
0	1	4	605	536	11	0	4	12	432	430	11	0	8	7	496	479	12	0	12	8	483	474	14	1	0	-5	1428	1414	20
0	1	5	735	707	13	0	4	13	237	277	14	0	8	8	262	253	12	0	12	9	0	21	52*	1	0	-3	1183	1224	17
0	1	6	1306	1320	19	0	4	14	114	136	23*	0	8	9	462	481	12	0	12	10	538	576	14	1	0	-1	549	319	12
0	1	7	625	634	13	0	4	15	123	63	17	0	8	10	379	374	10	0	12	11	137	134	18	1	0	1	1222	1231	18
0	1	8	603	595	14	0	5	-2	1844	1708	26	0	8	11	456	468	12	0	13	1	204	206	17	1	0	3	829	887	14
0	1	9	0	87	45*	0	5	1	1451	1282	20	0	8	12	239	257	13	0	13	2	0	110	56*	1	0	5	1878	1786	26
0	1	10	76	2	47*	0	5	3	119	121	8	0	8	13	387	369	10	0	13	3	255	255	13	1	0	7	2083	2069	29
0	1	11	144	106	17	0	5	4	1021	1025	15	0	8	14	0	56	48*	0	13	4	514	515	13	1	0	9	212	255	13
0	1	12	282	292	12	0	5	5	721	694	13	0	9	1	230	255	10	0	13	5	308	323	11	1	0	11	449	457	13
0	1	13	274	257	12	0	5	6	1189	1243	18	0	9	2	567	564	13	0	13	6	398	413	10	1	0	13	494	492	13
0	1	14	520	522	13	0	5	7	472	451	11	0	9	3	949	1034	16	0	13	7	269	286	12	1	0	15	523	580	14
0	1	15	284	292	10	0	5	8	248	263	10	0	9	4	193	151	9	0	13	8	170	179	18	1	1	-15	182	205	18
0	2	0	1593	1642	22	0	5	9	221	226	11	0	9	5	1050	1053	18	0	13	9	49	21	52*	1	1	-14	77	27	50*
0	2	1	2224	2562	30	0	5	10	213	216	14	0	9	6	149	121	14	0	13	10	0	44	50*	1	1	-13	262	284	18
0	2	2	913	1055	13	0	5	11	179	158	16	0	9	7	501	480	12	0	13	11	0	51	50*	1	1	-12	350	332	14
0	2	3	251	275	7	0	5	12	196	224	15	0	9	8	163	172	16	0	14	0	190	181	18	1	1	-11	685	663	16
0	2	4	200	150	7	0	5	13	345	332	10	0	9	9	178	187	16	0	14	1	692	683	15	1	1	-10	364	353	13
0	2	5	106	65	11	0	5	14	417	432	12	0	9	10	0	14	52*	0	14	2	259	272	14	1	1	-9	963	939	20
0	2	6	462	365	12	0	5	15	237	237	11	0	9	11	279	270	12	0	14	3	526	543	14	1	1	-8	696	673	17
0	2	7	398	455	10	0	6	0	1849	1848	26	0	9	12	0	40	53*	0	14	4	261	298	13	1	1	-7	1365	1423	21
0	2	8	688	672	15	0	6	1	85	58	15*	0	9	13	333	351	10	0	14	5	99	32	26*	1	1	-6	730	689	14
0	2	9	869	883	16	0	6	2	2094	1872	28	0	10	0	531	567	13	0	14	6	89	23	52*	1	1	-5	551	520	12
0	2	10	277	291	11	0	6	3	825	792	13	0	10	1	598	648	16	0	14	7	372	390	11	1	1	-4	461	416	11
0	2	11	479	493	13	0	6	4	447	442	11	0	10	2	814	780	16	0	14	8	102	62	51*	1	1	-3	498	548	10
0	2	12	184	203	15	0	6	5	287	306	8	0	10	3	1075	1082	18	0	14	9	425	446	12	1	1	-2	988	966	14
0	2	13	340	342	10	0	6	6	72	49	38*	0	10	4	249	249	9	0	14	10	311	311	11	1	1	-1	1866	1983	25
0	2	14	0	100	51*	0	6	7	0	51	42*	0	10	5	76	67	43*	0	15	1	189	156	18	1	1	0	1186	1062	16
0	2	15	0	68	48*	0	6	8	864	896	17	0	10	6	176	172	13	0	15	2	168	135	19	1	1	1	1291	1468	18
0	3	-2	1647	1585	23	0	6	9	150	150	17	0	10	7	326	312	10	0	15	3	453	473	12	1	1	2	1458	1328	20
0	3	1	868	864	13	0	6	10	661	716	17	0	10	8	389	380	11	0	15	4	133	89	20	1	1	3	170	194	9
0	3	3	719	748	11	0	6	11	64	39	43*	0	10	9	594	599	14	0	15	5	629	605	17	1	1	4	255	187	8
0	3	4	56	12	18*	0	6	12	529	543	14	0	10	10	268	291	13	0	15	6	117	108	25*	1	1	5	96	92	17*
0	3	5	886	862	14	0	6	13	170	144	16	0	10	11	561	558	14	0	15	7	361	344	11	1	1	6	287	291	8
0	3	6	0	32	38*	0	6	14	200	203	13	0	10	12	214	217	13	0	15	8	123	85	20	1	1	7	581	571	14
0	3	7	1023	1019	17	0	7	1	1438	1283	21	0	10	13	193	215	13	0	16	0	401	401	13	1	1	8	450	469	11
0	3	8	70	15	35*	0	7	2	289	299	8	0	11	1	0	36	50*	0	16	1	467	473	12	1	1	9	680	659	16
0	3	9	270	245	10	0	7	3	1277	1245	19	0	11	2	657	645	16	0	16	2	330	334	13	1	1	10	360	351	10
0	3	10	72	103	50*	0	7	4	930	960	15	0	11	3	394	389	10	0	16	3	426	427	11	1	1	11	424	404	11
0	3	11	258	269	12	0	7	5	303	326	8	0	11	4	962	995	18	0	16	4	218	232	16	1	1	12	87	173	50*
0	3	12	0	107	51*	0	7	6	922	897	16	0	11	5	541	545	12	0	16	5	67	33	50*	1	1	13	390	394	10
0	3	13	528	525	13	0	7	7	473	463	11	0	11	6	649	658	16	0	16	6	162	160	17	1	1	14	139	143	17
0	3	14	67	31	51*	0	7	8	437	462	11	0	11	7	0	97	51*	0	16	7	245	230	12	1	1	15	0	120	46*
0	3	15	521	525	12	0	7	9	192	177	13	0	11	8	386	390	11	0	17	1	47	61	47*	1	2	-15	267	261	13
0	4	-1	2525	2785	34	0	7	10	102	130	53*	0	11	9	122	75	22*	0	17	2	151	129	20	1	2	-14	594	584	16
0	4	0	2264	2369	31	0	7	11	119	137	23*	0	11	10	0	54	53*	0	17	3	160	165	20	1	2	-13	112	92	61*
1	2	-12	392	371	13	1	3	12	441	445	11	1	5	5	489	527	12	1	7	1	1718	1776	24	1	9	0	898	978	17
1	2	-11	0	40	60*	1	3	13	75	38	32*	1	5	6	516	575	13	1	7	2	148	168	9	1	9	1	72	68	27*
1	2	-10	112	7	57*	1	3	14	260	259	11	1	5	7	449	426	11	1	7	3	800	814	14	1	9	2	860	939	16
1	2	-9	79	43	45*	1	3	15	0	36	46*	1	5	8	19	68	45*	1	7	4	510	466	12	1	9	3	347	376	9
1	2	-8	109	62	22*	1	4	-15	188	176	16	1	5	9	1069	1094	19	1	7	5	134	144	11	1	9	4	538	559	14
1	2	-7	110	78	18	1	4	-14	473	479	13	1	5	10	293	305	11	1	7	6	0	15	42*	1	9	5	318	311	9
1	2	-6	1176	1116	18	1	4	-13	415	406	13	1	5	11	597	639	13	1	7	7	436	430	12	1	9	6	196	154	12
1	2	-5	26	133	42*	1	4	-12	367	357	13	1	5	12	259	249	12	1	7	8	793	800	17	1	9	7	178	196	15
1	2	-4	849	817	14	1	4	-11	0	40	61*	1	5	13	368	398	11	1	7	9	544	545	13	1	9	8	557	535	14
1	2	-3	528	552	11	1	4	-10	106	29	57*	1	5	14	67	65	34*	1	7	10	435	470	12	1	9	9	230	241	14
1	2	-2	409	431	9	1	4	-9	0	103	56*	1	6	-15	405	449	11	1	7	11	476	493	12	1	9	10	686	711	18
1	2	-1	308	366	8	1	4	-8	373	392	11	1	6	-14	96	143	54*	1	7	12	221	213	14	1	9	11	83	78	50*
1	2	0	601	597	11	1	4	-7	562	597	16	1	6	-13	503	454	14	1	7	13	305	291	11	1	9	12	426	456	11
1	2	1	667	602	10	1	4	-6	772	791	16	1	6	-12	91	125	47*	1	7	14	0	63	45*	1	9	13	90	44	47*
1	2	2	687	708	11	1	4	-5	1120	1088	18	1	6	-11	281	262	13	1	8	-14	451	460	13	1	10	-13	252	255	13
1	2	3	365	355	8	1	4	-4	1236	1215	19	1	6	-10	189	196	19	1	8	-13	0	103	55*	1	10	-12	366	314	12
1	2	4	712	709	13	1	4	-3	109	100	16	1	6	-9	63	38	43*	1	8	-12	396	351	12	1	10	-11	78	144	48*
1	2	5	949	840	15	1	4	-2	327	348	9	1	6	-8	274	275	14	1	8	-11	285	267	14	1	10	-10	119	155	29*
1	2	6	1136	1156	18	1	4	-1	173	127	13	1	6	-7	856	867	18	1	8	-10	229	213	16	1	10	-9	47	48	49*
1	2	7	736	734	15	1	4	0	56	48	40*	1	6	-6	478	518	13	1	8	-9	127	129	28*	1	10	-8	333	341	13
1	2	8	901	868	17	1	4	1	728	808	12	1	6	-5	1186	1261	20	1	8	-8	387	337	12	1	10	-7	443	432	12
1	2	9	185	187	14	1	4	2	1136	1093	16	1	6	-4	262	254	11	1	8	-7	352	349	12	1	10	-6	695	690	15
1	2	10	320	316	10	1	4	3	700	683	11	1	6	-3	832	748	16	1	8	-6	1221	1183	22	1	10	-5	627	615	15
1	2	11	90	111	52*	1	4	4	1148	1119	17	1	6	-2	22	147	47*	1	8	-5	422	430	12	1	10	-4	860	865	19
1	2	12	404	390	11	1	4	5	271	289	7	1	6	-1	292	290	9	1	8	-4	867	854	18	1	10	-3	50	76	41*
1	2	13	289	320	12	1	4	6	1381	1418	20	1	6	0	423	427	11	1	8	-3	738	755	17	1	10	-2	600	606	14
1	2	14	494	519	12	1	4	7	676	651	14	1	6	1	1295	1223	19	1	8	-2	313	282	10	1	10	-1	196	219	16
1	2	15	206	239	11	1	4	8	823	816	16	1	6	2	913	816	14	1	8	-1	0	38	45*	1	10	0	279	282	12
1	3	-15	86	5	53*	1	4	9	153	144	16	1	6	3	1316	1288	19	1	8	0	130	83	16	1	10	1	262	268	11
1	3	-14	0	18	62*	1	4	10	194	200	14	1	6	4	41	50	33*	1	8	1	433	451	11	1	10	2	901	879	17
1	3	-13	112	64	59*	1	4	11	0	68	51*	1	6	5	1006	1073	16	1	8	2	1125	1197	18	1	10	3	683	647	15
1	3	-12	741	741	21	1	4	12	443	466	12	1	6	6	142	132	11	1	8	3	780	757	14	1	10	4	1007	1031	18
1	3	-11	104	55	58*	1	4	13	0	53	49*	1	6	7	934	942	17	1	8	4	677	705	13	1	10	5	344	345	9
1	3	-10	1054	1033	21	1	4	14	469	462	13	1	6	8	141	128	16	1	8	5	721	695	14	1	10	6	398	396	11
1	3	-9	494	443	14	1	4	15	259	265	10	1	6	9	187	218	14	1	8	6	601	589	15	1	10	7	504	483	12
1	3	-8	1421	1392	23	1	5	-15	91	87	28*	1	6	10	197	236	16	1	8	7	144	158	17	1	10	8	165	153	17
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6	7	7	0	102	49*	6	10	-7	466	474	13	6	13	-8	86	28	52*	7	1	-5	219	226	10	7	3	0	1084	1047	18						
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6	9	-7	459	459	11	6	11	6	429	445	12	6	15	2	45	70	38*	7	2	3	290	278	10	7	4	8	377	368	10						
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7	5	0	355	337	9	7	7	8	251	258	10	7	10	1	0	67	55*	7	14	0	176	162	18	8	2	6	200	182	14						
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7	5	6	89	12	48*	7	8	-8	275	254	14	7	10	7	141	177	16	8	0	-4	0	37	42*	8	3	-11	358	334	12						
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7	6	-12	0	47	54*	7	8	-2	532	532	14	7	11	-5	190	175	18	8	0	8	292	291	10	8	3	-5	581	595	16						
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9	10	-6	188	207	15	10	2	4	177	194	14	10	6	-1	0	66	48*	11	2	0	297	292	11						
9	10	-5	199	183	15	10	2	5	0	129	49*	10	6	0	461	480	13	11	2	1	82	84	48*						
9	10	-4	533	559	14	10	3	-10	19	57	50*	10	6	1	64	25	47*	11	2	2	69	100	49*						
9	10	-3	282	273	12	10	3	-9	71	97	37*	10	6	2	421	430	11	11	3	-7	126	50	18						
9	10	-2	303	289	12	10	3	-8	135	113	20	10	6	3	132	124	17	11	3	-6	458	445	13						
9	10	-1	281	271	12	10	3	-7	205	216	14	10	7	-8	97	74	50*	11	3	-5	70	1	48*						
9	10	0	98	101	54*	10	3	-6	52	21	50*	10	7	-7	0	78	52*	11	3	-4	0	20	50*						
9	10	1	161	156	16	10	3	-5	573	577	13	10	7	-6	255	274	12	11	3	-3	0	3	50*						
9	10	2	72	13	38*	10	3	-4	0	43	51*	10	7	-5	324	295	11	11	3	-2	175	191	15						
9	11	-5	289	286	12	10	3	-3	460	500	13	10	7	-4	449	450	11	11	3	-1	41	83	49*						
9	11	-4	68	13	39*	10	3	-2	0	93	51*	10	7	-3	262	223	12	11	3	0	417	432	10						
9	11	-3	55	87	54*	10	3	-1	425	446	11	10	7	-2	365	360	10	11	3	1	85	22	47*						

C. [Bz_2SnCl_2(1,10-phenanthroline)].

Crystallographic Data and Refinement details for [Bz_2SnCl_2(1,10-phenanthroline)].

Formula	$C_{26}H_{22}Cl_2N_2Sn$
Formula weight	552.1
Crystal morphology	orange block
Crystal dimensions (mm)	0.08 x 0.31 x 0.37
Crystal system	monoclinic
Space group	$P2_1/n$ (C_{2h}^5, No. 14)
Temperature (°C)	20.0
a (Å)	10.356(3)
b (Å)	17.540(2)
c (Å)	13.817(9)
β (°)	105.93(5)
V (Å^3)	2413(1)
Z	4
D_{calc} (g cm^{-3})	1.519
F(000)	1104
Radiation	MoKα (λ = 0.7107Å)
μ (cm^{-1})	12.95
θ limits, data (°)	3.0 to 27.5
hkl range	0 to 13, 0 to 23, -18 to 18
Range of transmission factors	0.938 to 1.000
Scan technique	ω:2θ
Scan width (°)	1.15
No. of data measured	6083
No. of unique data	5778
R_{amal}	0.075
Program for structure solution	Direct Methods (SIR92)
No. of unique data used	2576
No. of parameters	271
R	0.045
R_w	0.044
G.O.F.	1.59
Min./Max. residual electron density (e Å^{-3})	-0.85 to +1.07

Fractional atomic coordinates ($Å^2$) for the non-hydrogen atoms in [Bz_2SnCl_2(1,10-phenanthroline)].

Atom	*x*	*y*	*z*
Sn	-0.10044(4)	-0.05832(2)	-0.27778(4)
Cl(1)	-0.0493(2)	-0.1831(1)	-0.3483(2)
Cl(2)	-0.3309(2)	-0.0761(1)	-0.2550(2)
N(1)	0.1119(5)	-0.0091(3)	-0.2759(4)
N(2)	-0.0826(5)	0.0695(3)	-0.2211(4)
C(1)	-0.1836(7)	-0.0196(5)	-0.4307(6)
C(2)	-0.2327(8)	0.0605(5)	-0.4427(6)
C(3)	-0.1516(9)	0.1201(6)	-0.4546(6)
C(4)	-0.196(1)	0.1947(6)	-0.4595(7)
C(5)	-0.323(2)	0.2090(7)	-0.4547(9)
C(6)	-0.408(1)	0.1514(8)	-0.4448(9)
C(7)	-0.3629(8)	0.0773(6)	-0.4395(7)
C(8)	-0.0230(9)	-0.0973(4)	-0.1256(7)
C(9)	0.1249(9)	-0.1033(5)	-0.0836(6)
C(10)	0.203(1)	-0.0434(5)	-0.0356(7)
C(11)	0.341(1)	-0.0516(8)	0.0028(8)
C(12)	0.400(1)	-0.120(11)	-0.008(1)
C(13)	0.327(2)	-0.1770(9)	-0.055(1)
C(14)	0.190(1)	-0.1719(5)	-0.0927(7)
C(15)	0.207(6)	-0.0503(5)	-0.2970(5)
C(16)	0.3325(8)	-0.0206(7)	-0.2926(7)
C(17)	0.3589(8)	0.0512(8)	-0.2679(7)
C(18)	0.2602(9)	0.0984(5)	-0.2457(6)
C(19)	0.1357(6)	0.0643(4)	-0.2475(6)
C(20)	0.274(1)	0.1755(8)	-0.2197(9)
C(21)	0.178(1)	0.2174(6)	-0.1991(8)
C(22)	0.0328(6)	0.1060(4)	-0.2228(6)
C(23)	0.050(1)	0.1832(4)	-0.1972(6)
C(24)	-0.056(1)	0.2226(5)	-0.1769(7)
C(25)	-0.171(1)	0.1852(5)	-0.1769(6)
C(26)	-0.1822(7)	0.1066(4)	-0.1990(5)

Anisotropic thermal parameters (Å) for the non-hydrogen atoms in [Bz_2SnCl_2.(1,10-phenanthroline)].

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Sn	0.0433(2)	0.0433(2)	0.0519(4)	-0.0020(2)	0.0143(2)	-0.0112(3)
Cl(1)	0.084(1)	0.057(1)	0.122(2)	0.004(1)	0.026(1)	-0.036(1)
Cl(2)	0.062(1)	0.092(2)	0.186(3)	-0.016(1)	0.060(2)	-0.021(2)
N(1)	0.043(3)	0.077(4)	0.005(4)	-0.004(3)	0.005(3)	0.007(3)
N(2)	0.062(3)	0.048(3)	0.008(4)	0.013(2)	0.003(3)	-0.007(3)
C(1)	0.062(4)	0.092(6)	0.034(6)	0.016(4)	-0.016(4)	-0.031(5)
C(2)	0.071(5)	0.093(6)	0.012(5)	0.025(5)	-0.018(4)	-0.015(5)
C(3)	0.106(7)	0.097(7)	0.010(6)	0.022(6)	0.000(5)	0.003(5)
C(4)	0.174(1)	0.096(8)	0.019(7)	0.010(7)	0.000(7)	0.014(6)
C(5)	0.202(2)	0.116(1)	0.033(8)	0.075(1)	0.010(1)	0.008(7)
C(6)	0.125(9)	0.173(1)	0.038(8)	0.091(9)	0.008(7)	0.010(9)
C(7)	0.071(5)	0.134(8)	0.043(7)	0.038(5)	-0.006(5)	-0.009(6)
C(8)	0.109(6)	0.070(5)	0.066(8)	0.013(5)	0.054(6)	0.019(5)
C(9)	0.115(7)	0.077(6)	0.023(6)	0.028(5)	0.036(5)	0.024(5)
C(10)	0.139(9)	0.083(7)	0.024(7)	0.019(6)	0.024(6)	0.015(5)
C(11)	0.139(1)	0.169(1)	0.023(7)	-0.007(9)	-0.008(7)	0.006(8)
C(12)	0.139(1)	0.207(2)	0.052(1)	0.052(1)	-0.028(8)	0.089(1)
C(13)	0.155(1)	0.164(1)	0.074(1)	0.088(1)	0.013(1)	0.015(9)
C(14)	0.127(8)	0.086(6)	0.043(7)	0.037(6)	0.021(6)	0.022(5)
C(15)	0.045(3)	0.105(6)	0.022(5)	0.001(4)	0.009(4)	-0.008(5)
C(16)	0.051(5)	0.182(1)	0.039(8)	-0.014(6)	0.011(5)	-0.004(7)
C(17)	0.054(4)	0.192(1)	0.026(7)	-0.042(7)	0.011(4)	0.005(8)
C(18)	0.092(6)	0.103(7)	0.006(5)	-0.054(5)	-0.003(5)	-0.003(5)
C(20)	0.141(1)	0.151(1)	0.035(9)	-0.085(9)	0.002(7)	0.004(8)
C(21)	0.183(1)	0.080(7)	0.034(8)	-0.083(8)	-0.007(8)	-0.006(6)
C(23)	0.149(8)	0.044(4)	0.009(6)	-0.020(5)	-0.004(5)	0.002(4)
C(24)	0.188(1)	0.045(5)	0.023(7)	0.010(6)	-0.032(7)	-0.008(5)
C(25)	0.142(8)	0.079(6)	0.012(6)	0.052(6)	-0.010(6)	-0.013(5)
C(26)	0.081(5)	0.068(5)	0.010(5)	0.024(4)	0.003(4)	-0.003(4)

Fractional atomic coordinates and B_{eq} values ($Å^2$) for the hydrogen atoms in [Bz_2SnCl_2(1,10-phenanthroline)].

Atom	*x*	*y*	*z*	*B*eq
H(1a)	-0.2586	-0.0525	-0.4623	6.4
H(1b)	-0.1144	-0.0246	-0.4657	6.4
H(3a)	-0.0614	0.1094	-0.4591	6.9
H(4a)	-0.1366	0.2361	-0.4664	9.5
H(5a)	-0.3546	0.2611	-0.4577	11.5
H(6a)	-0.4989	0.1624	-0.4426	10.9
H(7a)	-0.4228	0.0361	-0.4337	8.3
H(8a)	-0.0549	-0.0625	-0.0828	7.2
H(8b)	-0.0599	-0.1477	-0.1217	7.2
H(10a)	0.1618	0.0047	-0.0281	7.7
H(11a)	0.3948	-0.0091	0.0361	11.0
H(12a)	0.4967	-0.1254	0.0190	13.5
H(13a)	0.3721	-0.2242	-0.0638	12.7
H(14a)	0.1389	-0.2156	-0.1252	7.8
H(15a)	0.1903	-0.1034	-0.3157	5.2
H(16a)	0.4004	-0.0525	-0.3088	8.4
H(17a)	0.4462	0.0720	-0.2648	8.6
H(20a)	0.3600	0.1990	-0.2150	10.6
H(21a)	0.1941	0.2713	-0.1847	9.9
H(24a)	-0.0487	0.2766	-0.1630	9.1
H(25a)	-0.2444	0.2124	-0.1610	7.9
H(26a)	-0.2638	0.0798	-0.1979	5.2

Bond distances (Å) for [Bz_2SnCl_2(1,10-phenanthroline)].

Atom - Atom	Distance	Atom - Atom	Distance
Sn - Cl(1)	2.510(2)	C(9) - C(10)	1.38(1)
Sn - Cl(2)	2.511(2)	C(9) - C(14)	1.40(1)
Sn - N(1)	2.356(5)	C(10) - C(11)	1.39(1)
Sn - N(2)	2.365(5)	C(11) - C(12)	1.37(2)
Sn - C(1)	2.161(8)	C(12) - C(13)	1.32(2)
Sn - C(8)	2.146(9)	C(13) - C(14)	1.38(1)
N(1) - C(15)	1.323(8)	C(15) - C(16)	1.38(1)
N(1) - C(19)	1.347(8)	C(16) - C(17)	1.31(1)
N(2) - C(22)	1.362(7)	C(17) - C(18)	1.41(1)
N(2) - C(26)	1.325(8)	C(18) - C(19)	1.415(9)
C(1) - C(2)	1.49(1)	C(18) - C(20)	1.40(1)
C(2) - C(3)	1.38(1)	C(19) - C(22)	1.411(9)
C(2) - C(7)	1.39(1)	C(20) - C(21)	1.33(1)
C(3) - C(4)	1.38(1)	C(21) - C(23)	1.46(1)
C(4) - C(5)	1.36(2)	C(22) - C(23)	1.397(9)
C(5) - C(6)	1.37(2)	C(23) - C(24)	1.39(1)
C(6) - C(7)	1.38(1)	C(24) - C(25)	1.36(1)
C(8) - C(9)	1.49(1)	C(25) - C(26)	1.41(1)

Bond angles (°) for [Bz_2SnCl_2(1,10-phenanthroline)].

Atom - Atom - Atom	Angle	Atom - Atom - Atom	Angle
Cl(1) - Sn - Cl(2)	104.46(7)	Sn - C(8) - C(9)	118.2(5)
Cl(1) - Sn - N(1)	163.4(1)	C(8) - C(9) - C(10)	122.9(8)
Cl(1) - Sn - N(2)	94.3(1)	C(8) - C(9) - C(14)	119.6(9)
Cl(1) - Sn - C(1)	89.1(2)	C(10) - C(9) - C(14)	117.5(9)
Cl(1) - Sn - C(8)	93.8(1)	C(9) - C(10) - C(11)	120.8(9)
Cl(2) - Sn - N(1)	91.4(2)	C(10) - C(11) - C(12)	120(1)
Cl(2) - Sn - N(2)	161.7(1)	C(11) - C(12) - C(13)	121(1)
Cl(2) - Sn - C(1)	87.2(2)	C(12) - C(13) - C(14)	122(1)
Cl(2) - Sn - C(8)	92.3(2)	C(9) - C(14) - C(13)	120(1)
N(1) - Sn - N(2)	70.2(2)	N(1) - C(15) - C(16)	122.3(8)
N(1) - Sn - C(1)	90.9(2)	C(15) - C(16) - C(17)	119.9(9)
N(1) - Sn - C(8)	90.5(3)	C(16) - C(17) - C(18)	120.4(8)
N(2) - Sn - C(1)	90.0(2)	C(17) - C(18) - C(19)	117.3(8)
N(2) - Sn - C(8)	90.2(3)	C(17) - C(18) - C(20)	126.6(9)
C(1) - Sn - C(8)	178.5(3)	C(19) - C(18) - C(20)	116.1(9)
Sn - N(1) - C(15)	123.5(5)	N(1) - C(19) - C(18)	120.1(7)
Sn - N(1) - C(19)	116.7(4)	N(1) - C(19) - C(22)	118.5(6)
C(15) - N(1) - C(19)	119.8(5)	C(18) - C(19) - C(22)	121.4(7)
Sn - N(2) - C(22)	115.4(4)	C(18) - C(20) - C(21)	124(1)
Sn - N(2) - C(26)	123.2(5)	C(20) - C(21) - C(23)	121(1)
C(22) - N(2) - C(26)	121.0(6)	N(2) - C(22) - C(19)	119.0(6)
Sn - C(1) - C(2)	116.0(5)	N(2) - C(22) - C(23)	120.3(7)
C(1) - C(2) - C(3)	121.9(7)	C(19) - C(22) - C(23)	120.7(7)
C(1) - C(2) - C(7)	120.1(9)	C(21) - C(23) - C(22)	116.8(9)
C(3) - C(2) - C(7)	118.0(8)	C(21) - C(23) - C(24)	124.7(9)
C(2) - C(3) - C(4)	121.3(9)	C(22) - C(23) - C(24)	118.5(8)
C(3) - C(4) - C(5)	119(1)	C(23) - C(24) - C(25)	120.1(8)
C(4) - C(5) - C(6)	122(1)	C(24) - C(25) - C(26)	119.5(8)
C(5) - C(6) - C(7)	119(1)	N(2) - C(26) - C(25)	120.5(8)
C(2) - C(7) - C(6)	121(1)		

Observed and calculated structure factors for $[Bz_2SnCl_2(1,10\text{-phenanthroline})]$.

h	k	l	Fo	Fc	sigF
0	0	4	2943	2897	34
0	0	6	1115	1106	16
0	0	8	284	307	14
0	0	10	151	29	41*
0	0	12	442	456	28
0	0	14	242	290	99*
0	0	16	250	149	99*
0	1	3	845	856	11
0	1	4	2760	2767	32
0	1	5	800	824	13
0	1	6	419	410	11
0	1	7	1389	1324	20
0	1	8	590	576	15
0	1	9	348	402	17
0	1	10	215	185	34
0	1	11	730	808	20
0	1	12	0	32	99*
0	1	13	180	264	99*
0	1	14	0	115	99*
0	1	15	238	97	99*
0	1	16	221	82	99*
0	1	17	0	93	99*
0	2	2	1660	1677	20
0	2	3	221	248	6
0	2	4	2032	2033	24
0	2	6	1243	1213	17
0	2	7	667	656	15
0	2	8	452	429	12
0	2	9	131	37	72*
0	2	10	0	107	85*
0	2	11	200	124	99*
0	2	12	160	199	85*
0	2	13	0	29	99*
0	2	14	400	411	51
0	2	15	248	362	99*
0	2	16	0	175	99*
0	2	17	406	54	88*
0	3	1	264	267	7
0	3	2	103	81	8
0	3	3	1275	1237	16
0	3	4	1289	1261	16
0	3	5	915	936	14
0	3	6	1130	1102	16
0	3	7	1231	1234	18
0	3	8	1207	1152	20
0	3	9	716	706	17
0	3	10	852	840	20
0	3	11	133	36	71*
0	3	12	345	398	36
0	3	13	0	211	99*
0	3	14	199	241	99*
0	3	15	0	51	99*
0	3	16	310	6	90*
0	3	17	0	22	99*
0	4	0	329	312	8
0	4	1	1935	1920	23
0	4	2	213	221	6
0	4	3	1552	1603	19
0	4	4	52	69	30*
0	4	5	962	993	14
0	4	6	257	236	10
0	4	7	82	60	51*
0	4	8	266	228	15
0	4	9	278	234	20
0	4	10	0	142	82*
0	4	11	467	449	22
0	4	12	170	94	60*
0	4	13	219	230	99*
0	4	14	236	88	99*
0	4	15	0	161	99*
0	4	16	202	69	99*
0	4	17	345	137	93*
0	5	1	351	348	9
0	5	2	590	610	10
0	5	3	77	67	14*
0	5	4	932	947	13
0	5	5	117	158	15
0	5	6	1221	1179	18
0	5	7	171	198	17
0	5	8	1047	1033	20
0	5	9	0	51	75*
0	5	10	563	594	17
0	5	11	160	83	92*
0	5	12	248	296	41
0	5	13	202	106	99*
0	5	14	0	208	99*
0	5	15	138	35	99*
0	5	16	0	7	99*
0	6	0	1247	1207	16
0	6	1	1268	1275	16
0	6	2	1301	1333	16
0	6	3	944	956	13
0	6	4	1220	1225	16
0	6	5	594	578	13
0	6	6	756	736	15
0	6	7	208	216	15
0	6	8	335	323	14
0	6	9	0	21	72*
0	6	10	85	28	57*
0	6	11	228	191	38*
0	6	12	142	27	99*
0	6	13	249	267	54*
0	6	14	0	85	99*
0	6	15	294	207	67*
0	6	16	96	7	99*
0	7	1	70	166	37*
0	7	2	789	788	12
0	7	3	172	189	8
0	7	4	832	839	13
0	7	5	450	458	10
0	7	6	352	367	9
0	7	7	527	518	13
0	7	8	385	388	13
0	7	9	381	374	17
0	7	10	201	226	35*
0	7	11	331	380	29
0	7	12	223	172	48*
0	7	13	165	183	87*
0	7	14	41	55	99*
0	7	15	183	101	99*
0	7	16	0	75	99*
0	8	0	2410	2366	29
0	8	1	657	644	11
0	8	2	1556	1578	19
0	8	3	210	196	8
0	8	4	920	928	14
0	8	5	232	221	10
0	8	6	449	434	12
0	8	7	267	245	13
0	8	8	100	86	63*
0	8	9	0	121	77*
0	8	10	131	22	79*
0	8	11	151	176	97*
0	8	12	0	179	90*
0	8	13	99	125	87*
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6	12	8	0	80	82*	6	15	-7	67	67	46*	6	18	-6	248	262	13	7	1	-7	299	319	11	7	3	-12	159	15	85*
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7	19	-1	86	57	45*	8	2	-4	155	170	13	8	4	-3	354	370	9	8	6	-2	195	210	10	8	8	2	173	195	15
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12	8	0	0	57	46*	13	5	-3	52	23	43*																		
12	9	-8	0	3	51*	13	6	-5	80	140	43*																		
12	9	-7	0	33	47*																								
12	9	-6	0	3	44*																								
12	9	-5	116	111	16																								
12	9	-4	84	34	19*																								
12	9	-3	194	203	10																								
12	9	-2	85	31	43*																								
12	9	-1	214	212	12																								
12	10	-6	126	155	17																								
12	10	-5	167	163	12																								
12	10	-4	148	154	13																								
12	10	-3	79	103	41*																								
13	0	-9	105	135	61*																								
13	0	-7	245	233	12																								
13	0	-5	294	308	9																								
13	0	-3	308	318	9																								
13	0	-1	275	262	11																								
13	1	-9	59	68	58*																								
13	1	-8	148	173	20																								
13	1	-7	26	79	51*																								
13	1	-6	127	124	17																								
13	1	-5	0	54	42*																								
13	1	-4	45	43	42*																								
13	1	-3	0	10	42*																								
13	1	-2	72	50	45*																								
13	1	-1	0	25	50*																								
13	2	-9	81	118	44*																								
13	2	-8	85	103	53*																								
13	2	-7	170	178	16																								
13	2	-6	175	178	13																								

D. [Ph(Me)$SnCl_2$(1,10-phenanthroline)].

Crystallographic Data and Refinement details for [Ph(Me)$SnCl_2$(1,10-phenanthroline)].

Formula	$C_{19}H_{16}Cl_2N_2Sn$
Formula weight	461.9
Crystal morphology	colourless needle
Crystal dimensions (mm)	0.06 x 0.11 x 0.50
Crystal system	monoclinic
Space group	$P2_1/n$ (C_{2h}^5, No. 14)
Temperature (°C)	20.0
a (Å)	9.118(2)
b (Å)	11.023(2)
c (Å)	18.712(2)
β (°)	93.03(1)
V (Å^3)	1878.1(4)
Z	4
D_{calc} (g cm^{-3})	1.634
F(000)	912
Radiation	MoKα (λ = 0.7107Å)
μ (cm^{-1})	16.47
θ limits, data (°)	3.0 to 27.5
hkl range	0 to 12, 0 to 14, -24 to 24
Range of transmission factors	0.987 to 1.000
Scan technique	ω:2θ
Scan width (°)	1.00
No. of data measured	4842
No. of unique data	4565
R_{amal}	0.069
Program for structure solution	Direct Methods (SHELXS86)
No. of unique data used	2538
No. of parameters	218
R	0.036
R_w	0.036
G.O.F.	1.31
Min./Max. residual electron density (e Å^{-3})	-0.61 to +0.41

Fractional atomic coordinates ($Å^2$) for the non-hydrogen atoms in [Ph(Me)$SnCl_2$(1,10-phenanthroline)].

Atom	*x*	*y*	*z*
Sn	-0.21783(4)	0.82925(3)	0.61920(2)
Cl(1)	-0.2955(2)	1.0393(2)	0.5878(1)
Cl(2)	-0.1048(2)	0.8502(2)	0.73665(8)
N(1)	-0.1597(4)	0.6183(4)	0.6140(2)
N(2)	-0.3088(5)	0.7388(4)	0.5130(2)
C(1)	-0.0131(7)	0.8603(6)	0.5620(3)
C(2)	-0.4272(5)	0.7833(5)	0.6698(3)
C(3)	-0.4392(6)	0.6888(5)	0.7176(3)
C(4)	-0.5754(7)	0.6592(6)	0.7515(3)
C(5)	-0.6983(7)	0.7258(8)	0.7361(4)
C(6)	-0.6866(7)	0.8200(8)	0.6893(4)
C(7)	-0.5522(6)	0.8488(6)	0.6552(3)
C(8)	-0.0827(6)	0.5602(5)	0.6617(3)
C(9)	-0.0551(6)	0.4359(6)	0.6575(3)
C(10)	-0.1128(7)	0.3703(5)	0.6050(4)
C(11)	-0.1945(6)	0.4273(5)	0.5533(3)
C(12)	-0.2126(5)	0.5537(5)	0.5596(3)
C(13)	-0.2550(7)	0.3650(6)	0.4954(4)
C(14)	-0.3257(7)	0.4245(6)	0.4454(4)
C(15)	-0.2911(6)	0.6174(5)	0.5059(3)
C(16)	-0.3439(6)	0.5531(6)	0.4479(3)
C(17)	-0.4151(7)	0.6193(7)	0.3964(3)
C(18)	-0.4334(7)	0.7396(7)	0.4048(3)
C(19)	-0.3787(7)	0.7972(6)	0.4634(3)

Anisotropic thermal parameters ($Å^2$) for the non-hydrogen atoms in [Ph(Me)$SnCl_2$(1,10-phenanthroline)].

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Sn	0.0442(2)	0.0440(2)	0.0436(2)	-0.0101(2)	0.0019(1)	-0.0013(2)
Cl(1)	0.092(1)	0.050(1)	0.146(2)	-0.023(3)	-0.004(1)	0.018(1)
Cl(2)	0.054(2)	0.093(1)	0.056(3)	0.007(3)	0.015(2)	-0.016(3)
N(1)	0.043(2)	0.049(3)	0.036(2)	-0.013(2)	0.001(2)	0.004(2)
N(2)	0.065(3)	0.056(3)	0.029(2)	-0.025(2)	0.007(2)	-0.001(2)
C(1)	0.068(4)	0.071(5)	0.074(4)	-0.009(3)	-0.019(3)	0.018(4)
C(2)	0.042(3)	0.056(3)	0.040(3)	-0.005(2)	0.004(2)	-0.014(3)
C(3)	0.048(3)	0.058(4)	0.055(3)	-0.001(3)	-0.001(3)	-0.012(3)
C(4)	0.073(4)	0.073(4)	0.066(4)	0.021(4)	-0.011(3)	-0.018(4)
C(5)	0.043(4)	0.113(6)	0.084(5)	0.017(4)	-0.012(4)	-0.052(5)
C(6)	0.049(4)	0.103(6)	0.086(5)	-0.011(4)	0.009(3)	-0.035(5)
C(7)	0.046(3)	0.075(4)	0.065(4)	-0.016(3)	0.010(3)	-0.019(3)
C(8)	0.060(4)	0.067(4)	0.040(3)	-0.016(3)	0.011(3)	0.007(3)
C(9)	0.064(4)	0.070(4)	0.057(4)	-0.030(3)	-0.001(3)	0.024(3)
C(10)	0.075(4)	0.050(4)	0.067(4)	-0.025(3)	-0.007(3)	0.008(3)
C(11)	0.055(3)	0.048(3)	0.050(3)	-0.015(3)	-0.009(3)	-0.005(3)
C(12)	0.047(3)	0.046(3)	0.036(3)	-0.012(2)	-0.001(2)	-0.003(2)
C(13)	0.076(4)	0.057(4)	0.073(5)	-0.020(3)	-0.005(4)	-0.017(3)
C(14)	0.073(4)	0.081(5)	0.061(4)	-0.012(4)	0.005(3)	-0.037(4)
C(15)	0.044(3)	0.057(3)	0.038(3)	-0.021(3)	-0.003(2)	-0.006(3)
C(16)	0.055(3)	0.076(4)	0.039(3)	-0.019(3)	0.001(3)	-0.019(3)
C(17)	0.072(4)	0.115(6)	0.038(4)	-0.036(4)	0.010(3)	-0.022(4)
C(18)	0.080(5)	0.113(6)	0.040(4)	-0.046(4)	0.012(3)	-0.003(4)
C(19)	0.078(4)	0.072(4)	0.043(3)	-0.034(3)	0.009(3)	0.003(3)

Fractional atomic coordinates and *B*eq values ($Å^2$) for the hydrogen atoms in [Ph(Me)$SnCl_2$(1,10-phenanthroline)].

Atom	*x*	*y*	*z*	B_{eq}
H(1a)	-0.0003	0.0535	0.4462	5.7
H(1b)	-0.0122	0.1818	0.4836	5.7
H(1c)	0.0659	0.1700	0.4103	5.8
H(3a)	-0.3525	0.3579	0.2721	5.3
H(4a)	-0.5831	0.4074	0.2146	6.7
H(5a)	-0.7933	0.2949	0.2413	6.8
H(6a)	-0.7729	0.1323	0.3203	6.3
H(7a)	-0.5455	0.0851	0.3792	5.5
H(8a)	-0.0446	0.3939	0.2990	4.9
H(9a)	0.0053	0.6032	0.3080	5.2
H(10a)	-0.0978	0.7169	0.3970	5.9
H(13a)	-0.2450	0.7224	0.5079	5.8
H(14a)	-0.3658	0.6209	0.5936	6.5
H(17a)	-0.4511	0.4213	0.6453	6.5
H(18a)	-0.4850	0.2141	0.6301	6.4
H(19a)	-0.3923	0.1158	0.5316	5.4

Bond distances (Å) for [$PhMeSnCl_2$(1,10-phenanthroline)].

Atom - Atom	Distance	Atom - Atom	Distance
Sn - Cl(1)	2.500(2)	C(5) - C(6)	1.36(1)
Sn - Cl(2)	2.487(1)	C(6) - C(7)	1.388(9)
Sn - N(1)	2.386(4)	C(8) - C(9)	1.395(8)
Sn - N(2)	2.410(4)	C(9) - C(10)	1.349(8)
Sn - C(1)	2.130(6)	C(10) - C(11)	1.400(8)
Sn - C(2)	2.146(5)	C(11) - C(12)	1.408(7)
N(1) - C(8)	1.329(6)	C(11) - C(13)	1.418(8)
N(1) - C(12)	1.352(6)	C(12) - C(15)	1.445(7)
N(2) - C(15)	1.354(6)	C(13) - C(14)	1.336(8)
N(2) - C(19)	1.321(6)	C(14) - C(16)	1.428(9)
C(2) - C(3)	1.374(7)	C(15) - C(16)	1.402(7)
C(2) - C(7)	1.389(7)	C(16) - C(17)	1.396(8)
C(3) - C(4)	1.403(8)	C(17) - C(18)	1.345(9)
C(4) - C(5)	1.38(1)	C(18) - C(19)	1.381(9)

Bond angles (°) for [$PhMeSnCl_2$(1,10-phenanthroline)].

Atom - Atom - Atom	Angle	Atom - Atom - Atom	Angle
Cl(1) - Sn - Cl(2)	104.91(7)	C(3) - C(4) - C(5)	119.4(6)
Cl(1) - Sn - N(1)	163.4(1)	C(4) - C(5) - C(6)	120.2(6)
Cl(1) - Sn - N(2)	94.3(1)	C(5) - C(6) - C(7)	120.6(6)
Cl(1) - Sn - C(1)	89.1(2)	C(2) - C(7) - C(6)	120.3(6)
Cl(1) - Sn - C(2)	93.8(2)	N(1) - C(8) - C(9)	122.4(5)
Cl(2) - Sn - N(1)	91.4(1)	C(8) - C(9) - C(10)	119.4(5)
Cl(2) - Sn - N(2)	160.8(1)	C(9) - C(10) - C(11)	120.4(5)
Cl(2) - Sn - C(1)	92.1(2)	C(10) - C(11) - C(12)	116.8(5)
Cl(2) - Sn - C(2)	91.9(1)	C(10) - C(11) - C(13)	123.6(5)
N(1) - Sn - N(2)	69.4(1)	C(12) - C(11) - C(13)	119.6(5)
N(1) - Sn - C(1)	87.1(2)	N(1) - C(12) - C(11)	122.6(5)
N(1) - Sn - C(2)	88.8(2)	N(1) - C(12) - C(15)	118.5(4)
N(2) - Sn - C(1)	89.0(2)	C(11) - C(12) - C(15)	118.9(5)
N(2) - Sn - C(2)	86.0(2)	C(11) - C(13) - C(14)	121.3(6)
C(1) - Sn - C(2)	174.4(2)	C(13) - C(14) - C(16)	121.6(6)
Sn - N(1) - C(8)	124.5(4)	N(2) - C(15) - C(12)	118.2(5)
Sn - N(1) - C(12)	117.1(3)	N(2) - C(15) - C(16)	122.1(5)
C(8) - N(1) - C(12)	118.3(5)	C(12) - C(15) - C(16)	119.7(5)
Sn - N(2) - C(15)	116.4(3)	C(14) - C(16) - C(15)	118.9(6)
Sn - N(2) - C(19)	125.3(4)	C(14) - C(16) - C(17)	123.6(6)
C(15) - N(2) - C(19)	118.2(5)	C(15) - C(16) - C(17)	117.5(6)
Sn - C(2) - C(3)	120.3(4)	C(16) - C(17) - C(18)	119.6(6)
Sn - C(2) - C(7)	120.7(4)	C(17) - C(18) - C(19)	119.9(6)
C(3) - C(2) - C(7)	119.0(5)	N(2) - C(19) - C(18)	122.8(6)
C(2) - C(3) - C(4)	120.6(5)		

Observed and calculated structure factors for [PhMeSnCl$_2$(1,10-phenanthroline)].

h	k	l	Fo	Fc	sigF
0	0	4	1268	1278	14
0	0	6	1112	1123	14
0	0	8	1539	1524	18
0	0	10	222	222	9
0	0	12	434	434	11
0	0	14	548	535	12
0	0	16	578	535	13
0	0	18	541	553	13
0	0	20	167	122	18
0	0	22	227	206	17
0	0	24	0	106	60*
0	1	3	846	803	11
0	1	4	729	710	10
0	1	5	767	755	11
0	1	6	633	641	11
0	1	7	24	20	37*
0	1	8	238	243	8
0	1	9	712	693	13
0	1	10	1132	1132	16
0	1	11	0	136	51*
0	1	12	66	95	35*
0	1	13	220	229	11
0	1	14	399	371	10
0	1	15	63	38	35*
0	1	16	327	335	11
0	1	17	99	138	57*
0	1	18	585	594	13
0	1	19	274	279	16
0	1	20	278	285	13
0	1	21	141	136	23
0	1	22	100	116	32*
0	1	23	0	7	58*
0	1	24	172	149	20
0	2	0	1228	1267	13
0	2	1	1486	1523	16
0	2	2	711	710	10
0	2	3	976	974	12
0	2	4	45	24	33*
0	2	5	884	891	12
0	2	6	106	105	13
0	2	7	971	1015	14
0	2	8	1202	1214	16
0	2	9	420	436	10
0	2	10	365	377	9
0	2	11	478	494	11
0	2	12	338	349	9
0	2	13	151	174	16
0	2	14	306	314	11
0	2	15	588	596	14
0	2	16	216	231	14
0	2	17	0	6	49*
0	2	18	83	65	51*
0	2	19	299	285	13
0	2	20	170	191	19
0	2	21	73	8	55*
0	2	22	100	83	26*
0	2	23	148	140	22
0	2	24	85	86	57*
0	3	1	1030	1039	13
0	3	2	328	305	8
0	3	3	1247	1283	15
0	3	4	53	71	37*
0	3	5	609	618	12
0	3	6	0	55	37*
0	3	7	520	515	12
0	3	8	109	92	13
0	3	9	338	362	9
0	3	10	0	5	43*
0	3	11	738	756	15
0	3	12	131	125	16
0	3	13	604	609	12
0	3	14	0	20	46*
0	3	15	54	11	37*
0	3	16	102	24	23*
0	3	17	585	577	14
0	3	18	0	5	54*
0	3	19	159	122	17
0	3	20	37	31	40*
0	3	21	248	247	15
0	3	22	0	5	57*
0	3	23	89	58	33*
0	4	0	1272	1279	15
0	4	1	1278	1293	15
0	4	2	211	222	8
0	4	3	1323	1329	16
0	4	4	376	397	9
0	4	5	796	780	13
0	4	6	258	253	8
0	4	7	1047	1046	15
0	4	8	815	814	14
0	4	9	125	130	16
0	4	10	102	81	18*
0	4	11	543	551	12
0	4	12	284	290	10
0	4	13	0	47	46*
0	4	14	194	194	14
0	4	15	515	511	12
0	4	16	288	276	12
0	4	17	85	100	52*
0	4	18	205	202	16
0	4	19	364	371	12
0	4	20	55	33	51*
0	4	21	83	22	43*
0	4	22	111	89	25*
0	4	23	169	196	21
0	5	1	1225	1219	16
0	5	2	1473	1510	18
0	5	3	541	502	12
0	5	4	274	285	8
0	5	5	719	692	14
0	5	6	760	773	14
0	5	7	403	404	10
0	5	8	498	484	11
0	5	9	351	357	9
0	5	10	651	631	16
0	5	11	69	68	47*
0	5	12	0	98	50*
0	5	13	455	466	11
0	5	14	318	294	10
0	5	15	31	46	48*
0	5	16	289	296	12
0	5	17	295	308	13
0	5	18	237	216	14
0	5	19	60	64	51*
0	5	20	0	52	53*
0	5	21	138	138	22
0	5	22	0	94	57*
0	6	0	1039	1027	15
0	6	1	248	253	8
0	6	2	413	379	10
0	6	3	53	84	38*
0	6	4	779	763	14
0	6	5	437	420	10
0	6	6	417	401	11
0	6	7	181	147	11
0	6	8	935	957	16
0	6	9	142	141	15
0	6	10	196	185	13
0	6	11	199	192	12
0	6	12	471	472	11
0	6	13	0	48	50*
0	6	14	271	302	14
0	6	15	137	145	19
0	6	16	375	369	11
0	6	17	0	35	56*
0	6	18	78	102	53*
0	6	19	0	54	54*
0	6	20	223	220	14
0	6	21	0	7	46*
0	6	22	128	154	26*
0	7	1	368	352	9
0	7	2	707	723	15
0	7	3	220	233	10
0	7	4	133	140	15
0	7	5	145	131	13
0	7	6	759	743	16
0	7	7	98	106	20*
0	7	8	210	205	12
0	7	9	0	11	48*
0	7	10	519	515	13
0	7	11	322	325	11
0	7	12	145	113	16
0	7	13	58	34	49*
0	7	14	406	404	11
0	7	15	0	7	53*
0	7	16	203	225	17
0	7	17	222	190	14
0	7	18	158	182	21
0	7	19	0	1	53*
0	7	20	129	125	22*
0	7	21	0	19	53*
0	8	0	578	573	15
0	8	1	467	433	11
0	8	2	80	26	22*
0	8	3	211	212	11
0	8	4	545	546	12
0	8	5	198	212	12
0	8	6	54	137	49*
0	8	7	392	365	9
0	8	8	69	106	37*
0	8	9	424	410	10
0	8	10	0	124	53*
0	8	11	404	396	11
0	8	12	322	324	11
0	8	13	0	82	52*
0	8	14	138	122	18
0	8	15	333	307	12
0	8	16	150	163	19
0	8	17	72	24	53*
0	8	18	0	95	55*
0	8	19	154	173	20
0	8	20	0	76	54*
0	9	1	570	557	12
0	9	2	241	228	11
0	9	3	389	376	10
0	9	4	57	76	34*
0	9	5	599	567	13
0	9	6	197	200	13
0	9	7	298	305	11
0	9	8	143	153	18
0	9	9	751	707	18
0	9	10	71	9	48*
0	9	11	97	37	49*
0	9	12	145	114	16
0	9	13	343	341	11
0	9	14	112	88	23*
0	9	15	0	28	54*
0	9	16	60	27	51*
0	9	17	211	229	16
0	9	18	0	20	45*
0	10	0	420	427	11
0	10	1	359	366	10
0	10	2	62	45	32*
0	10	3	476	483	11
0	10	4	134	135	18
0	10	5	218	217	12
0	10	6	152	162	17
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3	1	-13	447	448	11	3	2	-5	1295	1292	15	3	3	4	802	802	12	3	4	14	224	233	13	3	6	-19	205	209	14				
3	1	-12	93	69	16*	3	2	-4	1425	1445	16	3	3	5	124	117	11	3	4	15	151	98	16	3	6	-18	56	11	41*				
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6	7	-7	132	82	15	6	8	15	0	26	56*	6	11	-10	137	126	19	7	1	-13	122	114	18	7	2	3	163	180	13
6	7	-6	299	296	11	6	9	-15	194	207	16	6	11	-9	90	41	50*	7	1	-12	272	257	10	7	2	4	163	149	13
6	7	-5	157	180	15	6	9	-14	66	103	37*	6	11	-8	59	143	53*	7	1	-11	562	554	12	7	2	5	344	350	10
6	7	-4	347	348	10	6	9	-13	0	21	53*	6	11	-7	235	218	13	7	1	-10	359	350	9	7	2	6	564	552	12
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6	7	3	269	244	11	6	9	-6	81	53	25*	6	11	0	172	168	16	7	1	-3	763	746	15	7	2	13	235	221	13
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8	2	-8	162	136	14	8	3	12	55	85	51*	8	5	1	10	132	50*	8	7	-2	0	92	53*	8	9	7	225	217	15
8	2	-7	58	40	42*	8	3	13	91	36	26*	8	5	2	0	26	47*	8	7	-1	279	313	13	8	9	8	0	57	50*
8	2	-6	156	177	15	8	3	14	0	34	51*	8	5	3	238	227	11	8	7	0	493	535	12	8	10	-6	67	36	49*
8	10	-5	183	175	15	9	1	13	0	58	54*	9	3	6	206	187	14	9	5	3	138	124	16	9	7	9	98	68	51*
8	10	-4	119	99	20*	9	1	14	66	47	44*	9	3	7	0	28	39*	9	5	4	142	190	19	9	8	-9	72	140	55*
8	10	-3	127	157	22*	9	2	-16	80	113	42*	9	3	8	295	306	12	9	5	5	74	11	49*	9	8	-8	0	59	49*
8	10	-2	83	63	45*	9	2	-15	67	11	28*	9	3	9	96	82	27*	9	5	6	6	30	52*	9	8	-7	70	86	50*
8	10	-1	133	126	21	9	2	-14	132	149	17	9	3	10	166	151	18	9	5	7	213	219	13	9	8	-6	122	147	21*
8	10	0	88	62	46*	9	2	-13	38	108	48*	9	3	11	63	79	43*	9	5	8	172	154	15	9	8	-5	84	127	49*
8	10	1	59	159	44*	9	2	-12	33	2	41*	9	3	12	147	158	21	9	5	9	79	19	48*	9	8	-4	0	28	46*
8	10	2	0	13	51*	9	2	-11	83	74	47*	9	3	13	83	17	49*	9	5	10	67	10	42*	9	8	-3	0	111	52*
8	10	3	114	96	21*	9	2	-10	246	253	12	9	3	14	141	134	20	9	5	11	208	181	16	9	8	-2	156	161	16
8	10	4	0	60	52*	9	2	-9	135	156	18	9	4	-15	63	7	33*	9	5	12	96	127	31*	9	8	-1	87	113	53*
8	10	5	93	122	51*	9	2	-8	77	28	25*	9	4	-14	150	174	17	9	6	-13	116	112	22*	9	8	0	0	55	50*
9	0	-15	0	14	46*	9	2	-7	123	107	19	9	4	-13	0	5	48*	9	6	-12	0	104	48*	9	8	1	150	154	17
9	0	-13	128	156	19	9	2	-6	399	387	10	9	4	-12	0	93	46*	9	6	-11	134	173	19	9	8	2	181	158	15
9	0	-11	223	225	11	9	2	-5	0	108	49*	9	4	-11	155	151	15	9	6	-10	0	22	48*	9	8	3	51	41	52*
9	0	-9	191	200	14	9	2	-4	55	36	43*	9	4	-10	217	218	13	9	6	-9	215	222	14	9	8	4	90	40	51*
9	0	-7	60	63	39*	9	2	-3	193	197	14	9	4	-9	0	46	48*	9	6	-8	0	21	47*	9	8	5	0	76	44*
9	0	-5	272	243	10	9	2	-2	359	364	10	9	4	-8	0	72	47*	9	6	-7	250	255	12	9	8	6	133	123	21
9	0	-3	449	458	11	9	2	-1	193	204	14	9	4	-7	36	70	48*	9	6	-6	0	53	49*	9	8	7	61	74	39*
9	0	-1	239	241	12	9	2	0	45	87	40*	9	4	-6	331	327	11	9	6	-5	181	186	15	9	9	-5	97	47	49*
9	0	1	433	451	11	9	2	1	166	140	15	9	4	-5	72	47	28*	9	6	-4	79	124	42*	9	9	-4	196	189	13
9	0	3	164	158	15	9	2	2	511	507	13	9	4	-4	73	52	45*	9	6	-3	282	289	11	9	9	-3	0	83	47*
9	0	5	307	294	11	9	2	3	239	241	12	9	4	-3	139	106	17	9	6	-2	114	38	18	9	9	-2	53	55	48*
9	0	7	0	69	52*	9	2	4	143	128	15	9	4	-2	313	310	11	9	6	-1	176	174	14	9	9	-1	0	16	49*
9	0	9	263	282	14	9	2	5	231	224	12	9	4	-1	0	37	49*	9	6	0	62	64	51*	9	9	0	193	188	16
9	0	11	75	136	55*	9	2	6	208	215	14	9	4	0	97	115	25*	9	6	1	281	274	11	9	9	1	56	72	34*
9	0	13	180	204	18	9	2	7	51	111	50*	9	4	1	153	142	17	9	6	2	0	6	47*	9	9	2	72	37	43*
9	1	-16	99	103	23*	9	2	8	213	206	15	9	4	2	372	405	11	9	6	3	184	203	16	9	9	3	83	43	51*
9	1	-15	200	213	13	9	2	9	198	209	16	9	4	3	82	111	51*	9	6	4	0	67	49*	10	0	-14	188	195	14
9	1	-14	57	67	33*	9	2	10	263	297	13	9	4	4	0	86	51*	9	6	5	224	235	14	10	0	-12	49	23	38*
9	1	-13	49	39	45*	9	2	11	45	20	52*	9	4	5	0	123	47*	9	6	6	59	91	52*	10	0	-10	246	256	13
9	1	-12	99	102	22*	9	2	12	102	161	52*	9	4	6	186	229	16	9	6	7	61	13	38*	10	0	-8	79	95	46*
9	1	-11	179	171	14	9	2	13	84	80	33*	9	4	7	69	66	50*	9	6	8	0	34	53*	10	0	-6	362	359	10
9	1	-10	0	33	47*	9	2	14	0	61	50*	9	4	8	0	123	50*	9	6	9	258	242	13	10	0	-4	65	17	31*
9	1	-9	289	306	11	9	3	-16	282	282	12	9	4	9	85	130	53*	9	6	10	88	28	44*	10	0	-2	247	254	13
9	1	-8	362	346	10	9	3	-15	84	39	48*	9	4	10	214	184	15	9	6	11	72	32	52*	10	0	0	280	277	12
9	1	-7	209	182	12	9	3	-14	95	98	23*	9	4	11	42	46	53*	9	7	-11	116	111	22*	10	0	2	277	279	12
9	1	-6	0	106	48*	9	3	-13	0	8	45*	9	4	12	0	16	54*	9	7	-10	0	61	49*	10	0	4	0	57	47*
9	1	-5	134	147	18	9	3	-12	177	168	14	9	4	13	34	77	54*	9	7	-9	0	111	50*	10	0	6	91	89	52*
9	1	-4	175	176	15	9	3	-11	127	116	18	9	5	-14	114	100	19	9	7	-8	161	123	15	10	0	8	176	194	18
9	1	-3	157	137	15	9	3	-10	65	73	49*	9	5	-13	69	65	32*	9	7	-7	217	219	13	10	0	10	164	180	18
9	1	-2	177	160	13	9	3	-9	53	32	45*	9	5	-12	67	89	47*	9	7	-6	0	4	44*	10	0	12	130	87	21
9	1	-1	494	488	13	9	3	-8	370	371	11	9	5	-11	0	62	49*	9	7	-5	68	155	52*	10	1	-14	0	60	50*
9	1	0	219	235	12	9	3	-7	0	36	52*	9	5	-10	97	41	21*	9	7	-4	89	50	45*	10	1	-13	60	40	33*
9	1	1	286	289	11	9	3	-6	0	26	50*	9	5	-9	264	268	12	9	7	-3	158	154	17	10	1	-12	71	128	50*
9	1	2	0	4	47*	9	3	-5	33	79	48*	9	5	-8	125	108	20	9	7	-2	89	93	52*	10	1	-11	0	24	54*
9	1	3	239	228	12	9	3	-4	345	331	10	9	5	-7	275	270	12	9	7	-1	200	212	15	10	1	-10	0	53	48*
9	1	4	165	156	15	9	3	-3	93	82	24*	9	5	-6	98	64	23*	9	7	0	184	207	16	10	1	-9	158	191	17
9	1	5	65	102	50*	9	3	-2	0	122	49*	9	5	-5	211	178	12	9	7	1	283	299	12	10	1	-8	261	270	12
9	1	6	66	97	50*	9	3	-1	25	1	39*	9	5	-4	228	241	14	9	7	2	142	164	20	10	1	-7	118	129	20*
9	1	7	318	335	12	9	3	0	544	528	13	9	5	-3	0	28	46*	9	7	3	296	296	11	10	1	-6	0	31	49*
9	1	8	158	143	18	9	3	1	33	18	44*	9	5	-2	0	21	45*	9	7	4	0	14	52*	10	1	-5	10	130	52*
9	1	9	98	64	50*	9	3	2	62	96	36*	9	5	-1	320	327	11	9	7	5	93	86	26*	10	1	-4	238	249	13
9	1	10	159	102	16	9	3	3	0	1	48*	9	5	0	184	172	14	9	7	6	0	128	53*	10	1	-3	84	30	45*
9	1	11	72	125	41*	9	3	4	325	333	11	9	5	1	161	149	16	9	7	7	190	231	19	10	1	-2	86	97	27*
9	1	12	0	25	41*	9	3	5	0	45	49*	9	5	2	60	42	49*	9	7	8	0	36	57*	10	1	-1	218	210	13
10	1	0	302	294	12	10	3	5	66	44	41*	10	6	-3	0	6	50*	11	2	-3	57	106	51*						
10	1	1	86	54	26*	10	3	6	85	27	48*	10	6	-2	190	211	16	11	2	-2	17	106	46*						
10	1	2	119	111	21*	10	3	7	198	226	16	10	6	-1	82	103	28*	11	2	-1	0	75	54*						
10	1	3	80	182	51*	10	3	8	69	22	37*	10	6	0	67	105	35*	11	2	0	199	189	13						
10	1	4	235	240	14	10	3	9	0	7	44*	10	6	1	64	90	40*	11	2	1	115	99	22*						
10	1	5	0	12	47*	10	3	10	54	38	39*	10	6	2	276	298	13	11	2	2	167	188	17						
10	1	6	82	104	33*	10	4	-12	47	38	48*	10	6	3	134	150	21	11	2	3	91	43	48*						
10	1	7	94	95	51*	10	4	-11	0	114	51*	10	6	4	144	181	21	11	2	4	144	127	18						
10	1	8	111	136	25*	10	4	-10	0	84	53*	10	6	5	0	79	53*	11	2	5	128	145	22*						
10	1	9	76	9	50*	10	4	-9	139	119	18	10	6	6	107	130	27*	11	2	6	0	59	56*						
10	1	10	182	151	16	10	4	-8	87	21	23*	10	6	7	133	107	20	11	2	7	45	9	37*						
10	1	11	0	94	58*	10	4	-7	203	192	14	10	7	-6	63	22	40*	11	3	-8	203	176	13						
10	2	-13	65	109	46*	10	4	-6	125	135	21	10	7	-5	69	34	45*	11	3	-7	0	18	57*						
10	2	-12	24	17	43*	10	4	-5	229	200	12	10	7	-4	214	190	13	11	3	-6	0	105	52*						
10	2	-11	182	172	15	10	4	-4	0	17	55*	10	7	-3	0	14	48*	11	3	-5	115	86	21*						
10	2	-10	125	116	18	10	4	-3	221	207	12	10	7	-2	0	46	49*	11	3	-4	214	202	13						
10	2	-9	99	120	24*	10	4	-2	0	35	50*	10	7	-1	99	92	26*	11	3	-3	53	28	47*						
10	2	-8	0	82	49*	10	4	-1	0	37	50*	10	7	0	200	190	15	11	3	-2	149	117	15						
10	2	-7	290	304	11	10	4	0	64	89	40*	10	7	1	85	47	50*	11	3	-1	76	46	32*						
10	2	-6	167	146	15	10	4	1	302	301	11	10	7	2	128	123	20	11	3	0	147	147	19						
10	2	-5	232	210	12	10	4	2	0	77	48*	10	7	3	0	44	52*	11	3	1	58	49	51*						
10	2	-4	0	24	49*	10	4	3	66	68	34*	10	7	4	91	166	54*	11	3	2	159	180	17						
10	2	-3	191	189	13	10	4	4	28	65	38*	11	0	-9	38	49	37*	11	3	3	77	10	50*						
10	2	-2	152	159	18	10	4	5	220	219	12	11	0	-7	231	251	14	11	3	4	148	169	19						
10	2	-1	46	34	50*	10	4	6	52	32	39*	11	0	-5	98	195	53*	11	3	5	0	5	50*						

10	2	0	76	69	44*	10	4	7	75	24	51*	11	0	-3	238	262	13	11	3	6	119	97	23*
10	2	1	338	344	11	10	4	8	123	105	21*	11	0	-1	0	14	54*	11	4	-7	19	90	52*
10	2	2	227	235	13	10	4	9	131	161	22*	11	0	1	267	263	12	11	4	-6	203	183	15
10	2	3	6	103	42*	10	4	10	0	48	56*	11	0	3	67	37	46*	11	4	-5	0	67	52*
10	2	4	36	10	48*	10	5	-11	89	101	50*	11	0	5	114	139	25*	11	4	-4	88	32	44*
10	2	5	200	200	14	10	5	-10	43	82	45*	11	0	7	30	32	53*	11	4	-3	0	34	48*
10	2	6	89	119	31*	10	5	-9	55	88	35*	11	1	-10	104	35	20*	11	4	-2	162	160	17
10	2	7	100	41	25*	10	5	-8	236	245	14	11	1	-9	159	147	15	11	4	-1	62	90	38*
10	2	8	124	99	21*	10	5	-7	132	123	19	11	1	-8	133	115	17	11	4	0	135	153	21
10	2	9	190	220	18	10	5	-6	0	39	50*	11	1	-7	46	26	48*	11	4	1	34	108	52*
10	2	10	0	118	55*	10	5	-5	130	108	18	11	1	-6	42	106	51*	11	4	2	177	167	15
10	2	11	103	56	25*	10	5	-4	196	180	13	11	1	-5	167	166	16	11	4	3	73	21	49*
10	3	-13	96	94	23*	10	5	-3	126	111	19	11	1	-4	0	68	52*	11	4	4	42	119	45*
10	3	-12	0	43	48*	10	5	-2	60	109	50*	11	1	-3	174	129	14	11	5	-4	162	173	18
10	3	-11	0	72	47*	10	5	-1	138	145	19	11	1	-2	104	77	52*	11	5	-3	0	3	50*
10	3	-10	0	39	47*	10	5	0	123	128	20	11	1	-1	173	194	16	11	5	-2	0	29	41*
10	3	-9	274	294	12	10	5	1	81	27	27*	11	1	0	89	63	27*	11	5	-1	159	165	16
10	3	-8	56	64	48*	10	5	2	16	74	46*	11	1	1	104	7	23*	11	5	0	0	130	54*
10	3	-7	242	229	12	10	5	3	123	118	20	11	1	2	117	110	22*	11	5	1	57	62	52*
10	3	-6	21	58	48*	10	5	4	127	129	20	11	1	3	163	166	16	11	5	2	20	48	36*
10	3	-5	168	171	16	10	5	5	0	72	50*	11	1	4	62	113	53*						
10	3	-4	0	70	51*	10	5	6	97	111	25*	11	1	5	0	20	53*						
10	3	-3	126	110	19	10	5	7	77	107	42*	11	1	6	81	91	33*						
10	3	-2	88	4	44*	10	5	8	0	79	56*	11	1	7	174	182	18						
10	3	-1	286	304	12	10	6	-9	55	31	44*	11	2	-9	0	38	43*						
10	3	0	92	47	48*	10	6	-8	0	40	46*	11	2	-8	97	116	49*						
10	3	1	120	120	22*	10	6	-7	49	33	46*	11	2	-7	101	147	54*						
10	3	2	0	10	45*	10	6	-6	258	269	13	11	2	-6	251	255	13						
10	3	3	297	299	12	10	6	-5	0	34	46*	11	2	-5	0	21	50*						
10	3	4	46	29	46*	10	6	-4	87	45	24*	11	2	-4	0	110	51*						

Chapter 5

Examination of the Influence of Crystal Packing Forces on Geometric Parameters: A Comparison Between the Crystallographic and Theoretical Structures of some Diorganotinchloro(N,N-dialkyldithiocarbamates), $R_2Sn(S_2CNR'_2)Cl$.

5.1 Introduction

In the previous chapters two series of diimine adducts of R_2SnCl_2 have been investigated [1-3]. These offer the advantage of adopting one structural motif, i.e. based on a *trans*-C_2 octahedral geometry, and hence correlations between structural parameters and electronic parameters associated with the tin center (by varying the nature of the tin-bound R groups to alter the Lewis acidity) may be made without significant changes in molecular geometry. The combined crystallographic/theoretical approach has now been extended to include a series of $R_2Sn(S_2CNR'_2)Cl$ compounds which incorporate a dithiolate ligand in the tin atom geometry. The dithiocarbamate ligand may coordinate in the monodentate mode via one sulfur atom only, in a bidentate mode via both sulfur atoms forming similar Sn-S interactions, and in an asymmetric mode owing to the formation of dissimilar Sn-S bond distances. In this sense, the $R_2Sn(S_2CNR'_2)Cl$ compounds represent a series of structures with increased flexibility in their coordination environments compared with the diimine adducts studied earlier. Two variables have been explored in the present combined crystallographic/theoretical study, namely the changing of the tin-bound R substituents to moderate the Lewis acidity of the tin center and the nature of the R' groups to moderate the Lewis basicity of the dithiocarbamate ligands.

5.2 Results and Discussion

Details of the experimental procedure employed in the synthesis of the compounds reported in this chapter are provided in Chapter 2. Spectroscopic characterizations are also provided in Chapter 2.

In the following the structural characteristics of a series of $R_2Sn(S_2CNR'_2)Cl$ compounds as determined by crystallographic techniques will be discussed and correlations made between i) the Lewis acidity of the tin atom (moderated by changes in R) and ii) the Lewis basicity of the dithiocarbamate ligand (moderated by changes in R') and the derived interatomic parameters involving the tin atom will be made. The theoretical structures of the compounds will then be described and similar correlations

made as for the experimental structures. Finally, the differences between the experimental and calculated structures will be discussed.

5.2.1 Crystallographic Studies

A series of structurally similar molecules $R_2Sn(S_2CNR'_2)Cl$ as determined by X-Ray crystallography are described and then compared to analogous literature structures. The experimental procedure employed in the data collection and the structure determinations are summarised in Chapter 2. Presented below are the experimental details unique to the $R_2Sn(S_2CNR'_2)Cl$, where R= Me and Cy, R' = Et and Cy ; and R= ^{t}Bu, R'_2 = Et and Cy structure determinations. Details specific to each structure determination are summarised in Table 5.1. Crystal data and refinement details specific for these molecular structure determinations are provided in the Appendix of this chapter. All diagrams are drawn with ORTEP [4] at the 35% probability level.

In this section, a description of the five crystal and molecular structures of $R_2Sn(S_2CNR'_2)Cl$, where R= Me and Cy, R' = Et and Cy ; and R= ^{t}Bu R'_2 = Et and Cy will be given as well as a summary of five related literature structures R = ^{t}Bu, [1,5] and Ph [5-6] where R' = Et and Cy and R = Ph[7] where R'_2 = Et and Cy. Table 5.2 lists selected interatomic parameters for all ten structures. It is appropriate to mention here that a correction for secondary extinction was applied in the refinement of $Cy_2Sn(S_2CNR'_2)Cl$ such that the extinction coefficient was 1.24401×10^{-8}.

TABLE 5.1: Crystallographic Data for $R_2Sn(S_2CNR'_2)Cl$ for R= Me and Cy, R' = Et and Cy ; and R= ^tBu R'_2 = Et and Cy

	$R_2Sn(S_2CNR'_2)Cl$				
Crystallographic Data	**$Me_2Sn(S_2CNEt_2)Cl$**	**$Me_2Sn(S_2CNCy_2)Cl$**	**$^tBu_2Sn(S_2CNCy(Et))Cl$**	**$Cy_2Sn(S_2CNEt_2)Cl$**	**$Cy_2Sn(S_2CNCy_2)Cl$**
Formula	$C_7H_{16}ClNS_2Sn$	$C_{15}H_{28}ClNS_2Sn$	$C_{17}H_{34}ClNS_2Sn$	$C_{17}H_{32}ClNS_2Sn$	$C_{25}H_{44}ClNS_2Sn$
Formula weight	332.5	440.7	470.7	468.7	576.5
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/c$	$P2_1/c$	$P2_1/n$	$P2_1/c$	$P2_1/n$
a, Å	10.896(2)	6.758(6)	13.481(5)	17.107(6)	11.411(7)
b, Å	9.869(4)	19.046(3)	11.466(5)	11.134(2)	16.942(5)
c, Å	12.722(2)	15.190(5)	15.351(8)	11.953(6)	14.712(5)
α, (°)	90	90	90	90	90
β, (°)	105.08(1)	98.09(4)	107.51(4)	104.00(3)	100.45(3)
γ, (°)	90	90	90	90	90
V, Å^3	1320.8(5)	1930(2)	2262(1)	2209(2)	2797(1)
Z	4	4	4	4	4
D_{calcd}, g cm^{-3}	1.672	1.512	1.382	1.409	1.370
Radiation, Å	Mo, 0.7107	Mo, 0.7107	Mo, 0.7107	Cu, 1.5418	Mo, 0.7107
μ, cm^{-1}	24.11	16.65	14.29	120.55	11.70
Trans coeff	0.981 – 1	0.977 – 1	0.955 – 1	0.921 – 1	0.986 – 1
2θ range, (°)	6.0 – 55.0	6.0 – 55.0	6.0 – 55.0	6.0 – 120	6.0 – 55.0
No. reflns meas	3401	4996	5699	3683	6998
No. unique reflns	3240	4622	5478	3496	6681
No of reflns used	1367	1881	2707	1914	2550
No. of variables	109	176	199	200	271
R	0.039	0.038	0.049	0.042	0.045
R_W	0.037	0.033	0.053	0.034	0.038
Residual e$^-$/Å^3	0.45	0.46	0.73	0.40	0.54

TABLE 5.2: Crystallographically Determined Interatomic Parameters (Å, deg.) for $R_2Sn(S_2CNR'_2)Cl$ for R= Me, ^{t}Bu [ab], Cy, Ph [bde], R' = Et and Cy and ; and R= ^{t}Bu and Ph R'_2 = Et and Cy

	$R_2Sn(S_2CNR'_2)Cl$											
Bond Distance	R=Me, R'=Et (y = 2)	R=Me, R'=Cy (y = 2)	R= ^{t}Bu[ab], R'=Et (y = 5)		R=^{t}Bu, R'=Et,Cy (y = 2)	R = ^{t}Bu[ac], R' = Cy (y = 5)		R =Ph[b], R'=Et (y = 7)	R=Ph[d], R'=Et,Cy (y = 7)	R=Ph[e], R'=Cy (y = 7)	R=Cy, R'=Et (y = 7)	R=Ph[e], R'=Cy (y = 7)
Sn-Cl(1)	2.479(2)	2.467(2)	2.498(2)	2.505(2)	2.472(2)	2.482(3)	2.492(3)	2.440(1)	2.446(3)	2.437(2)	2.459(3)	2.493(2)
Sn-S(1)	2.463(2)	2.463(2)	2.479(2)	2.482(2)	2.479(2)	2.471(3)	2.477(3)	2.445(1)	2.460(3)	2.440(1)	2.470(2)	2.472(2)
Sn-S(2)	2.703(2)	2.696(2)	2.732(2)	2.734(2)	2.756(2)	2.722(3)	2.743(3)	2.716(1)	2.681(3)	2.657(2)	2.768(2)	2.680(2)
Sn-C(1)	2.111(9)	2.112(8)	2.191(8)	2.195(8)	2.182(8)	2.19(1)	2.19(1)	2.131(5)	2.125(9)	2.100(5)	2.11(1)	2.166(7)
Sn-C(y)	2.112(8)	2.102(8)	2.201(9)	2.20(1)	2.192(7)	2.16(1)	2.21(1)	2.127(5)	2.141(9)	2.106(5)	2.15(1)	2.143(8)
S(1)-C	1.750(8)	1.734(7)	1.731(6)	1.738(6)	1.739(7)	1.740(9)	1.73(1)	1.744(5)	1.73(1)	1.719(5)	1.727(9)	1.740(8)
S(2)-C	1.707(8)	1.716(7)	1.701(6)	1.699(7)	1.713(7)	1.71(1)	1.72(1)	1.701(4)	1.714(9)	1.709(5)	1.696(9)	1.712(8)
C-N(1)	1.31(1)	1.336(8)	1.326(7)	1.325(8)	1.320(8)	1.31(1)	1.31(1)	1.327(5)	1.33(1)	1.308(6)	1.32(1)	1.339(9)
Bond Angle												
Cl(1)-Sn-S(1)	88.32(8)	87.96(8)	84.65(6)	85.63(6)	84.57(8)	83.9(1)	85.0(1)	88.41(4)	87.47(9)	85.97(5)	87.37(8)	85.67(8)
Cl(1)-Sn-S(2)	157.52(8)	156.80(7)	153.19(6)	154.15(6)	152.57(7)	152.0(1)	152.3(1)	157.82(4)	157.34(9)	153.57(5)	155.54(8)	154.42(8)
Cl(1)-Sn-C(1)	96.9(3)	95.6(2)	97.6(2)	97.1(2)	98.4(2)	96.4(3)	96.3(4)	98.2(1)	97.4(3)	94.5(1)	96.1(3)	95.4(2)
Cl(1)-Sn-C(y)	96.5(3)	97.2(2)	96.5(2)	96.5(2)	97.7(2)	98.6(3)	96.9(3)	96.8(1)	96.8(3)	98.0(1)	98.8(3)	94.7(2)
S(1)-Sn-S(2)	69.35(7)	68.87(6)	68.54(5)	68.54(5)	68.01(6)	68.04(8)	67.50(9)	69.58(4)	69.87(9)	68.86(5)	68.17(7)	68.86(7)
S(1)-Sn-C(1)	113.4(2)	116.4(2)	115.1(2)	114.5(2)	116.6(2)	115.3(4)	120.1(4)	122.7(1)	124.1(2)	125.6(1)	114.8(2)	123.5(2)
S(1)-Sn-C(y)	117.6(3)	117.0(2)	115.0(2)	115.6(2)	116.8(2)	119.8(4)	113.5(4)	118.0(1)	113.2(2)	113.9(1)	114.8(3)	112.1(2)
S(2)-Sn-C(1)	94.5(3)	93.8(2)	93.5(1)	93.0(2)	94.0(2)	95.1(3)	95.2(4)	96.1(1)	95.6(3)	93.8(1)	94.0(3)	96.7(2)
S(2)-Sn-C(y)	91.8(3)	94.6(2)	95.3(2)	95.5(2)	94.8(2)	96.0(3)	96.6(3)	91.4(1)	92.1(2)	99.5(1)	92.1(3)	97.0(2)
C(1)-Sn-C(y)	127.4(4)	125.3(3)	128.8(3)	128.7(3)	125.3(3)	123.9(5)	125.6(6)	117.6(2)	121.3(3)	119.8(2)	128.5(4)	124.0(3)

a two molecules in the asymmetric unit; *b* [5]; *c* [1]; *d* [7]; *e* [6]

TABLE 5.2: Cont'd.

	$R_2Sn(S_2CNR'_2)Cl$											
Bond Angles	R=Me, R'=Et (y = 2)	R=Me, R'=Cy (y = 2)	R= $^tBu^{ab}$, R'=Et (y = 5)		R=^tBu, R'=Et,Cy (y = 2)	R = $^tBu^{ac}$, R' = Cy (y = 5)		R =Ph^b, R'=Et (y = 7)	R=Ph^d, R'=Et,Cy (y = 7)	R=Ph^e, R'=Cy (y = 7)	R=Cy, R'=Et (y = 7)	R=Ph^e, R'=Cy (y = 7)
Sn-S(1)-C	90.3(3)	91.1(3)	90.5(3)	90.4(3)	91.7(2)	91.6(3)	92.6(4)	89.9(2)	89.5(3)	91.6(2)	91.0(3)	90.8(3)
Sn-S(2)-C	83.5(3)	83.9(2)	83.0(3)	83.1(3)	83.3(3)	84.1(3)	84.2(4)	82.2(1)	82.6(3)	84.7(2)	82.0(3)	84.7(3)
S(1)-C-S(2)	116.9(5)	115.9(4)	118.0(4)	117.9(4)	116.5(4)	115.3(5)	114.9(6)	118.0(2)	118.0(5)	114.7(3)	118.8(5)	115.4(5)
S(1)-C-N(1)	119.4(6)	122.0(5)	119.9(5)	119.4(5)	120.4(5)	121.1(8)	123.0(8)	118.7(3)	120.2(7)	122.9(4)	119.2(7)	122.6(6)
S(2)-C-N(2)	123.8(6)	122.1(5)	122.1(5)	122.7(5)	123.1(5)	123.6(7)	122.1(8)	123.3(3)	121.8(8)	122.4(4)	122.0(6)	122.0(6)
Torsion Angles												
C/N/C/C (Et)	96.4(9)		-91.2(9)		82.1(9)			94.5(5)	-82(1)		-93.5(9)	
	92.8(9)		-94.5(9)					90.7(5)			89(1)	
C/N/C/C (Cy)		66.7(9)			-131.7(7)	73(1)	-130(1)		-115(1)	103.6(7)		77(1)
		-65.0(9)			101.6(7)	-57(1)	102(1)		120(1)	-110.7(7)		-71(1)
		113.8(7)				- 134.1(9)	75(9)			-73.8(8)		105.2(9)
		-116.6(7)				98(1)	-56(1)			73.3(8)		-113(1)

a two molecules in the asymmetric unit; *b* [5]; *c* [1]; *d* [7]; *e* [6]

5.2.1a [$Me_2Sn(S_2CNEt_2)Cl$]

Unsolvated colourless crystals were obtained from the slow evaporation of an chloroform/acetonitrile (4/1 *v/v*) solution of the compound [$Me_2Sn(S_2CNEt_2)Cl$]; melting point: 97-99 °C.

The molecular structure of [$Me_2Sn(S_2CNEt_2)Cl$] is shown in Fig. 5.1. The tin atom is coordinated by a chloride atom, two sulfur atoms derived from an asymmetrically chelating dithiocarbamate ligand and two methyl groups. The coordination geometry is based on a trigonal bipyramid with the chloride atom and the less tightly held S(2) atom defining the axial positions such that Cl-Sn-S(2) is 157.52(8)°. The tin atom lies 0.1604(6) Å out of the SC_2 trigonal plane in the direction of the chloride atom. The dithiocarbamate ligand chelates the tin atom in an asymmetric mode with the Sn-S(1) bond distance of 2.463(2) Å being significantly shorter than the Sn-S(2) distance of 2.703(2) Å. The closest non-hydrogen contact in the lattice occurs between the S(2) and $C(4)^{i}$ atoms (symmetry operation *i*: x, $-0.5 - y$, $-0.5 + z$) of 3.561(8) Å. The closest contact involving the chloride atom of 2.89 Å involves a translationally related $H(4a)^{ii}$ atom (symmetry operation *ii*: x, $1 + y$, z). The structural motif found here for [$Me_2Sn(S_2CNEt_2)Cl$] is repeated for all other $R_2Sn(S_2CNR'_2)Cl$ structures described in this report.

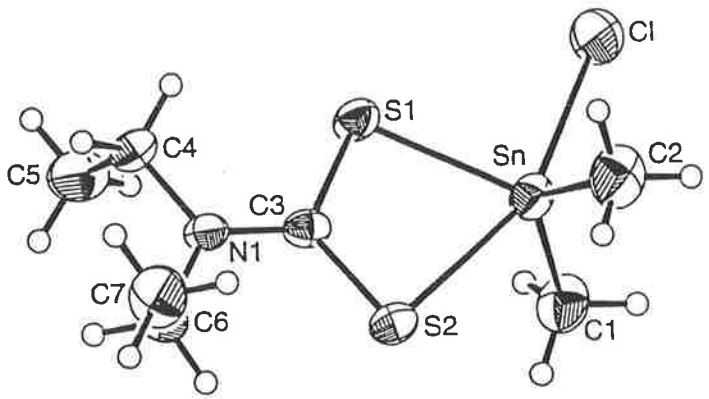


Figure 5.1
The molecular structure of [$Me_2Sn(S_2CNEt_2)Cl$]

5.2.1b. $[Me_2Sn(S_2CNCy_2)Cl]$

Colourless crystals were then obtained from the slow evaporation of a chloroform solution for $[Me_2Sn(S_2CNCy_2)Cl]$; melting point: 203-204°C.

The structure of $[Me_2Sn(S_2CNCy_2)Cl]$ is illustrated in Fig. 5.2. The structural motif found here for $[Me_2Sn(S_2CNCy_2)Cl]$ is consistent with the structural motif found in $[Me_2Sn(S_2CNEt_2)Cl]$ which is described in section 5.2.1a. In this structure the tin atom lies 0.1449(6) Å out of the trigonal plane towards the chloride atom. The closest non-hydrogen contact in the lattice of 3.58(2) Å occurs between a pair of centrosymmetrically related C(6) atoms (symmetry operation: 1 - x, 1 - y, 1 - z); a Cl...H^i contact of 2.99 Å is noted (symmetry operation i: 1 - x, -0.5 + y, 0.5 - z).

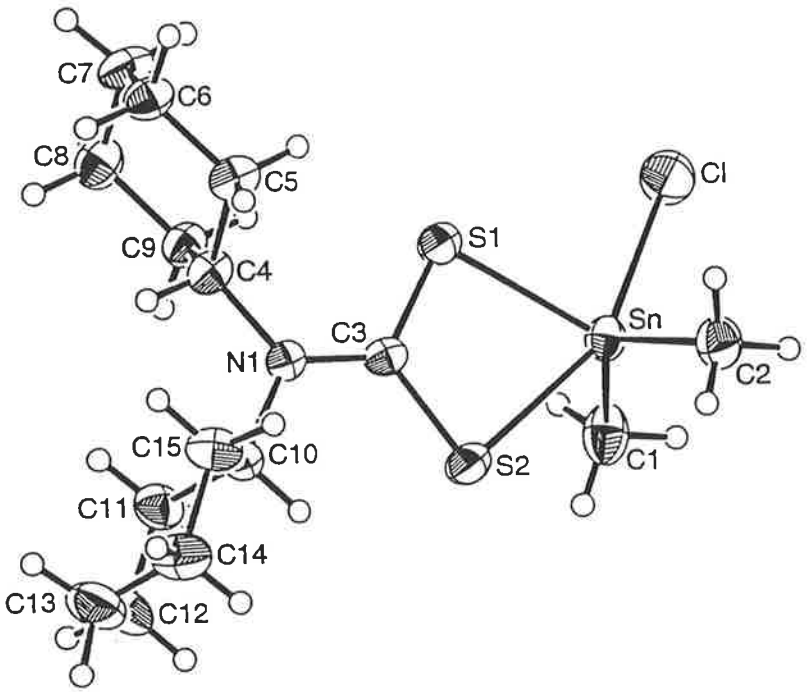


Figure 5.2

The molecular structure of $[Me_2Sn(S_2CNCy_2)Cl]$

5.2.1c. [$Cy_2Sn(S_2CNEt_2)Cl$]

Colourless crystals were obtained from the slow evaporation of an acetonitrile solution for [$Cy_2Sn(S_2CNEt_2)Cl$]; melting point: 114 - 115°C.

Figure 5.3 shows the molecular structure of [$Cy_2Sn(S_2CNEt_2)Cl$]. It is apparent that the structural motif of [$Cy_2Sn(S_2CNEt_2)Cl$] is consistent with that found in [$Me_2Sn(S_2CNEt_2)Cl$] which is described in section 5.2.1a. The tin atom lies 0.1726(8) Å out of the trigonal plane towards the chloride atom. There are no non-hydrogen contacts less than 3.6 Å in the lattice and the closest Cl...H contact of 2.95 Å involves the $H(14a)^i$ atom (symmetry operation *i*: *x*, 0.5 - *y*, -0.5 + *z*).

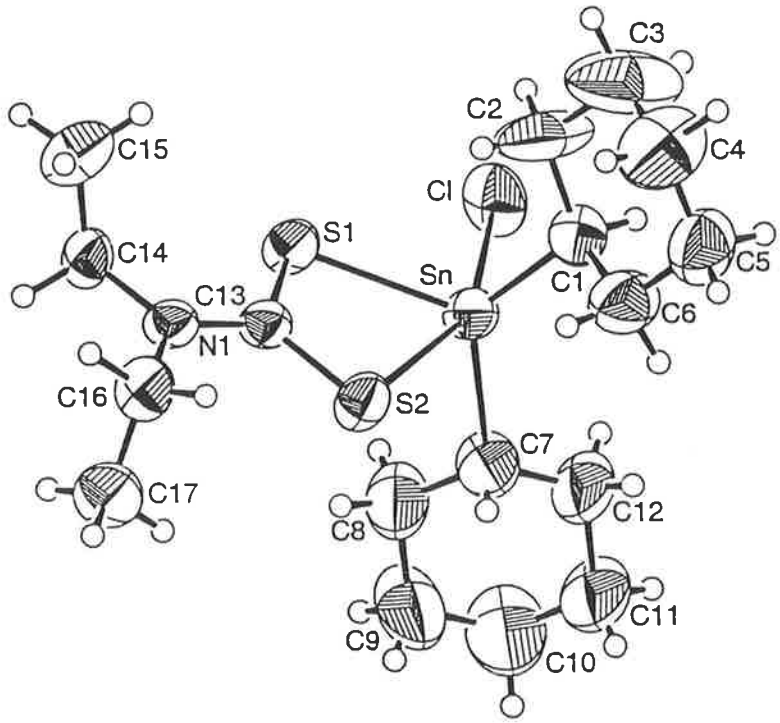


Figure 5.3
The molecular structure of [$Cy_2Sn(S_2CNEt_2)Cl$]

5.2.1d. $[Cy_2Sn(S_2CNCy_2)Cl]$

Colourless crystals were obtained from the slow evaporation of an chloroform/acetonitrile (4/1 v/v) solution of $[Cy_2Sn(S_2CNCy_2)Cl]$; melting point: 232 - 204 °C.

Figure 5.4 shows the molecular structure of $[Cy_2Sn(S_2CNCy_2)Cl]$ and again the structural motif is consistent with that found in $[Me_2Sn(S_2CNEt_2)Cl]$. Here $[Cy_2Sn(S_2CNCy_2)Cl]$ tin atoms lies 0.0812(5) Å out of the S_2C trigonal plane in the direction of the chloride atom. There are no intermolecular contacts less than 3.6 Å involving the non-hydrogen atoms and the closest Cl...H contact of 3.03 Å occurs between Cl and H(15a)^i (symmetry operation *i*: -0.5 + *x*, 0.5 - *y*, -0.5 + *z*).

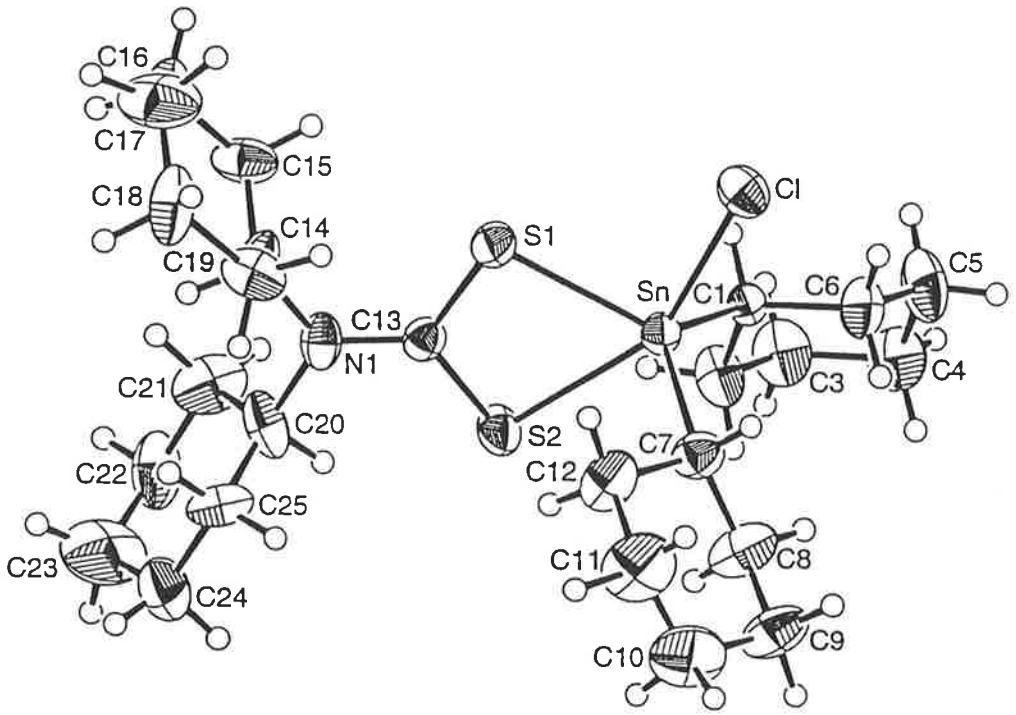


Figure 5.4

The molecular structure of $[Cy_2Sn(S_2CNCy_2)Cl]$

5.2.1e. [^{t}Bu$_2$Sn(S$_2$CN(Et)Cy)Cl]

Colourless crystals were obtained from the slow evaporation a chloroform/ethanol (9/1 *v/v*) solution of [^{t}Bu$_2$Sn(S$_2$CN(Et)Cy)Cl]; melting point: 127 - 128°C.

The structure of [^{t}Bu$_2$Sn(S$_2$CN(Et)Cy)Cl], containing an unsymmetrical dithiocarbamate ligand, is illustrated in Fig. 5.5. Again the structural motif as observed throughout this series is preserved in this structure. The tin atom lies 0.1538(5) Å above the SC_2 trigonal plane in the direction of the chloride atom. In the lattice there are no non-hydrogen contacts less than 3.6 Å and the closest Cl...H contact of 3.28 Å involves the H(3b)^i atom (symmetry operation *i*: -0.5 - *x*, -0.5 + *y*, 1.5 - *z*).

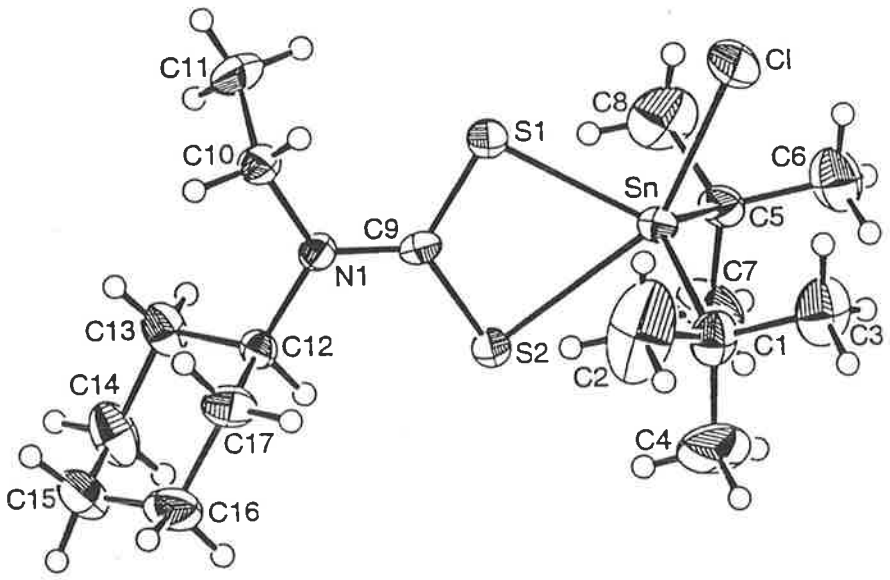


Figure 5.5

The molecular structure of [^{t}Bu$_2$Sn(S$_2$CN(Et)Cy)Cl]

5.2.1e. Other $R_2Sn(S_2CNR'_2)Cl$ structures: [$^tBu_2Sn(S_2CNEt_2)Cl$] [5], $^tBu_2Sn(S_2CNCy_2)Cl$ [1], $Ph_2Sn(S_2CNEt_2)Cl$ [5], $Ph_2Sn(S_2CN(Et)Cy)Cl$ [7] and $Ph_2Sn(S_2CNCy_2)Cl$ [6]

In addition to the five structures reported above, the structural motif described above is also found in five literature structures pertinent to the present work. The geometric details of the [$^tBu_2Sn(S_2CNEt_2)Cl$] [5], [$tBu_2Sn(S_2CNCy_2)Cl$] [1], [$Ph_2Sn(S_2CNEt_2)Cl$] [5], [$Ph_2Sn(S_2CN(Et)Cy)Cl$] [1] and [$Ph_2Sn(S_2CNCy_2)Cl$] [7] are summarised in Table 5.2. The specific details of each structure are given in the original references and important structural features are discussed in section 5.2.1g in the context of correlations made with the calculated interatomic parameters.

5.2.1g Structural Correlations Derived from the Crystal Structure Determinations.

The availability of ten molecular structures enables two key effects to be examined. The first effect investigated is an analysis of the variation of the Sn-ligand parameters as the Lewis basicity of the dithiocarbamate ligand is altered. Secondly, the influence of changing the nature of the tin-bound organo substituents on the derived interatomic parameters can be ascertained.

An examination of the Sn-ligand parameters for the three $Ph_2Sn(S_2CNR'_2)Cl$ structures, listed in Table 5.2, shows some interesting features [7]. The three independent Sn-Cl distances are equal within experimental error and similarly the three Sn-S(1) distances are spread over a narrow range. The systematic variation between the structures is found in the length of the Sn-S(2) bonds. Thus, Sn-S(2) decreases from 2.716(1) Å for R' = Et, to 2.681(3) Å for R'_2 = Et, Cy and then to 2.657(2) Å for R' = Cy. Given that the Sn-C interactions are invariant, the Sn-S(2) bonds may be described as hypervalent interactions that increase in magnitude as the Lewis basicity of the dithiocarbamate ligand increases. The increase in Lewis basicity is readily correlated with the greater stabilisation of the following canonical form Figure 5.6 below:

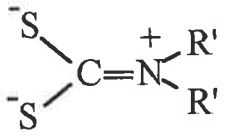


Figure 5.6

A Canonical stricture for $^-[S_2CNR'_2]$

as the ethyl substituents are successively substituted by the cyclohexyl groups, i.e. consistent with the greater inductive effect of the latter. While there is a systematic variation in the Sn-S(2) distances, no definitive trends in bond angles are noted with any differences between them being normally small, i.e. < 2°. Given the above trend exists in the $Ph_2Sn(S_2CNR'_2)Cl$ structures it was thought of interest to determine whether similar variations are found in related systems.

The three different dithiocarbamate ligands found in the $Ph_2Sn(S_2CNR'_2)Cl$ series are also present in three $^tBu_2Sn(S_2CNR'_2)Cl$ structures; there are two molecules in the asymmetric unit of both [$^tBu_2Sn(S_2CNEt_2)Cl$] [5] and [$^tBu_2Sn(S_2CNCy_2)Cl$] [1]. By contrast to the narrow range of Sn-Cl distances in the $Ph_2Sn(S_2CNR'_2)Cl$ series of structures, the Sn-Cl distances range from 2.472(2) Å to 2.505(2) Å. However, the Sn S(1) distances are experimentally equivalent with a range of values 2.471(3) Å to 2.482(2) Å. The systematic shortening of the Sn-S(2) distances found above for the R = Ph series is not reproduced in the present structures as seen in the differences between the Sn-S(1) and Sn-S(2) distances of 0.253(3) Å and 0.252(3) Å for R' = Et, 0.277(3) Å for R'_2 = Et, Cy, and 0.251(4) Å and 0.266(4) Å for R' = Cy. Clearly, no systematic trends in the mode of coordination of the dithiocarbamate ligands pertain in the $^tBu_2Sn(S_2CNR'_2)Cl$ structures.

As for the R = ^{t}Bu series of structures, no systematic trends are found in the two [$Me_2Sn(S_2CNEt_2)Cl$] and [$Me_2Sn(S_2CNCy_2)Cl$] structures. The Sn-Cl distances are equal within experimental error as are each of the two pairs of Sn-S distances, the difference between the Sn-S(1) and Sn-S(2) distances being 0.240(3) Å and 0.233(3) Å, respectively. By contrast to these observations, the difference between the Sn-S(1) and Sn-S(2) distances is 0.298(3) Å in the structure of [$Cy_2Sn(S_2CNEt_2)Cl$] and 0.208(3) Å

in [$Cy_2Sn(S_2CNCy_2)Cl$], i.e. consistent with the trends found in the $Ph_2Sn(S_2CNR'_2)Cl$ structures. Noteworthy, however, is that while the Sn-S(1) distances are experimentally equivalent in these structures, the Sn-Cl distance of 2.459(3) Å in the R' = Et structure is significantly shorter than that found in the R' = Cy structure, i.e. 2.493(2) Å. A possible source for this discrepancy is found in the nature of the *inter-* and *intra-* molecular Cl...H interactions in these structures. In the R' = Et structure, there are no intramolecular Cl...H interactions < 3.2 Å but three intermolecular interactions less than 3.1 Å (i.e. 2.95 Å, 3.01 Å and 3.04 Å). By contrast, in the R' = Cy structure, with the longer Sn-Cl bond distance, the Cl...H interactions are more significant with two intermolecular Cl...H interactions less than 3.1 Å (i.e. 3.03 Å and 3.09 Å) as well as two intramolecular contacts of 2.90 Å and 3.07 Å.

In summary, while the moderation of the Lewis basicity of the ligands results in systematic variations in the degree of asymmetry in the mode of coordination of the dithiocarbamate ligands for the R = Ph and R = Cy series of structures, no such trends are found in the R = Me and R = ^{t}Bu series. The availability of two series of structures of the general formulae $R_2Sn(S_2CNEt_2)Cl$ and $R_2Sn(S_2CNCy_2)Cl$ enables an examination of the influence of changing the Lewis acidity of the tin center by altering the nature of R on the Sn-ligand parameters.

An examination of the Sn-Cl and Sn-S(1) distances in the $R_2Sn(S_2CNEt_2)Cl$ and $R_2Sn(S_2CNCy_2)Cl$ structures shows that shorter distances are found in the R = Ph structures (for constant R'), a trend consistent with the enhanced Lewis acidity at the tin center in the R = Ph structures. Generally, this trend is repeated in the Sn-S(2) distances. Considering the differences between the Sn-S(1) and Sn-S(2) distances for the $R_2Sn(S_2CNEt_2)Cl$ structures, i.e. the degree of asymmetry, the order is R = Me [0.240(3) Å] ≅ ^{t}Bu [0.253(3) Å] < Ph [0.271(1) Å] < Cy [0.298(3) Å] which contrasts the order for the $R_2Sn(S_2CNCy_2)Cl$ series, i.e R = Cy [0.208(3) Å] ≅ Ph [0.217(2) Å] < Me [0.233(3) Å] < ^{t}Bu [0.251(4) Å and 0.266(4) Å].

From the above correlations, it is clear that another influence is in effect in these structures which precludes a systematic variation of the derived interatomic parameters about the tin centers. In order to ascertain whether crystal packing effects exert a significant influence on these parameters, the geometry optimised structures of the $R_2Sn(S_2CNR'_2)Cl$ were investigated.

5.2.2 Geometry Optimisations

Experimental details pertaining to the geometry optimisation calculations presented below are discussed in Chapter 2. The results of the optimisations are discussed below.

In order to ascertain the influence of crystal packing effects on the molecular geometries and, therefore, the geometric parameters describing the tin atoms, all seven $R_2Sn(S_2CNR'_2)Cl$ structures have been subjected to geometry optimisation calculations at the HF level of theory employing the LanL2DZ basis set. This protocol has been demonstrated to be effective for the R_2SnCl_2(2,2'-bipyridyl) systems, (chapters 3 and 4 and earlier work [4]).

The calculated interatomic parameters for the geometry optimised structures of the $R_2Sn(S_2CNR'_2)Cl$ compounds are listed in Table 5.3. A brief description of each structure is given below and general trends discussed later.

5.2.2a. [$Me_2Sn(S_2CNEt_2)Cl$] and [$Me_2Sn(S_2CNCy_2)Cl$]

The geometry optimised structure of [$Me_2Sn(S_2CNEt_2)Cl$] is shown in Fig. 5.7 from which it can be seen that the essential features found in the solid state are retained in the gas phase molecule. The optimised molecule is more symmetric in that there is mirror symmetry in the $SnCl(S_2CN)$ portion of the molecule such that these atoms define the mirror plane with the methyl groups related to each other across this plane. Further, the orientation of the ethyl groups is more symmetric as judged from a comparison of the C-N-C-C torsion angles listed in Tables 5.2 and 5.3. A similar description pertains in the

structure of $[Me_2Sn(S_2CNCy_2)Cl]$, Fig. 5.8, allowing for the presence of the cyclohexyl groups. For the $Me_2Sn(S_2CNR'_2)Cl$ structures the Sn-Cl distances are shorter in the theoretical structures as opposed to the Sn-Cl bond lengths found in the crystalline structure.

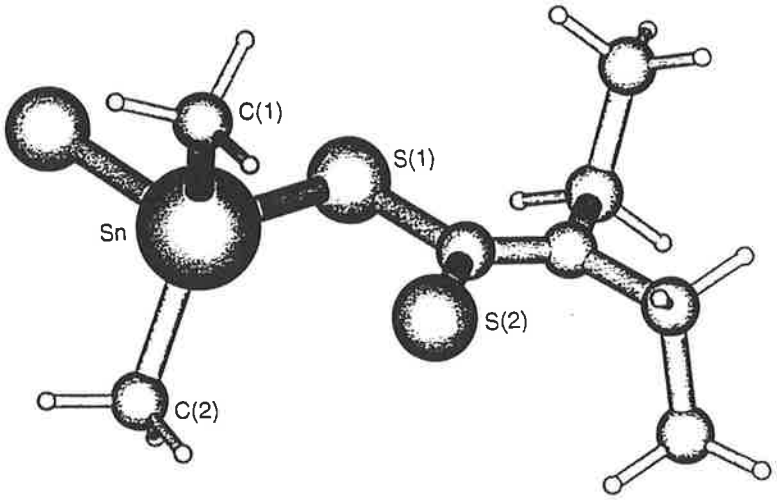


Figure 5.7

The optimised structure of $[Me_2Sn(S_2CNEt_2)Cl]$

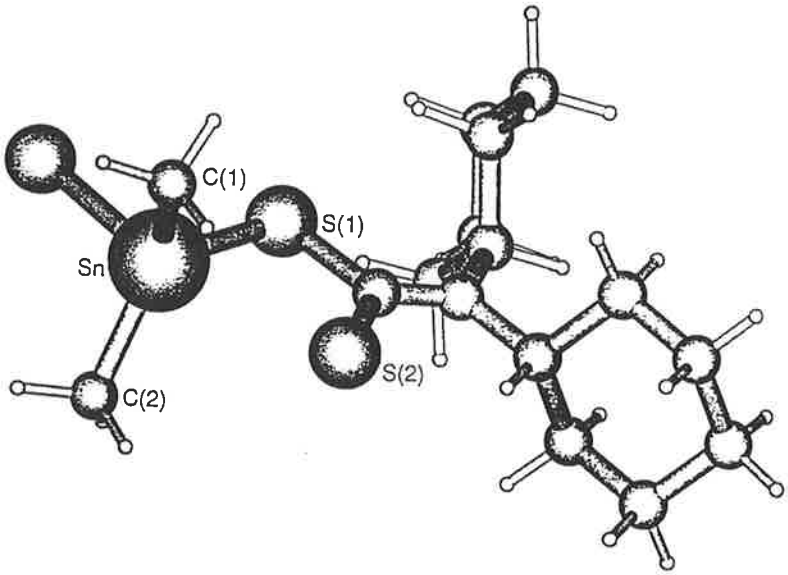


Figure 5.8

The optimised structure of $[Me_2Sn(S_2CNCy_2)Cl]$

TABLE 5.3: Interatomic Parameters (Å, deg.) for $R_2Sn(S_2CNR'_2)Cl$ for R= Me, ^tBu [ab], Cy, Ph, R' = Et and Cy and ; and R= ^tBu and Ph R'_2 = Et and Cy as Derived from Geometry Optimisation Calculations

	$R_2Sn(S_2CNR'_2)Cl$										
Bond Distance	R=Me, R'=Et (y = 2)	R=Me, R'=Cy (y = 2)	R= $^tBu^{ab}$, R'=Et (y = 5)	R=^tBu, R'=Et,Cy (y = 2)	R = $^tBu^{ab}$, R' = Cy (y = 5)		R =Ph, R'=Et (y = 7)	R=Ph, R'=Et,Cy (y = 7)	R=Ph, R'=Cy (y = 7)	R=Cy, R'=Et (y = 7)	R=Cy, R'=Cy (y = 7)
Sn-Cl(1)	2.445	2.456	2.475	2.479	2.485	2.486	2.451	2.455	2.463	2.461	2.482
Sn-S(1)	2.530	2.532	2.556	2.555	2.556	2.557	2.539	2.539	2.541	2.540	2.544
Sn-S(2)	3.034	2.946	3.045	3.012	2.960	2.957	2.978	2.947	2.893	3.041	2.940
Sn-C(1)	2.110	2.110	2.178	2.177	2.177	2.177	2.113	2.115	2.116	2.141	2.149
Sn-C(y)	2.110	2.110	2.178	2.178	2.177	2.177	2.113	2.114	2.116	2.142	2.145
S(1)-C	1.811	1.814	1.802	1.804	1.814	1.805	1.804	1.806	1.807	1.807	1.808
S(2)-C	1.761	1.779	1.762	1.767	1.771	1.779	1.762	1.768	1.780	1.762	1.779
C-N(1)	1.317	1.317	1.318	1.319	1.318	1.318	1.316	1.317	1.316	1.319	1.318
Bond Angle											
Cl(1)-Sn-S(1)	92.2	90.8	86.6	86.3	85.7	85.6	88.7	88.4	87.6	90.5	88.4
Cl(1)-Sn-S(2)	157.7	157.1	151.3	151.3	151.1	151.0	154.8	154.7	154.3	155.7	154.0
Cl(1)-Sn-C(1)	100.7	99.9	99.8	100.7	99.6	99.9	100.2	99.9	99.4	101.6	96.8
Cl(1)-Sn-C(y)	100.8	99.9	100.9	99.5	99.9)	99.6	100.1	99.8	99.4	99.3	97.0
S(1)-Sn-S(2)	65.6	66.2	64.8	65.0	65.4	65.4	66.1	66.3	66.7	65.3	66.0
S(1)-Sn-C(1)	114.5	115.4	115.6	115.4	116.0	115.9	116.5	116.9	117.4	115.0	115.2
S(1)-Sn-C(y)	114.5	115.4	115.2	115.9	115.9	116.0	116.5	116.8	117.4	115.6	118.2
S(2)-Sn-C(1)	89.3	90.6	93.0	92.3	93.4	93.2	91.9	92.4	92.8	89.0	98.0
S(2)-Sn-C(y)	89.3	90.6	92.0	93.3	93.2	93.5	91.4	91.7	92.8	92.3	91.8
C(1)-Sn-C(y)	125.1	124.7	125.7	125.6	125.4	125.4	123.1	122.8	122.4	124.5	125.1

a two molecules in the asymmetric unit; *b* [1]

TABLE 5.3: Cont'd.

	$R_2Sn(S_2CNR'_2)Cl$										
Bond Angles	R=Me, R'=Et (y = 2)	R=Me, R'=Cy (y = 2)	R= $^tBu^{ab}$, R'=Et (y = 5)	R=^{t}Bu, R'=Et,Cy (y = 2)	R = $^tBu^{ab}$, R' = Cy (y = 5)		R =Ph, R'=Et (y = 7)	R=Ph, R'=Et,Cy (y = 7)	R=Ph, R'=Cy (y = 7)	R=Cy, R'=Et (y = 7)	R=Cy, R'=Cy (y = 7)
Sn-S(1)-C	96.3	96.1	96.9	96.8	96.6	96.7	95.4	95.3	95.2	95.5	96.2
Sn-S(2)-C	81.3	83.7	82.0	82.8	84.5	84.3	82.3	83.1	84.5	81.5	84.1
S(1)-C-S(2)	116.8	114.0	116.3	115.4	113.6	113.6	116.3	115.3	113.6	116.7	113.8
S(1)-C-N(1)	119.0	121.6	119.7	119.9	120.5	122.2	119.8	120.0	122.4	119.3	122.0
S(2)-C-N(2)	124.2	124.4	124.0	124.8	125.9	124.2	123.9	124.7	124.0	124.0	124.2
Torsion Angles											
C/N/C/C (Et)	90.0		-90.2	-114.1			90.1	-82.7		-90.1	
	90.2		-90.2				90.1			-90.2	
C/N/C/C (Cy)		116.4		-133.0	65.2	-116.5		-100.8	65.3		65.4
		-116.5		100.8	-65.2	116.4		132.9	-65.3		-65.4
		65.5			-116.4	65.4			-116.4		-116.5
		-65.4			116.4	-65.4			116.4		116.3

a two molecules in the asymmetric unit; *b* [1]

5.2.2b [$Cy_2Sn(S_2CNEt_2)Cl$] and [$Cy_2Sn(S_2CNCy_2)Cl$]

The optimised geometries of the two [$Cy_2Sn(S_2CNR'_2)Cl$] derivatives, where R' = Et and Cy are shown in Figs 5.8 and 5.9 respectively. In these molecules, the Sn-bound cyclohexyl groups are orientated so as to place the methine-H atoms on either side of the molecule so that the mirror symmetry observed for the earlier molecules no longer pertains. In the $Cy_2Sn(S_2CNR'_2)Cl$ molecules, and indeed in all molecules containing cyclohexyl rings, the rings adopt the chair conformation. An examination of the torsion angles listed in Table 5.3 reveals a remarkable level of consistency for N-bound substituents and also indicates the degree of symmetrisation that has occurred upon geometry optimisation compared with the solid state results, Table 5.2. The orientations of the N-bound substituents were deliberately perturbed to alternative positions and the molecules then optimised in order to confirm that global minima had been attained rather than local minima. The relatively narrow range of torsion angles for each of the three dithiocarbamate ligands inspires confidence in the reliability of the calculations. In addition to the changes in angles in order to accommodate the symmetrisation of the molecules, changes in the Sn-ligand bond distances are also evident. As has been noted previously, bond elongation may occur owing, at least in part, to the theoretical model employed in the study [1] and thus, elongation of the Sn-ligand bond distances are not due to the removal of intermolecular forces alone. This point is borne out by the following discussion which shows that some Sn-ligand distances actually contract compared with their solid state structures.

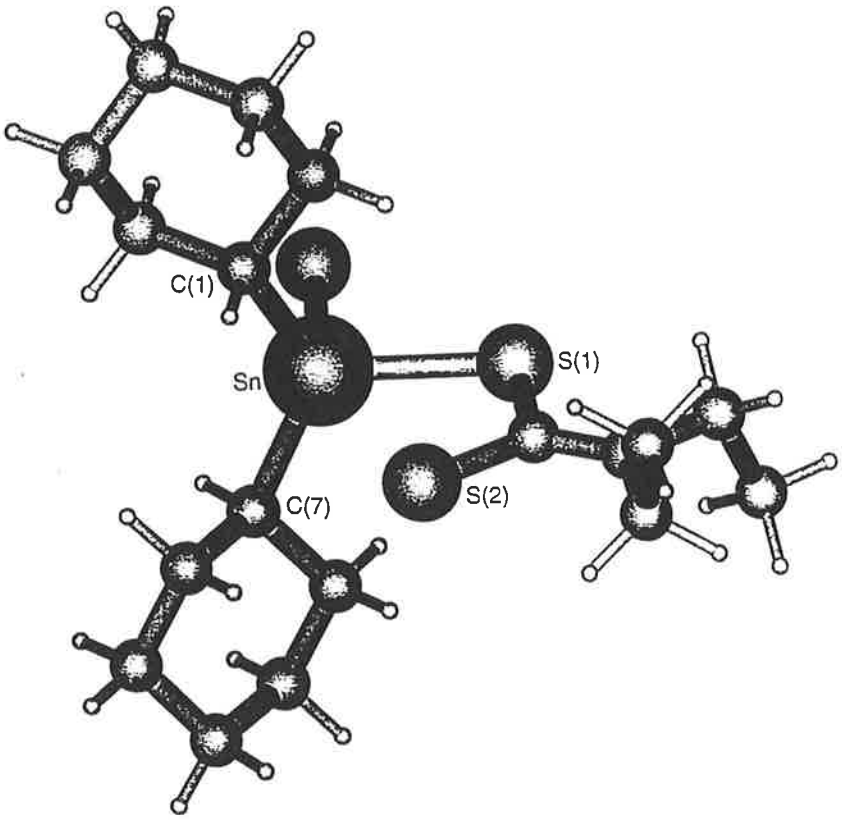


Figure 5.8

The optimised structure of $[Cy_2Sn(S_2CNEt_2)Cl]$

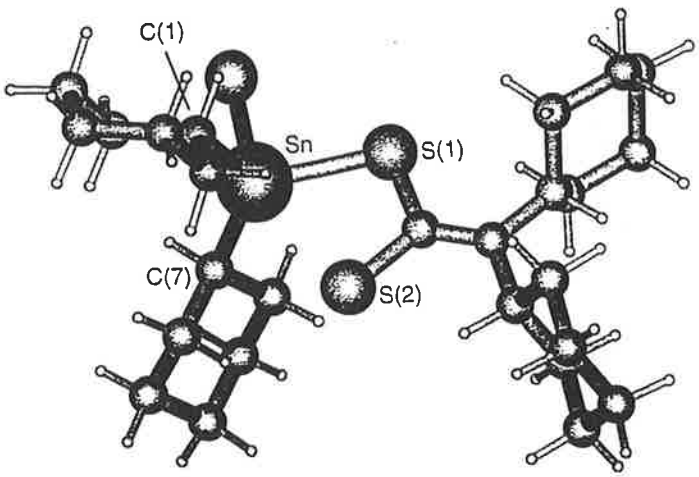


Figure 5.9

The optimised structure of $[Cy_2Sn(S_2CNCy_2)Cl]$

5.2.2c [$^tBu_2Sn(S_2CNEt_2)Cl$] , [$^tBu_2Sn(S_2CNEt(Cy))Cl$] and [$^tBu_2Sn(S_2CNCy_2)Cl$] [1]

The geometry optimised structures of the [$^tBu_2Sn(S_2CNEt_2)Cl$] and [$^tBu_2Sn(S_2CNEt(Cy))Cl$] molecules are shown in Figs 5.10 and 5.11; the results of the geometry optimisation of [$^tBu_2Sn(S_2CNCy_2)Cl$] have been reported earlier [1, Chapter 3]. Symmetrisation of the structures relative to their structures observed in the crystalline state is found, allowing once again for the N-bound substituents. It is noteworthy that there are two molecules in the crystallographic asymmetric unit of [$^tBu_2Sn(S_2CNEt_2)Cl$] [5] and that geometry optimisation calculations for both of these converged to the same theoretical structure in the gas phase. This result duplicates that found earlier for [$^tBu_2Sn(S_2CNCy_2)Cl$] [1] and demonstrates that there is no inherent chemical reason for the adoption of different molecular structures in the solid state.

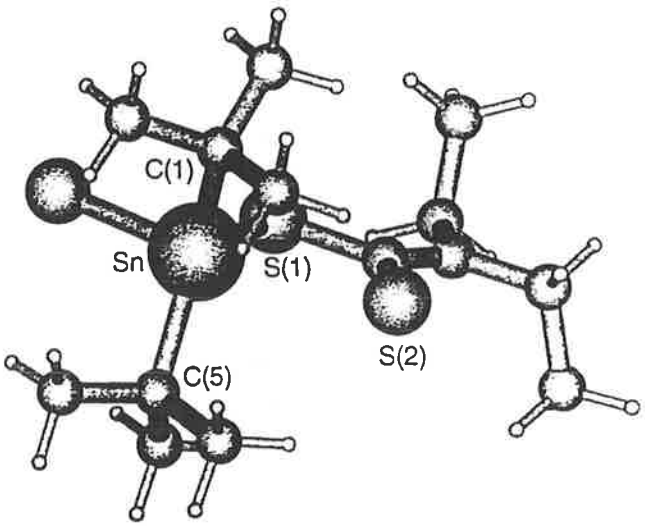


Figure 5.10

The optimised structure of [$^tBu_2Sn(S_2CNEt_2)Cl$]

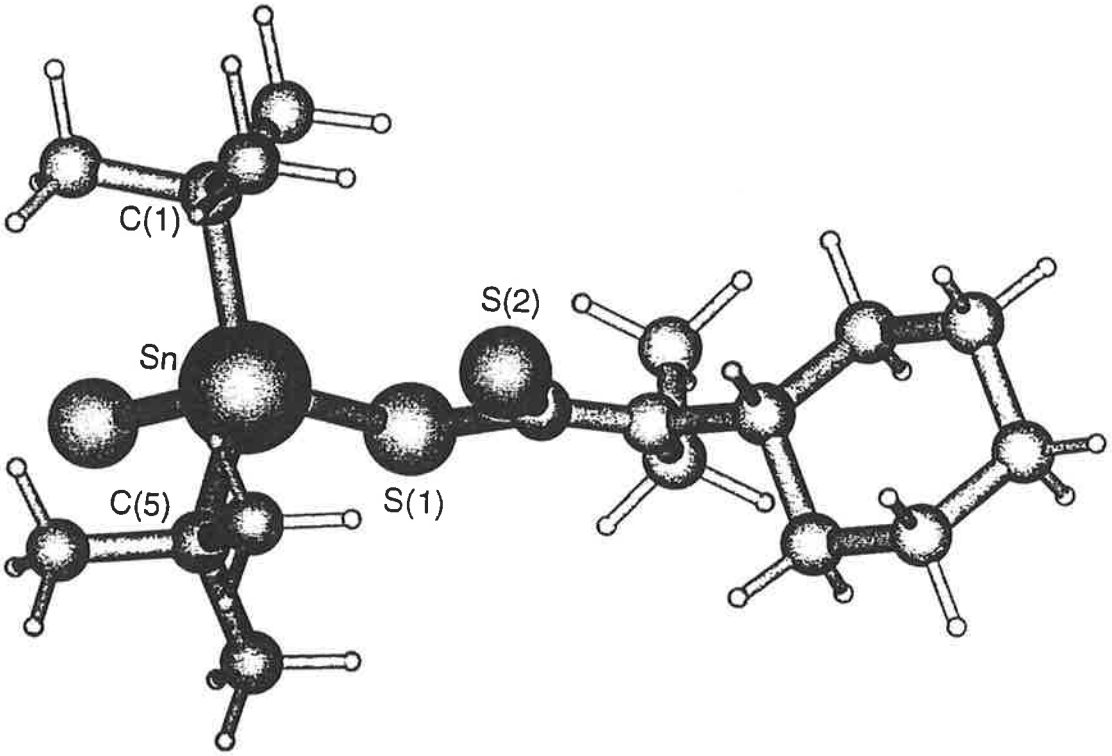


Figure 5.11

The optimised structure of $[^tBu_2Sn(S_2CNEt(Cy))Cl]$

5.2.2d. $[Ph_2Sn(S_2CNEt_2)Cl]$, $[Ph_2Sn(S_2CN(Et)Cy)Cl]$ and $[Ph_2Sn(S_2CNCy_2)Cl]$

The optimised structures of three $[Ph_2Sn(S_2CNR'_2)Cl]$ compounds, where R' = Et, Cy and R'_2 = Et, Cy are shown in Figs 5.12 – 5.14 respectively. It can be seen that the essential features found in the solid state are retained in the gas phase molecule. The optimised molecule is more symmetric in that there is mirror symmetry in the $SnCl(S_2CN)$ portion of the molecule such that these atoms define the mirror plane with the phenyl groups related to each other across this plane. The three orientations emphasise the symmetry in the tin regions of the molecules, a feature that is lacking in the N-bound groups. The Sn-Cl distances are longer in the theoretical structures, than those found in the crystalline structure determinations discussed in section 5.2.1. In all cases the theoretical structure is lower in energy than the crystallographic determined structure, as indicated in Table 5.4.

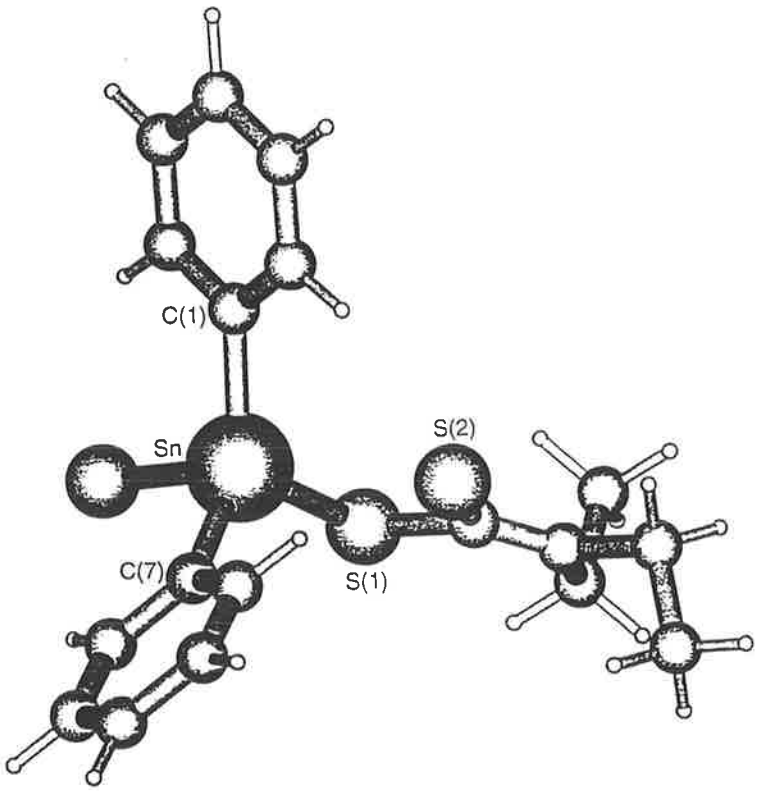


Figure 5.12

The optimised structure of $[Ph_2Sn(S_2CNEt_2)Cl]$

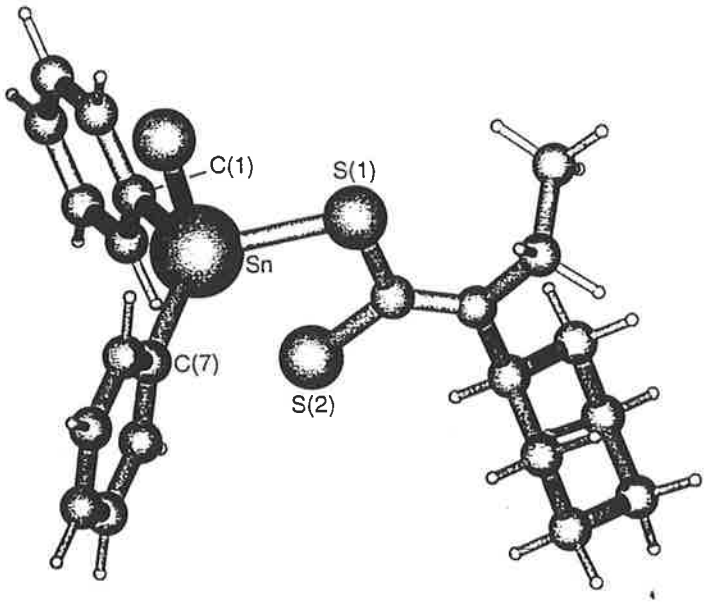


Figure 5.13

The optimised structure of $[Ph_2Sn(S_2CN(Et)Cy)Cl]$

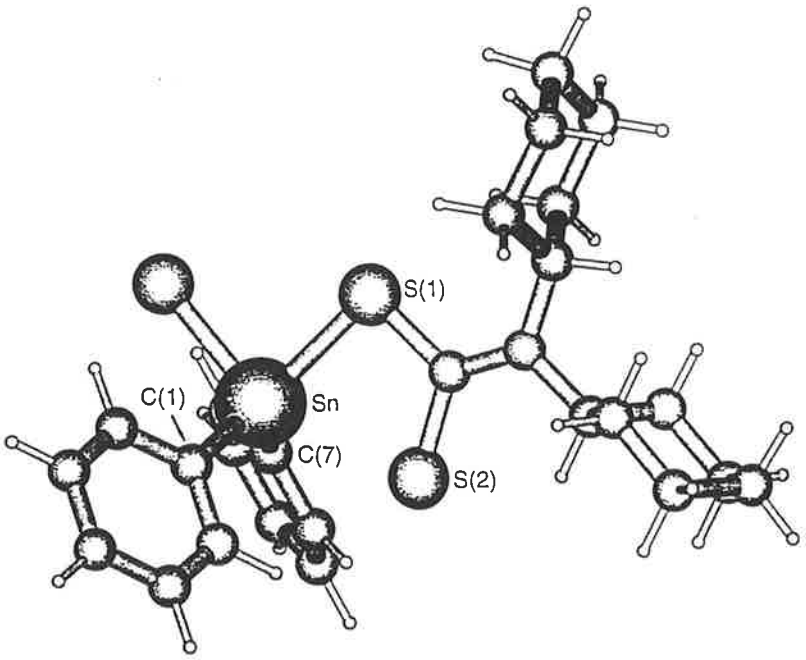


Figure 5.14

The optimised structure of $[Ph_2Sn(S_2CNCy_2)Cl]$

5.2.2e. Structural correlation derived from Geometry Optimisations

In common with previous studies of this type [1-3], the Sn-S distances generally elongate in the gas phase compared with the solid state. Of particular interest, is that the variation in the Sn-Cl distances are not systematic. Thus, while in the $Me_2Sn(S_2CNR'_2)Cl$ structures the Sn-Cl distances are shorter in the theoretical structures, the opposite is true for the $Ph_2Sn(S_2CNR'_2)Cl$ molecules. Further, in the other two series both elongation and contraction in the Sn-Cl bond distances is noted. The Sn-C distances are not sufficiently different to ascertain any trends between the solid and gas phases, however, in the gas phase the Sn-C distances vary systematically in the order R = Me < Ph < Cy < ^{t}Bu. In the dithiocarbamate ligands, the S(1)-C [1.80 Å - 1.81 Å] and C-N [1.32 Å] distances are consistent across the series of $R_2Sn(S_2CNR'_2)Cl$ molecules but there is a systematic variation in the S(2)-C [1.76 Å - 1.78 Å] distances; see later. Using the data collected in Table 5.3, the trends investigated for the crystallographically-determined structures may be re-examined using the calculated values.

The key result ascertained from the crystallographically-determined structures was a lack of a systematic variation in the derived interatomic parameters as the Lewis acidity of the tin center and/or the Lewis basicity of the dithiocarbamate ligands were varied. The opposite is true in the theoretical gas phase structures.

Considering first each series of $R_2Sn(S_2CNR'_2)Cl$ structures. As the Lewis basicity (coordinating ability) of the dithiocarbamate ligands is increased, i.e. as the ethyl substituents are successively replaced by cyclohexyl residues, the Sn-Cl distances systematically increase for each series of $R_2Sn(S_2CNR'_2)Cl$ structures. Keeping R constant but varying R' does not alter significantly the magnitude of the Sn-S(1) bond distances, however, Sn-S(2) distances do vary systematically, i.e. Sn-S(2) decreases as the Lewis basicity of the dithiocarbamate ligand increases. A model for the bonding of the dithiocarbamate ligands in each series of $R_2Sn(S_2CNR'_2)Cl$ may thus be formulated.

The strength of the covalent Sn-S(1) interaction is determined by the nature of the tin-bound substituent and the magnitude of the weaker Sn-S(2) interaction is determined by the Lewis basicity of the dithiocarbamate ligand. In other words, based on the theoretical study, the degree of asymmetry in the mode of coordination of the dithiocarbamate is dictated by the Lewis basicity of the ligand and not the Lewis acidity of the tin center. The changes in the degree of asymmetry in the mode of coordination are reflected by small but systematic variations in the S(2)-C distances and in the Sn-S-C, S-C-S and S(1)-C-N angles. Thus, as the asymmetry is decreased, the S(2)-C distance concomitantly tend to increase and the Sn-S(1)-C, Sn-S(2)-C, S-C-S and S(1)-C-N angles decrease (marginally), increase, decrease and increase, respectively.

The final trend to be ascertained concerns the influence of moderating the Lewis acidity of the tin center as the nature of R is varied and R' is held constant. A close examination of the Sn-ligand bond distances shows that, systematically, the longer distances are found in the ^{t}Bu structures. The Sn-Cl and Sn-S(1) distances follow the trends R = Me, Ph < Cy < ^{t}Bu and R = Me < Ph, Cy < tBu, respectively and the Sn-S(2) increase in the order R = Ph < Me/Cy < ^{t}Bu. On electronic arguments alone, it would be anticipated that the tin center in the R = Me compound would be of lowest Lewis acidity owing to the electron donating ability of the methyl group and conversely, the tin center in the R = Ph structure would be of highest Lewis acidity. The above trends, indicating that there is little difference in the Sn-ligand parameters for the R = Me and Ph compounds, suggest that another factor over above crystal packing effects must be taken into account. In these congested five-coordinate structures where the organic substituents occupy positions in the equatorial planes of the distorted trigonal bipyramidal geometries, it is clear that steric hindrance between the larger tin-bound substituents, resulting in reorganisation of electron density about the tin center, must also play an important role in moderating the Lewis acidity of the tin center. In support of this proposal is the observation made above concerning the length of the Sn-C bonds found in the theoretical structures, i.e. R = Me < Ph < Cy < ^{t}Bu, noting that the

difference in the Sn-C distances in the R = Me and Ph compounds is not great. This important feature of organotin systems will be the focus of further studies in this area.

5.2.2f Energy considerations

Table 5.4 presents data relating to the calculated energy differences between the crystallographically-determined structures (i.e. single-point calculations) and the energy minimised structures. As has been argued in previous contributions in this area, the rather large energy differences between the solid state and gas phase structures may not be correlated to the influence of crystal packing effects [1-2]. Errors in the theoretical model and in the crystallographic experiment (notably the treatment of hydrogen atoms) contribute to the discrepancy. The energy differences for all the systems investigated, except for [^{t}Bu$_2$Sn(S$_2$CNEt$_2$)Cl], are comparable to those reported for related systems. The unusual feature of the energy differences calculated for the crystallographic and theoretical structures of [^{t}Bu$_2$Sn(S$_2$CNEt$_2$)Cl] is the small magnitude. As mentioned above, there are two independent molecules comprising the asymmetric unit in the structure of [^{t}Bu$_2$Sn(S$_2$CNEt$_2$)Cl] [5]. The energy difference between to the two molecules is calculated to be 40.0 kJ mol^{-1}, a result comparable to that calculated for related systems. The geometry optimisation calculations for both molecules converged to the same structure and the energy difference between the solid state and gas phase structures is approximately an order of magnitude lower than that found for related systems. In order to determine whether this result is an artefact of the theoretical model employed (i.e. HF, which does not allow for electron correlation) comparable calculations were conducted on molecules of [^{t}Bu$_2$Sn(S$_2$CNEt$_2$)Cl] and [^{t}Bu$_2$Sn(S$_2$CN(Et)Cy)Cl] employing Density Functional Theory (DFT). The results of these calculations are also listed in Table 4 and show that comparable energy differences are found regardless of the theoretical model employed, an observation that is consistent with work reported in this thesis.

TABLE 5.4: Calculated Energies (hartrees, kJ mol^{-1}) Employing the LanL2DZ[a] Basis Set for $R_2Sn(S_2CNR'_2)Cl$ for R= Me, ^tBu , Cy, Ph, R' = Et and Cy; and R= ^tBu, Ph where R'_2 = Et and Cy

	Calculated Energies		
$R_2Sn(S_2CNR'_2)Cl$	**Single point (hartrees)**	**Optimised geometry (hartrees)**	**Δ (kJ mol^{-1})**
$[Me_2Sn(S_2CNEt_2)Cl]$	-366.3717	-366.5547	480.5
$[Me_2Sn(S_2CNCy_2)Cl]$	-676.0764	-676.4022	855.4
$[Cy_2Sn(S_2CNEt_2)Cl]$	-753.9350	-754.4427	1333.0
$[Cy_2Sn(S_2CNCy_2)Cl]$	-1063.6840	-1064.2871	1583.4
$[^tBu_2Sn(S_2CNEt_2)Cl]$ [a] *Molecule a*	-600.6201	-600.6651	118.2
	-604.9891	*-605.0535*	*169.1*
$[^tBu_2Sn(S_2CNEt_2)Cl]$ [a] *Molecule* b	-600.6353	-600.6651	78.2
	-604.9996	*-605.0535*	*141.5*
$[^tBu_2Sn(S_2CN(Et)Cy)Cl]$ [a]	-755.0327	-755.5908	1465.3
	-760.2861	*-760.9769*	*1813.6*
$[^tBu_2Sn(S_2CNCy_2)Cl]$ [1] *Molecule a*	-910.0397	-910.5122	1240.6
$[^tBu_2Sn(S_2CNCy_2)Cl]$ [1] *Molecule b*	-910.0337	-910.5125	1257.1
$[Ph_2Sn(S_2CNEt_2)Cl]$	-747.0866	-747.4574	973.5
$[Ph_2Sn(S_2CN(Et)Cy)Cl]$	-901.9582	-902.3832	1115.8
$[Ph_2Sn(S_2CNCy_2)Cl]$	-1056.8155	-1057.3051	1285.5

[a] values obtained from HF except those given in italics which were obtained using DFT (see Text)

5.3 Conclusion

This combined crystallographic/theoretical study of a series of $R_2Sn(S_2CNR'_2)Cl$ compounds points to the significant influence of crystal packing forces on molecular geometry. Based on the X-ray crystallographic study, attempts at correlating changes in Sn-ligand parameters with the nature of both R and R' were unsuccessful. Geometry optimisation calculations were conducted on the $R_2Sn(S_2CNR'_2)Cl$ compounds in order to determine whether any trends in the Sn-ligand parameters may exist in the absence of intermolecular forces. The geometry optimisation calculations showed that more symmetric structures are invariably found in the gas phase compared with the solid state. Further, generally, there was an elongation in the Sn-ligand bond distances which, in part, may be ascribed to the theoretical model used. More interesting is the fact that in contrast to the solid state results, clear and systematic correlations in the Sn-ligand parameters owing to the variation of R' in the dithiocarbamate ligands are discernible again pointing to the influence of crystal packing effects on the tin atom geometry. Similarly, consistent trends are found as the Lewis acidity of the tin center is moderated but these can not be correlated directly with the electron withdrawing capability of the tin-bound R groups. This latter result indicates that Lewis acidity at the tin center is also influenced by the steric demands of these substituents.

5.4 References

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Appendix - Chapter 5

Crystal data and refinement details for:

A. $[Me_2Sn(S_2CNEt_2)Cl]$

B. $[Me_2Sn(S_2CNCy_2)Cl]$

C. $[Cy_2Sn(S_2CNEt_2)Cl]$

D. $[Cy_2Sn(S_2CNCy_2)Cl]$

E. $[^tBu_2Sn(S_2CN(Et)Cy)Cl]$

A. $[Me_2Sn(S_2CNEt_2)Cl]$

Crystallographic Data and Refinement details for $[Me_2Sn(S_2CNEt_2)Cl]$.

Formula	$C_7H_{16}ClNS_2Sn$
Formula weight	332.5
Crystal morphology	colourless plate
Crystal dimensions (mm)	0.03 x 0.06 x 0.35
Crystal system	monoclinic
Space group	$P2_1/c$ (C_{2h}^5, No. 14)
Temperature (°C)	20.0
a (Å)	10.896(2)
b (Å)	9.869(4)
c (Å)	12.722(2)
β (°)	105.08(1)
V (Å^3)	1320.8(5)
Z	4
D_{calc} (g cm^{-3})	1.672
$F(000)$	656
Radiation	MoKα (λ = 0.7107Å)
μ (cm^{-1})	24.11
θ limits, data (°)	3.0 to 27.5
hkl range	0 to 14, 0 to 13, -17 to 17
Range of transmission factors	0.981 to 1.000
Scan technique	ω:2θ
Scan width (°)	1.00
No. of data measured	3401
No. of unique data	3240
R_{amal}	0.090
Program for structure solution	Direct Methods (SHELXS86)
No. of unique data used	1367
No. of parameters	109
R	0.039
R_w	0.037
G.O.F.	1.29
Min./Max. residual electron density (e Å^{-3})	-0.66 to +0.45

Fractional atomic coordinates ($Å^2$) for the non-hydrogen atoms in $Me_2Sn(S_2CNEt_2)Cl$].

Atom	*x*	*y*	*z*
Sn	0.27935(5)	0.11981(6)	0.64322(5)
Cl(1)	0.2882(3)	0.2535(3)	0.8101(2)
S(1)	0.2397(2)	-0.0835(2)	0.7417(2)
S(2)	0.2646(2)	-0.1032(2)	0.5172(2)
N(1)	0.2199(6)	-0.3145(7)	0.6325(5)
C(1)	0.1119(8)	0.2083(9)	0.5453(7)
C(2)	0.4683(8)	0.1577(10)	0.6376(8)
C(3)	0.2394(7)	-0.1840(9)	0.6284(6)
C(4)	0.1979(7)	-0.3824(8)	0.7282(6)
C(5)	0.0578(8)	-0.4020(11)	0.7198(7)
C(6)	0.2225(9)	-0.4024(9)	0.5402(7)
C(7)	0.3539(11)	-0.4625(10)	0.5514(8)

Anisotropic thermal parameters ($Å^2$) for the non-hydrogen atoms in $[Me_2Sn(S_2CNEt_2)Cl]$.

Atom	$U11$	$U22$	$U33$	$U12$	$U13$	$U23$
Sn	0.0460(3)	0.0503(3)	0.0532(4)	0.0009(4)	0.0117(2)	0.0089(4)
Cl(1)	0.114(2)	0.059(2)	0.074(2)	0.004(2)	0.028(2)	-0.009(1)
S(1)	0.074(2)	0.049(1)	0.040(1)	0.006(1)	0.024(1)	0.002(1)
S(2)	0.084(2)	0.070(2)	0.038(1)	-0.011(2)	0.026(1)	0.002(1)
N(1)	0.052(4)	0.048(4)	0.033(4)	0.006(4)	0.009(3)	0.001(4)
C(1)	0.058(6)	0.065(6)	0.088(7)	0.012(5)	0.004(5)	0.020(6)
C(2)	0.051(5)	0.095(8)	0.101(8)	-0.011(6)	0.018(5)	0.016(7)
C(3)	0.037(4)	0.062(6)	0.035(5)	-0.001(4)	0.013(4)	-0.001(5)
C(4)	0.050(4)	0.053(5)	0.044(5)	0.009(5)	0.010(4)	0.013(5)
C(5)	0.064(6)	0.12(1)	0.066(6)	-0.018(7)	0.015(5)	0.005(6)
C(6)	0.082(6)	0.064(6)	0.046(5)	-0.007(6)	0.017(5)	-0.010(5)
C(7)	0.122(9)	0.067(7)	0.086(8)	0.015(7)	0.052(7)	-0.013(6)

Fractional atomic coordinates and B_{eq} values (Å^2) for the hydrogen atoms in [$Me_2Sn(S_2CNEt_2)Cl$].

Atom	x	y	z	B_{eq}
H(1a)	0.1248	0.3048	0.5389	5.9
H(1b)	0.0916	0.1673	0.4736	5.9
H(1c)	0.0423	0.1932	0.5785	5.9
H(2a)	0.5265	0.1236	0.7035	7.6
H(2b)	0.4844	0.1123	0.5749	7.6
H(2c)	0.4808	0.2544	0.6319	7.6
H(4a)	0.2388	-0.4704	0.7356	4.3
H(4b)	0.2349	-0.3280	0.7921	7.6
H(5a)	0.0157	-0.3145	0.7116	6.8
H(5b)	0.0202	-0.4581	0.6571	6.8
H(5c)	0.0477	-0.4458	0.7853	7.8
H(6a)	0.1621	-0.4755	0.5367	5.7
H(6b)	0.1985	-0.3496	0.4737	5.7
H(7a)	0.3782	-0.5163	0.6173	7.6
H(7b)	0.3521	-0.5196	0.4889	7.6
H(7c)	0.4149	-0.3900	0.5549	5.7

Bond distances (Å) for $[Me_2Sn(S_2CNEt_2)Cl]$.

Aom - Atom	Distance	Atom - Atom	Distance
Sn - Cl(1)	2.479(2)	S(2) - C(3)	1.707(8)
Sn - S(1)	2.463(2)	N(1) - C(3)	1.31(1)
Sn - S(2)	2.703(2)	N(1) - C(4)	1.462(9)
Sn - C(1)	2.111(9)	N(1) - C(6)	1.47(1)
Sn - C(2)	2.112(8)	C(4) - C(5)	1.51(1)
S(1) - C(3)	1.750(8)	C(6) - C(7)	1.52(1)

Bond angles (°) for $[Me_2Sn(S_2CNEt_2)Cl]$.

Atom - Atom - Atom	Angle	Atom - Atom - Atom	Angle
Cl(1) - Sn - S(1)	88.32(8)	Sn - S(1) - C(3)	90.3(3)
Cl(1) - Sn - S(2)	157.52(8)	Sn - S(2) - C(3)	83.5(3)
Cl(1) - Sn - C(1)	96.9(3)	C(3) - N(1) - C(4)	123.2(7)
Cl(1) - Sn - C(2)	96.5(3)	C(3) - N(1) - C(6)	120.9(7)
S(1) - Sn - S(2)	69.35(7)	C(4) - N(1) - C(6)	115.9(7)
S(1) - Sn - C(1)	113.4(2)	S(1) - C(3) - S(2)	116.9(5)
S(1) - Sn - C(2)	117.6(3)	S(1) - C(3) - N(1)	119.4(6)
S(2) - Sn - C(1)	94.5(3)	S(2) - C(3) - N(1)	123.8(6)
S(2) - Sn - C(2)	91.8(3)	N(1) - C(4) - C(5)	112.4(7)
C(1) - Sn - C(2)	127.4(4)	N(1) - C(6) - C(7)	111.7(7)

Observed and calculated structure factors for $[Me_2Sn(S_2CNEt_2)Cl]$.

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	758	748	9	0	4	2	128	101	14	0	7	13	60	52	69*	1	0	-6	1057	1062	13	1	2	-2	34	62	33*
0	0	4	418	441	9	0	4	3	276	278	9	0	8	0	624	646	14	1	0	-4	659	641	9	1	2	-1	1064	1056	12
0	0	6	851	824	12	0	4	4	551	531	13	0	8	1	0	56	48*	1	0	-2	2264	2316	25	1	2	0	38	27	33*
0	0	8	831	828	13	0	4	5	280	256	10	0	8	2	141	146	19	1	0	2	2350	2351	26	1	2	1	775	766	10
0	0	10	606	634	15	0	4	6	458	439	12	0	8	3	190	208	16	1	0	4	476	475	11	1	2	2	669	668	10
0	0	12	0	87	51*	0	4	7	0	90	56*	0	8	4	382	373	11	1	0	6	451	451	12	1	2	3	1783	1844	20
0	0	14	84	175	43*	0	4	8	782	792	17	0	8	5	201	232	18	1	0	8	850	843	16	1	2	4	283	284	9
0	0	16	0	28	52*	0	4	9	174	155	23	0	8	6	402	403	11	1	0	10	614	635	13	1	2	5	0	137	49*
0	1	2	425	454	9	0	4	10	513	509	13	0	8	7	0	6	59*	1	0	12	406	419	11	1	2	6	354	334	10
0	1	3	886	905	12	0	4	11	26	84	66*	0	8	8	83	59	60*	1	0	14	149	172	20	1	2	7	721	707	15
0	1	4	62	68	44*	0	4	12	96	2	50*	0	8	9	0	24	62*	1	1	-16	0	31	62*	1	2	8	49	14	60*
0	1	5	0	32	47*	0	4	13	124	170	67*	0	8	10	167	114	22	1	1	-15	150	113	29*	1	2	9	429	429	12
0	1	6	926	928	14	0	4	14	173	192	33*	0	8	11	78	26	71*	1	1	-14	153	166	22	1	2	10	108	31	65*
0	1	7	965	924	15	0	4	15	0	2	71*	0	8	12	60	10	67*	1	1	-13	0	10	51*	1	2	11	354	364	15
0	1	8	473	451	12	0	5	1	724	738	12	0	9	1	350	352	10	1	1	-12	159	162	18	1	2	12	0	41	67*
0	1	9	14	63	47*	0	5	2	862	828	13	0	9	2	194	202	15	1	1	-11	86	73	50*	1	2	13	88	139	57*
0	1	10	0	61	61*	0	5	3	572	564	13	0	9	3	249	259	13	1	1	-10	103	98	23*	1	2	14	0	33	65*
0	1	11	186	248	21	0	5	4	503	511	13	0	9	4	0	56	56*	1	1	-9	769	740	13	1	2	15	135	110	71*
0	1	12	327	321	13	0	5	5	77	65	50*	0	9	5	43	31	55*	1	1	-8	185	202	11	1	3	-15	112	101	68*
0	1	13	148	202	27*	0	5	6	86	94	54*	0	9	6	108	158	60*	1	1	-7	292	283	8	1	3	-14	284	271	13
0	1	14	70	18	58*	0	5	7	725	718	17	0	9	7	294	304	14	1	1	-6	441	434	10	1	3	-13	115	111	27*
0	1	15	125	57	66*	0	5	8	289	275	14	0	9	8	26	131	63*	1	1	-5	766	760	11	1	3	-12	233	242	14
0	2	0	242	232	6	0	5	9	101	56	53*	0	9	9	115	9	59*	1	1	-4	1429	1441	16	1	3	-11	72	41	52*
0	2	1	1531	1534	17	0	5	10	0	14	65*	0	9	10	172	103	27	1	1	-3	651	626	9	1	3	-10	283	281	11
0	2	2	259	259	7	0	5	11	82	221	66*	0	9	11	155	117	29*	1	1	-2	227	211	6	1	3	-9	419	421	10
0	2	3	906	912	12	0	5	12	94	135	45*	0	10	0	208	209	14	1	1	-1	1058	1022	12	1	3	-8	304	298	9
0	2	4	467	478	9	0	5	13	149	169	28*	0	10	1	347	358	10	1	1	1	1310	1345	15	1	3	-7	0	26	43*
0	2	5	1429	1441	18	0	5	14	133	22	68*	0	10	2	79	71	44*	1	1	2	778	818	10	1	3	-6	432	459	9
0	2	6	309	317	10	0	6	0	741	746	12	0	10	3	64	47	52*	1	1	3	174	181	11	1	3	-5	584	614	11
0	2	7	58	94	54*	0	6	1	758	769	13	0	10	4	91	6	33*	1	1	4	862	873	13	1	3	-4	2067	2054	23
0	2	8	266	280	14	0	6	2	282	281	9	0	10	5	178	170	20	1	1	5	592	612	13	1	3	-3	892	867	12
0	2	9	422	411	12	0	6	3	191	169	13	0	10	6	96	14	57*	1	1	6	867	877	14	1	3	-2	408	400	9
0	2	10	172	149	23	0	6	4	371	348	9	0	10	7	0	58	59*	1	1	7	0	16	56*	1	3	-1	428	447	9
0	2	11	196	230	22	0	6	5	761	754	15	0	10	8	174	190	29	1	1	8	246	224	15	1	3	0	557	520	9
0	2	12	0	79	64*	0	6	6	79	2	40*	0	10	9	172	219	28	1	1	9	734	732	18	1	3	1	937	896	12
0	2	13	410	430	13	0	6	7	0	97	61*	0	10	10	0	67	65*	1	1	10	259	265	18	1	3	2	310	316	8
0	2	14	110	14	36*	0	6	8	90	114	51*	0	11	1	0	42	52*	1	1	11	207	206	22	1	3	3	258	250	9
0	2	15	0	121	75*	0	6	9	295	321	15	0	11	2	267	257	12	1	1	12	0	40	67*	1	3	4	1483	1510	18
0	3	1	1079	1049	13	0	6	10	0	34	65*	0	11	3	126	140	24*	1	1	13	0	46	65*	1	3	5	595	591	14
0	3	2	1170	1142	14	0	6	11	120	173	65*	0	11	4	150	146	21	1	1	14	100	124	64*	1	3	6	428	412	10
0	3	3	626	639	11	0	6	12	20	31	65*	0	11	5	0	17	47*	1	1	15	108	121	71*	1	3	7	265	244	13
0	3	4	962	958	13	0	6	13	116	179	78*	0	11	6	114	134	66*	1	2	-16	0	9	60*	1	3	8	203	245	19
0	3	5	72	59	48*	0	6	14	0	41	70*	0	11	7	0	69	68*	1	2	-15	113	150	40*	1	3	9	381	390	13
0	3	6	1001	980	15	0	7	1	194	191	12	0	11	8	146	89	25*	1	2	-14	0	28	55*	1	3	10	328	337	15
0	3	7	609	611	16	0	7	2	522	507	11	0	12	0	0	95	61*	1	2	-13	0	72	55*	1	3	11	63	159	67*
0	3	8	380	346	11	0	7	3	368	369	10	0	12	1	138	80	25*	1	2	-12	0	83	51*	1	3	12	140	95	32*
0	3	9	55	132	62*	0	7	4	96	77	29*	0	12	2	52	43	60*	1	2	-11	567	563	15	1	3	13	42	40	66*
0	3	10	140	138	29*	0	7	5	123	105	26*	0	12	3	0	31	60*	1	2	-10	31	55	49*	1	3	14	196	239	32
0	3	11	0	193	69*	0	7	6	697	694	17	0	12	4	0	182	67*	1	2	-9	244	236	10	1	3	15	89	111	69*
0	3	12	90	196	69*	0	7	7	338	324	13	0	12	5	0	61	49*	1	2	-8	70	44	42*	1	4	-15	0	49	54*
0	3	13	116	112	67*	0	7	8	222	244	18	1	0	-16	140	153	29*	1	2	-7	721	729	12	1	4	-14	0	57	56*
0	3	14	131	197	66*	0	7	9	165	156	24	1	0	-14	178	139	18	1	2	-6	538	528	11	1	4	-13	66	86	57*
0	3	15	0	62	72*	0	7	10	118	70	64*	1	0	-12	486	485	12	1	2	-5	861	854	12	1	4	-12	198	202	17
0	4	0	1623	1663	18	0	7	11	36	63	63*	1	0	-10	881	859	15	1	2	-4	338	363	8	1	4	-11	0	58	55*
0	4	1	166	161	10	0	7	12	188	242	31	1	0	-8	830	825	13	1	2	-3	1301	1326	15	1	4	-10	429	443	11

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
1	4	-9	86	81	50*	1	6	-13	107	103	57*	1	8	-11	146	78	29*	1	10	-2	251	214	17	2	1	-16	121	55	32*
1	4	-8	436	457	12	1	6	-12	123	58	64*	1	8	-10	110	135	69*	1	10	-1	259	244	16	2	1	-15	88	120	67*
1	4	-7	59	40	39*	1	6	-11	316	317	18	1	8	-9	97	19	54*	1	10	0	0	44	63*	2	1	-14	86	75	54*
1	4	-6	395	422	10	1	6	-10	214	221	22	1	8	-8	271	259	18	1	10	1	161	175	24	2	1	-13	149	168	30*
1	4	-5	187	182	9	1	6	-9	119	65	62*	1	8	-7	0	5	64*	1	10	2	235	238	19	2	1	-12	310	294	15
1	4	-4	497	505	11	1	6	-8	0	60	62*	1	8	-6	384	386	14	1	10	3	326	345	16	2	1	-11	270	277	16
1	4	-3	37	69	40*	1	6	-7	498	496	13	1	8	-5	172	197	23	1	10	4	123	89	62*	2	1	-10	0	36	57*
1	4	-2	1426	1438	17	1	6	-6	100	40	55*	1	8	-4	42	6	57*	1	10	5	0	46	70*	2	1	-9	348	334	11
1	4	-1	69	63	37*	1	6	-5	394	397	11	1	8	-3	237	218	16	1	10	6	110	5	43*	2	1	-8	170	187	16
1	4	0	126	133	12	1	6	-4	236	251	14	1	8	-2	391	393	12	1	10	7	142	150	34*	2	1	-7	717	766	15
1	4	1	0	16	40*	1	6	-3	759	782	16	1	8	-1	70	10	47*	1	10	8	94	68	50*	2	1	-6	986	972	15
1	4	2	1649	1625	19	1	6	-2	39	39	49*	1	8	0	154	171	21	1	10	9	0	52	68*	2	1	-5	231	238	9
1	4	3	233	243	10	1	6	-1	481	504	12	1	8	1	71	39	57*	1	11	-8	50	147	61*	2	1	-4	266	276	8
1	4	4	995	984	14	1	6	0	56	30	47*	1	8	2	353	340	13	1	11	-7	0	59	62*	2	1	-3	758	769	11
1	4	5	264	284	11	1	6	1	241	206	13	1	8	3	224	177	18	1	11	-6	0	5	64*	2	1	-2	766	759	11
1	4	6	0	170	57*	1	6	2	91	25	32*	1	8	4	187	174	24	1	11	-5	223	185	20	2	1	-1	1363	1358	16
1	4	7	72	29	57*	1	6	3	958	952	18	1	8	5	124	101	38*	1	11	-4	252	245	19	2	1	0	748	748	11
1	4	8	637	613	13	1	6	4	174	175	23	1	8	6	130	211	41*	1	11	-3	158	130	27*	2	1	1	361	371	9
1	4	9	38	92	64*	1	6	5	0	67	65*	1	8	7	0	79	71*	1	11	-2	0	22	63*	2	1	2	540	536	12
1	4	10	217	223	20	1	6	6	0	66	71*	1	8	8	230	284	25	1	11	-1	39	7	60*	2	1	3	715	748	14
1	4	11	0	33	66*	1	6	7	431	452	15	1	8	9	0	34	71*	1	11	0	162	158	24	2	1	4	493	509	12
1	4	12	90	199	70*	1	6	8	74	39	70*	1	8	10	103	63	71*	1	11	1	0	10	62*	2	1	5	402	407	11
1	4	13	114	55	62*	1	6	9	163	182	34*	1	8	11	104	59	72*	1	11	2	133	104	28*	2	1	6	447	425	12
1	4	14	123	116	46*	1	6	10	225	222	27	1	8	12	182	153	24	1	11	3	90	75	54*	2	1	7	667	633	16
1	5	-15	81	104	44*	1	6	11	194	233	32	1	9	-11	152	1	25	1	11	4	130	155	66*	2	1	8	372	385	17
1	5	-14	67	73	66*	1	6	12	0	70	76*	1	9	-10	109	126	68*	1	11	5	113	163	39*	2	1	9	40	103	80*
1	5	-13	0	37	58*	1	6	13	161	153	33*	1	9	-9	236	246	21	1	11	6	0	52	65*	2	1	10	113	133	69*
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4	1	9	139	211	72*	4	3	3	682	667	17	4	5	0	235	228	14	4	7	2	144	115	28*	4	10	-9	219	232	20
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4	1	11	128	123	79*	4	3	5	250	248	18	4	5	2	388	398	12	4	7	4	345	334	16	4	10	-7	215	211	20
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4	1	13	0	175	82*	4	3	7	276	301	21	4	5	4	495	501	12	4	7	6	224	252	25	4	10	-5	100	88	62*
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4	2	-14	66	100	65*	4	3	11	0	29	81*	4	5	8	153	264	78*	4	7	10	118	53	70*	4	10	-1	63	112	60*
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4	10	2	0	51	65*	5	1	-3	731	729	13	5	3	-8	182	180	17	5	5	-9	453	453	12	5	7	-6	0	113	62*
4	10	3	132	177	34*	5	1	-2	571	562	13	5	3	-7	423	415	11	5	5	-8	373	385	12	5	7	-5	270	272	15
4	10	4	0	21	55*	5	1	-1	0	68	44*	5	3	-6	72	29	49*	5	5	-7	494	486	12	5	7	-4	555	536	14
4	10	5	167	156	27	5	1	0	100	108	21*	5	3	-5	428	434	10	5	5	-6	67	126	56*	5	7	-3	420	430	11
4	10	6	57	30	55*	5	1	1	1229	1248	17	5	3	-4	1431	1450	19	5	5	-5	0	81	54*	5	7	-2	0	107	57*
4	10	7	75	79	63*	5	1	2	795	789	15	5	3	-3	667	668	14	5	5	-4	509	524	13	5	7	-1	0	78	59*
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4	11	-6	0	136	64*	5	1	5	219	221	15	5	3	0	48	30	41*	5	5	-1	0	65	53*	5	7	2	370	366	14
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4	11	-2	174	179	22	5	1	9	281	265	17	5	3	4	307	314	14	5	5	3	267	251	17	5	7	6	303	302	18
4	11	-1	65	83	56*	5	1	10	226	224	23	5	3	5	331	316	15	5	5	4	202	167	22	5	7	7	187	212	30
4	11	0	96	111	49*	5	1	11	157	219	36*	5	3	6	403	398	14	5	5	5	143	174	35*	5	7	8	86	24	72*
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5	1	-11	0	145	64*	5	3	-16	105	9	30*	5	4	11	0	9	78*	5	6	11	81	30	52*	5	9	-3	295	276	14
5	1	-10	0	106	60*	5	3	-15	0	40	65*	5	4	12	74	103	70*	5	7	-13	172	202	24	5	9	-2	85	38	49*
5	1	-9	660	635	18	5	3	-14	146	143	31*	5	5	-15	0	27	60*	5	7	-12	254	303	19	5	9	-1	105	69	33*
5	1	-8	199	215	16	5	3	-13	170	146	24	5	5	-14	84	23	64*	5	7	-11	102	75	61*	5	9	0	305	296	14
5	1	-7	647	637	16	5	3	-12	420	410	13	5	5	-13	0	19	62*	5	7	-10	0	13	59*	5	9	1	313	323	15
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5	9	4	0	33	68*	6	1	-11	148	178	27*	6	3	-13	20	31	63*	6	5	-12	91	73	61*	6	7	-7	28	78	60*
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5	9	6	128	105	35*	6	1	-9	522	531	13	6	3	-11	198	170	19	6	5	-10	283	267	15	6	7	-5	184	241	21
5	9	7	123	128	36*	6	1	-8	58	81	57*	6	3	-10	351	339	13	6	5	-9	396	390	13	6	7	-4	54	142	60*
5	9	8	0	5	60*	6	1	-7	439	436	11	6	3	-9	409	403	12	6	5	-8	195	199	19	6	7	-3	0	105	59*
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5	10	-4	90	50	58*	6	1	-1	1048	1056	16	6	3	-3	89	49	27*	6	5	-2	226	195	14	6	7	3	22	101	65*
5	10	-3	0	30	62*	6	1	0	1174	1154	17	6	3	-2	534	523	12	6	5	-1	627	607	14	6	7	4	288	290	18
5	10	-2	0	24	58*	6	1	1	246	232	11	6	3	-1	730	722	15	6	5	0	266	265	15	6	7	5	144	133	34*
5	10	-1	227	214	16	6	1	2	203	223	13	6	3	0	523	534	12	6	5	1	120	156	61*	6	7	6	0	83	68*
5	10	0	64	4	61*	6	1	3	465	462	13	6	3	1	282	288	13	6	5	2	140	73	27*	6	7	7	0	69	71*
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5	10	6	0	2	63*	6	1	9	227	218	19	6	3	7	159	109	31*	6	5	8	208	183	27	6	8	-9	98	74	52*
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6	1	-14	0	168	71*	6	2	12	93	14	65*	6	4	11	114	6	42*	6	7	-10	166	165	24	6	9	3	176	176	25
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6	10	-6	102	7	56*	7	1	5	103	9	57*	7	3	6	259	248	18	7	5	9	110	76	58*	7	8	-2	194	145	18
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6	10	-4	104	13	57*	7	1	7	232	256	18	7	3	8	199	132	24	7	6	-13	85	157	47*	7	8	0	394	418	14
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6	10	2	0	51	63*	7	2	-14	0	12	65*	7	4	-13	0	99	64*	7	6	-7	113	91	61*	7	8	6	133	122	31*
6	10	3	155	176	26*	7	2	-13	237	225	20	7	4	-12	43	6	61*	7	6	-6	0	94	60*	7	8	7	0	77	63*
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6	11	-2	0	107	56*	7	2	-6	0	4	55*	7	4	-5	253	255	13	7	6	1	314	330	15	7	9	-4	0	26	60*
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7	1	-7	572	573	14	7	3	-6	99	84	53*	7	5	-3	247	233	14	7	7	6	61	174	69*	7	11	-1	0	52	54*
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7	1	-3	337	356	10	7	3	-2	542	555	13	7	5	1	539	549	13	7	8	-10	0	139	64*	8	0	-10	127	20	29*
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8	0	2	370	366	11	8	2	9	119	94	33*	8	5	-11	0	12	61*	8	7	0	309	319	16	9	0	-2	222	181	14
8	0	4	209	184	16	8	2	10	82	28	59*	8	5	-10	127	220	66*	8	7	1	220	187	20	9	0	0	521	527	14
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8	0	8	106	140	56*	8	3	-14	0	188	68*	8	5	-8	167	153	23	8	7	3	0	40	66*	9	0	4	312	310	13
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8	2	-2	90	121	56*	8	4	2	489	493	13	8	7	-11	72	79	51*	8	10	-2	49	76	54*	9	2	-1	392	382	12						
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9	3	-10	140	146	30*	9	5	-1	261	241	16	9	8	-2	0	33	61*	10	2	-11	304	296	16	10	4	1	0	10	64*						
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9	3	-3	310	325	13	9	5	6	0	71	67*	9	9	-7	129	148	24*	10	2	-4	0	76	57*	10	5	-12	0	22	56*						
9	3	-2	409	407	12	9	5	7	133	168	32*	9	9	-6	0	87	58*	10	2	-3	479	488	12	10	5	-11	39	53	59*						
9	3	-1	196	180	18	9	6	-12	0	102	50*	9	9	-5	86	70	56*	10	2	-2	57	61	56*	10	5	-10	154	163	25.						
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9	3	4	0	75	65*	9	6	-7	83	31	58*	9	9	0	104	36	31*	10	2	3	394	385	13	10	5	-5	157	163	23						
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9	3	8	121	153	30*	9	6	-3	112	133	59*	10	0	-12	38	89	64*	10	2	7	105	195	59*	10	5	-1	131	152	31*						
9	3	9	0	15	55*	9	6	-2	0	16	61*	10	0	-10	82	145	65*	10	2	8	47	19	51*	10	5	0	226	186	18						
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9	4	-11	148	32	25*	9	6	2	0	6	66*	10	0	-2	446	431	11	10	3	-10	165	197	26	10	5	4	0	115	64*						
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9	4	-7	111	88	58*	9	6	6	98	81	41*	10	0	6	142	124	21	10	3	-6	0	78	59*	10	6	-10	94	40	58*						
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9	4	-3	0	37	57*	9	7	-9	0	5	57*	10	1	-12	113	98	61*	10	3	-2	102	4	56*	10	6	-6	0	126	61*						
9	4	-2	109	48	58*	9	7	-8	141	87	24*	10	1	-11	73	18	47*	10	3	-1	215	212	18	10	6	-5	113	138	31*						
9	4	-1	59	106	60*	9	7	-7	95	90	51*	10	1	-10	163	142	25	10	3	0	284	285	15	10	6	-4	144	117	24						
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9	4	1	149	119	26*	9	7	-5	73	46	46*	10	1	-8	254	253	16	10	3	2	200	165	19	10	6	-2	64	52	60*						
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9	4	6	203	184	22	9	7	0	0	48	64*	10	1	-3	345	325	12	10	3	7	33	31	58*	10	6	3	222	230	19						
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9	4	8	116	121	62*	9	7	2	176	177	25	10	1	-1	238	210	15	10	4	-12	26	84	61*	10	6	5	102	9	57*						
9	5	-13	0	46	58*	9	7	3	0	89	65*	10	1	0	365	376	12	10	4	-11	62	87	63*	10	7	-10	49	94	55*						
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9	5	-10	69	9	51*	9	7	6	116	89	29*	10	1	3	0	106	58*	10	4	-8	275	246	15	10	7	-7	0	38	63*						
9	5	-9	0	115	66*	9	8	-10	123	100	23*	10	1	4	240	250	17	10	4	-7	0	36	63*	10	7	-6	59	23	56*						
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10	7	-2	130	46	27*	11	2	-9	219	210	19	11	5	-9	87	5	50*	12	1	-8	217	195	18	12	4	0	0	129	51*						
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10	7	4	155	106	20	11	2	-3	253	255	16	11	5	-3	95	65	38*	12	1	-2	0	66	58*	12	5	-7	45	81	55*						
10	8	-8	0	99	57*	11	2	-2	0	44	61*	11	5	-2	30	154	61*	12	1	-1	0	48	61*	12	5	-6	0	8	58*						
10	8	-7	0	2	56*	11	2	-1	0	125	61*	11	5	-1	208	207	20	12	1	0	192	187	19	12	5	-5	82	88	58*						
10	8	-6	156	175	21	11	2	0	0	22	59*	11	5	0	54	28	61*	12	1	1	140	152	25*	12	5	-4	149	164	23						
10	8	-5	29	9	57*	11	2	1	377	405	13	11	5	1	109	90	33*	12	1	2	0	150	51*	12	5	-3	184	218	21						
10	8	-4	90	44	56*	11	2	2	0	16	61*	11	5	2	19	146	65*	12	1	3	0	7	55*	12	5	-2	118	74	29*						
10	8	-3	0	75	55*	11	2	3	144	45	22	11	5	3	138	162	28*	12	1	4	96	88	52*	12	5	-1	63	35	49*						
10	8	-2	213	266	18	11	2	4	58	20	47*	11	5	4	70	131	60*	12	2	-11	164	205	23	12	5	0	0	78	60*						
10	8	-1	34	36	60*	11	2	5	193	201	18	11	6	-10	68	12	44*	12	2	-10	39	20	58*	12	5	1	56	130	57*						
10	8	0	76	97	49*	11	2	6	0	29	55*	11	6	-9	99	153	57*	12	2	-9	175	158	20	12	5	2	0	82	55*						
10	8	1	67	23	48*	11	3	-12	135	188	28*	11	6	-8	0	39	61*	12	2	-8	0	20	61*	12	6	-7	125	129	23*						
10	8	2	108	130	56*	11	3	-11	0	143	60*	11	6	-7	70	114	46*	12	2	-7	54	130	61*	12	6	-6	93	81	53*						
10	9	-4	73	65	50*	11	3	-10	0	151	63*	11	6	-6	102	11	55*	12	2	-6	0	48	56*	12	6	-5	109	136	57*						
10	9	-3	93	135	53*	11	3	-9	0	6	62*	11	6	-5	183	214	20	12	2	-5	207	210	18	12	6	-4	0	49	56*						
10	9	-2	0	7	54*	11	3	-8	93	50	50*	11	6	-4	0	52	59*	12	2	-4	0	31	59*	12	6	-3	98	131	32*						
11	0	-12	0	132	63*	11	3	-7	94	216	65*	11	6	-3	94	163	52*	12	2	-3	177	179	20	12	6	-2	78	42	38*						
11	0	-10	57	121	49*	11	3	-6	174	190	22	11	6	-2	76	20	41*	12	2	-2	88	23	58*	12	6	-1	114	157	28*						
11	0	-8	212	239	20	11	3	-5	73	105	59*	11	6	-1	0	109	53*	12	2	-1	286	312	15	12	6	0	12	1	56*						
11	0	-6	113	130	61*	11	3	-4	158	91	21	11	6	0	0	44	62*	12	2	0	66	35	59*	13	0	-10	46	20	57*						
11	0	-4	332	333	13	11	3	-3	89	128	61*	11	6	1	136	206	29*	12	2	1	124	75	27*	13	0	-8	158	155	22						
11	0	-2	59	156	61*	11	3	-2	269	269	15	11	6	2	0	15	61*	12	2	2	79	41	47*	13	0	-6	0	2	57*						
11	0	0	307	307	14	11	3	-1	211	208	19	11	6	3	54	15	57*	12	2	3	195	215	17	13	0	-4	182	173	19						
11	0	2	183	149	18	11	3	0	122	132	62*	11	7	-8	105	23	27*	12	2	4	0	31	54*	13	0	-2	151	163	23						
11	0	4	131	156	25*	11	3	1	0	82	62*	11	7	-7	102	67	57*	12	3	-11	85	3	56*	13	0	0	155	132	20						
11	0	6	100	211	31*	11	3	2	87	158	64*	11	7	-6	132	158	26*	12	3	-10	0	87	61*	13	0	2	0	127	54*						
11	1	-13	81	43	49*	11	3	3	116	160	64*	11	7	-5	0	38	57*	12	3	-9	105	148	35*	13	1	-10	0	107	58*						
11	1	-12	139	170	30*	11	3	4	86	121	58*	11	7	-4	0	11	54*	12	3	-8	210	177	18	13	1	-9	0	24	55*						
11	1	-11	118	122	62*	11	3	5	117	38	27*	11	7	-3	111	95	57*	12	3	-7	112	43	57*	13	1	-8	0	4	57*						
11	1	-10	169	162	24	11	3	6	0	61	55*	11	7	-2	127	146	27*	12	3	-6	0	38	58*	13	1	-7	177	154	18						
11	1	-9	0	24	64*	11	4	-12	111	96	56*	11	7	-1	147	120	22	12	3	-5	0	99	60*	13	1	-6	154	175	22						
11	1	-8	0	61	62*	11	4	-11	0	43	59*	11	7	0	0	81	61*	12	3	-4	197	207	19	13	1	-5	112	164	58*						
11	1	-7	321	314	13	11	4	-10	0	122	63*	11	7	1	0	5	56*	12	3	-3	74	153	58*	13	1	-4	76	56	49*						
11	1	-6	313	317	14	11	4	-9	0	15	60*	11	8	-5	45	39	49*	12	3	-2	47	40	62*	13	1	-3	85	3	55*						
11	1	-5	205	200	18	11	4	-8	233	239	18	11	8	-4	0	165	55*	12	3	-1	0	42	62*	13	1	-2	82	156	58*						
11	1	-4	74	27	49*	11	4	-7	70	57	41*	11	8	-3	67	18	51*	12	3	0	113	143	33*	13	1	-1	99	137	57*						
11	1	-3	61	94	57*	11	4	-6	24	113	58*	11	8	-2	0	32	55*	12	3	1	94	131	60*	13	1	0	48	113	56*						
11	1	-2	295	308	14	11	4	-5	103	35	58*	12	0	-12	53	13	58*	12	3	2	91	164	51*	13	1	1	96	23	28*						
11	1	-1	251	242	15	11	4	-4	325	344	13	12	0	-10	0	144	63*	12	3	3	0	11	55*	13	1	2	72	73	36*						
11	1	0	207	198	17	11	4	-3	93	45	50*	12	0	-8	117	172	63*	12	3	4	87	49	44*	13	2	-9	81	118	57*						
11	1	1	172	130	19	11	4	-2	146	145	26*	12	0	-6	231	264	18	12	4	-10	142	167	23	13	2	-8	105	26	59*						
11	1	2	198	200	19	11	4	-1	0	60	59*	12	0	-4	144	141	24*	12	4	-9	76	34	57*	13	2	-7	140	199	25*						
11	1	3	206	211	18	11	4	0	263	260	17	12	0	-2	254	244	15	12	4	-8	69	73	43*	13	2	-6	99	19	55*						
11	1	4	132	141	25*	11	4	1	0	28	61*	12	0	0	178	179	20	12	4	-7	105	2	58*	13	2	-5	89	106	49*						
11	1	5	81	70	36*	11	4	2	140	141	27*	12	0	2	111	123	56*	12	4	-6	164	210	22	13	2	-4	0	55	57*						
11	1	6	74	75	40*	11	4	3	49	7	42*	12	0	4	142	170	20	12	4	-5	104	24	31*	13	2	-3	158	189	21						
11	2	-13	149	191	24	11	4	4	57	105	59*	12	1	-12	59	104	58*	12	4	-4	100	60	57*	13	2	-2	63	26	58*						

13	2	-1	0	24	54*
13	2	0	73	17	56*
13	2	1	220	231	15
13	2	2	0	15	53*
13	3	-9	0	18	55*
13	3	-8	46	55	55*
13	3	-7	88	102	55*
13	3	-6	0	145	61*
13	3	-5	0	84	56*
13	3	-4	0	28	57*
13	3	-3	0	26	57*
13	3	-2	116	117	59*
13	3	-1	97	108	56*
13	3	0	86	110	36*
13	3	1	0	5	53*
13	4	-8	67	162	55*
13	4	-7	0	32	54*
13	4	-6	78	14	41*
13	4	-5	56	28	56*
13	4	-4	185	181	17
13	4	-3	83	22	36*
13	4	-2	0	123	57*
13	4	-1	0	17	55*
13	4	0	0	122	54*
13	5	-5	98	161	53*
13	5	-4	0	51	54*
13	5	-3	0	3	52*
14	0	-6	102	145	28*
14	0	-4	54	106	53*
14	0	-2	148	122	18
14	1	-6	0	53	51*
14	1	-5	0	56	53*
14	1	-4	15	133	54*
14	1	-3	184	159	15
14	1	-2	0	67	53*
14	2	-5	153	158	17
14	2	-4	0	20	53*

B. $[Me_2Sn(S_2CNCy_2)Cl]$

Crystallographic Data and Refinement details for $[Me_2Sn(S_2CNCy_2)Cl]$.

Formula	$C_{15}H_{28}ClNS_2Sn$
Formula weight	440.7
Crystal morphology	colourless rod
Crystal dimensions (mm)	0.04 x 0.05 x 0.32
Crystal system	monoclinic
Space group	$P2_1/c$ (C_{2h}^5, No. 14)
Temperature (°C)	20.0
a (Å)	6.758(6)
b (Å)	19.046(7)
c (Å)	15.190(5)
β (°)	98.09(4)
V (Å^3)	1930(2)
Z	4
D_{calc} (g cm^{-3})	1.512
$F(000)$	896
Radiation	MoKα (λ = 0.7107Å)
μ (cm^{-1})	16.65
θ limits, data (°)	3.0 to 27.5
hkl range	0 to 9, 0 to 25, -20 to 20
Range of transmission factors	0.977 to 1.000
Scan technique	ω:2θ
Scan width (°)	1.05
No. of data measured	4996
No. of unique data	4622
R_{amal}	0.044
Program for structure solution	Direct Methods (SHELXS86)
No. of unique data used	1881
No. of parameters	176
R	0.038
R_w	0.033
G.O.F.	2.09
Min./Max. residual electron density (e Å^{-3})	-1.20 to +0.46

Fractional atomic coordinates and B_{eq} values ($Å^2$) for the hydrogen atoms in $[Me_2Sn(S_2CNCy_2)Cl]$.

Atom	*x*	*y*	*z*
Sn	0.11256(7)	0.24749(3)	0.09591(3)
Cl(1)	0.2257(4)	0.1336(1)	0.1620(2)
S(1)	0.3370(3)	0.30488(10)	0.2165(1)
S(2)	0.1000(3)	0.3883(1)	0.0784(1)
N(1)	0.3756(8)	0.4450(3)	0.2019(4)
C(1)	0.228(1)	0.2317(4)	-0.0248(5)
C(2)	-0.190(1)	0.2380(4)	0.1129(5)
C(3)	0.281(1)	0.3868(4)	0.1698(5)
C(4)	0.537(1)	0.4481(4)	0.2794(5)
C(5)	0.472(1)	0.4283(4)	0.3668(6)
C(6)	0.640(1)	0.4399(4)	0.4426(5)
C(7)	0.828(1)	0.4008(5)	0.4260(5)
C(8)	0.893(1)	0.4220(4)	0.3381(6)
C(9)	0.725(1)	0.4116(4)	0.2617(5)
C(10)	0.323(1)	0.5146(4)	0.1581(5)
C(11)	0.496(1)	0.5465(4)	0.1190(6)
C(12)	0.427(1)	0.6120(5)	0.0680(6)
C(13)	0.331(2)	0.6640(4)	0.1237(7)
C(14)	0.162(1)	0.6307(4)	0.1643(6)
C(15)	0.228(1)	0.5643(4)	0.2169(6)

Anisotropic thermal parameters ($Å^2$) for the non-hydrogen atoms in $[Me_2Sn(S_2CNCy_2)Cl]$.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Sn	0.0424(2)	0.0439(2)	0.0441(3)	-0.0023(4)	0.0076(2)	-0.0066(4)
Cl(1)	0.087(2)	0.052(1)	0.101(2)	0.008(1)	-0.013(2)	0.007(1)
S(1)	0.057(1)	0.045(1)	0.047(1)	-0.0004(10)	-0.004(1)	0.0005(10)
S(2)	0.060(1)	0.051(1)	0.043(1)	-0.001(1)	-0.008(1)	-0.0013(10)
N(1)	0.036(4)	0.043(3)	0.038(4)	0.003(3)	0.007(3)	0.000(3)
C(1)	0.058(5)	0.078(7)	0.069(6)	-0.018(4)	0.021(5)	-0.019(5)
C(2)*	0.051(5)	0.065(6)	0.067(5)	-0.008(4)	0.010(4)	0.001(5)
C(3)	0.037(5)	0.047(4)	0.028(4)	0.005(4)	0.010(3)	-0.002(4)
C(4)	0.036(5)	0.067(5)	0.035(5)	0.003(4)	0.012(4)	-0.005(4)
C(5)	0.041(5)	0.066(5)	0.043(5)	0.012(4)	0.012(4)	-0.002(5)
C(6)	0.054(5)	0.071(6)	0.037(5)	0.006(5)	0.007(4)	-0.001(4)
C(7)	0.055(6)	0.084(7)	0.050(6)	0.011(5)	-0.009(4)	0.009(5)
C(8)	0.044(5)	0.071(6)	0.066(7)	0.001(4)	0.004(5)	-0.002(5)
C(9)	0.045(5)	0.064(6)	0.039(5)	-0.002(4)	0.008(4)	-0.002(4)
C(10)	0.051(5)	0.042(4)	0.036(5)	-0.004(4)	0.003(4)	0.001(4)
C(11)	0.057(6)	0.066(6)	0.050(6)	-0.002(5)	0.019(5)	0.008(5)
C(12)	0.085(7)	0.068(6)	0.070(7)	-0.016(5)	0.015(6)	0.024(6)
C(13)	0.118(9)	0.048(5)	0.076(8)	0.000(5)	0.007(7)	0.017(5)
C(14)	0.093(8)	0.060(5)	0.055(6)	0.024(5)	0.009(5)	-0.001(5)
C(15)	0.067(7)	0.061(6)	0.045(6)	0.018(5)	0.021(5)	0.005(5)

* the disordered carbon atoms are refined istropically

Fractional atomic coordinates ($Å^2$) for the non-hydrogen atoms in $[Me_2Sn(S_2CNCy_2)Cl]$.

Atom	x	y	z	B_{eq}
H(1a)	0.1673	0.1902	0.0543	6.3584
H(1b)	0.1978	0.2723	-0.0629	6.3584
H(1c)	0.3715	0.2254	-0.0126	6.3584
H(4a)	-0.2616	0.2798	0.0903	5.7678
H(5a)	-0.2470	0.1972	0.0807	5.7678
H(5b)	-0.1997	0.2327	0.1756	5.7678
H(6a)	0.5728	0.4974	0.2854	4.2811
H(6b)	0.3587	0.4569	0.3765	4.7002
H(7a)	0.4343	0.3792	0.3651	4.7002
H(7b)	0.6694	0.4897	0.4479	5.1055
H(8a)	0.5986	0.4229	0.4974	5.1055
H(8b)	0.9344	0.4113	0.4738	6.1358
H(9a)	0.8005	0.3507	0.4249	6.1358
H(9b)	0.9313	0.4711	0.3410	5.7548
H(10a)	1.0064	0.3935	0.3278	5.7548
H(11a)	0.6982	0.3618	0.2540	4.6602
H(11b)	0.7657	0.4305	0.2078	4.6602
H(12a)	0.2211	0.5047	0.1080	4.0982
H(12b)	0.6025	0.5583	0.1665	5.3628
H(13a)	0.5457	0.5130	0.0792	5.3628
H(13b)	0.5412	0.6341	0.0474	7.0138
H(14a)	0.3303	0.5989	0.0173	7.0138
H(14b)	0.4309	0.6811	0.1710	7.7153
H(15a)	0.2789	0.7031	0.0865	7.7153
H(15b)	0.1128	0.6643	0.2040	6.5932
	0.0557	0.6187	0.1170	6.5932
	0.1130	0.5420	0.2365	5.3224
	0.3243	0.5764	0.2682	5.3224

* Some H atoms were not included as these were on disordered carbon atoms.

Bond distances (Å) for $[Me_2Sn(S_2CNCy_2)Cl]$.

Atom - Atom	Distance	Atom - Atom	Distance
Sn - Cl(1)	2.467(4)	C(4) - C(9)	1.49(2)
Sn - S(1)	2.463(2)	C(5) - C(6)	1.52(2)
Sn - S(2)	2.696(2)	C(6) - C(7)	1.53(2)
Sn - C(1)	2.112(8)	C(7) - C(8)	1.51(2)
Sn - C(2)	2.102(8)	C(8) - C(9)	1.53(2)
S(1) - C(3)	1.734(7)	C(10) - C(11)	1.54(2)
S(2) - C(3)	1.716(7)	C(10) - C(15)	1.49(2)
N(1) - C(3)	1.336(8)	C(11) - C(12)	1.51(2)
N(1) - C(4)	1.49(1)	C(12) - C(13)	1.49(2)
N(1) - C(10)	1.50(1)	C(13) - C(14)	1.50(2)
C(4) - C(5)	1.52(2)	C(14) - C(15)	1.53(2)

Bond angles (°) for $[Me_2Sn(S_2CNCy_2)Cl]$.

Atom - Atom - Atom	Angle	Atom - Atom - Atom	Angle
Cl(1) - Sn - S(1)	87.96(8)	S(2) - C(3) - N(1)	122.1(5)
Cl(1) - Sn - S(2)	156.80(7)	N(1) - C(4) - C(5)	112(1)
Cl(1) - Sn - C(1)	95.6(2)	N(1) - C(4) - C(9)	114(1)
Cl(1) - Sn - C(2)	97.2(2)	C(5) - C(4) - C(9)	114(1)
S(1) - Sn - S(2)	68.87(6)	C(4) - C(5) - C(6)	110(1)
S(1) - Sn - C(1)	116.4(2)	C(5) - C(6) - C(7)	112(1)
S(1) - Sn - C(2)	117.0(2)	C(6) - C(7) - C(8)	110(1)
S(2) - Sn - C(1)	93.8(2)	C(7) - C(8) - C(9)	112(1)
S(2) - Sn - C(2)	94.6(2)	C(4) - C(9) - C(8)	109(1)
C(1) - Sn - C(2)	125.3(3)	N(1) - C(10) - C(11)	112(1)
Sn - S(1) - C(3)	91.1(3)	N(1) - C(10) - C(15)	113(1)
Sn - S(2) - C(3)	83.9(2)	C(11) - C(10) - C(15)	113(1)
C(3) - N(1) - C(4)	126(1)	C(10) - C(11) - C(12)	109(1)
C(3) - N(1) - C(10)	119.5(9)	C(11) - C(12) - C(13)	113(1)
C(4) - N(1) - C(10)	114.7(9)	C(12) - C(13) - C(14)	111(1)
S(1) - C(3) - S(2)	115.9(4)	C(13) - C(14) - C(15)	111(1)
S(1) - C(3) - N(1)	122.0(5)	C(10) - C(15) - C(14)	110(1)

Observed and calculated structure factors for $[Me_2Sn(S_2CNCy_2)Cl]$.

h	k	l	Fo	Fc	sigF
0	0	4	1905	1845	14
0	0	6	1406	1389	13
0	0	8	259	265	12
0	0	10	887	818	16
0	0	12	502	495	12
0	0	14	139	14	31*
0	0	16	520	504	14
0	0	18	59	42	70*
0	1	3	285	288	7
0	1	5	0	67	43*
0	1	7	444	429	11
0	1	8	1550	1513	15
0	1	9	69	126	53*
0	1	10	365	369	12
0	1	11	86	142	63*
0	1	12	532	514	13
0	1	13	0	35	65*
0	1	14	523	517	13
0	1	15	69	81	69*
0	1	16	0	40	72*
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3	12	-13	0	77	76*	3	13	11	0	109	84*	3	15	8	164	109	87*	3	17	9	146	125	82*	3	20	-2	117	154	59*
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3	20	0	117	62	78*	4	0	8	510	530	15	4	2	-3	0	103	54*	4	4	-17	57	40	65*	4	5	4	434	418	13
3	20	1	106	62	62*	4	0	10	593	609	15	4	2	-2	208	208	19	4	4	-16	155	185	32*	4	5	5	314	304	18
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4	17	-10	0	141	82*	4	19	5	0	101	89*	5	1	-10	358	420	17	5	2	13	51	44	65*	5	4	4	476	466	13
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5	17	-8	261	288	31	6	0	-4	130	178	42*	6	2	1	0	20	66*	6	4	-1	132	132	38*	6	6	-1	117	38	69*
5	17	-7	118	48	81*	6	0	-2	679	690	17	6	2	2	242	264	21	6	4	0	99	39	66*	6	6	0	349	345	17
5	17	-6	153	76	77*	6	0	0	249	229	21	6	2	3	13	38	66*	6	4	1	119	164	73*	6	6	1	244	267	22
5	17	-5	32	18	80*	6	0	2	261	288	21	6	2	4	505	556	14	6	4	2	308	316	18	6	6	2	410	440	15

5	17	-4	244	179	27	6	0	4	539	565	14	6	2	5	133	44	68*	6	4	3	47	111	70*	6	6	3	196	162	25
5	17	-3	55	17	83*	6	0	6	117	8	59*	6	2	6	45	86	74*	6	4	4	291	307	19	6	6	4	306	351	20
5	17	-2	0	153	85*	6	0	8	286	314	22	6	2	7	33	68	50*	6	4	5	173	17	26	6	6	5	105	65	46*
5	17	-1	144	45	81*	6	0	10	152	189	77*	6	2	8	294	349	19	6	4	6	130	105	68*	6	6	6	58	34	70*
5	17	0	108	113	77*	6	0	12	87	45	69*	6	2	9	30	96	50*	6	4	7	0	86	75*	6	6	7	153	64	30*
5	17	1	26	89	87*	6	1	-16	0	122	69*	6	2	10	21	115	60*	6	4	8	290	315	19	6	6	8	229	304	24
5	17	2	228	188	31	6	1	-15	118	30	35*	6	2	11	0	40	82*	6	4	9	0	26	71*	6	6	9	164	133	30*
5	17	3	0	61	82*	6	1	-14	158	194	28*	6	2	12	39	124	53*	6	4	10	80	126	59*	6	6	10	182	201	28
5	17	4	0	161	87*	6	1	-13	0	26	67*	6	3	-16	134	129	26*	6	4	11	113	18	65*	6	6	11	84	96	70*
5	17	5	0	5	85*	6	1	-12	0	59	69*	6	3	-15	0	25	64*	6	4	12	172	191	26	6	7	-15	0	15	61*
5	17	6	11	219	90*	6	1	-11	0	58	66*	6	3	-14	182	203	23	6	5	-15	100	25	59*	6	7	-14	119	182	35*
5	17	7	0	28	78*	6	1	-10	458	471	14	6	3	-13	78	5	48*	6	5	-14	117	161	63*	6	7	-13	110	50	60*
5	18	-9	0	21	88*	6	1	-9	0	22	71*	6	3	-12	109	39	64*	6	5	-13	0	67	64*	6	7	-12	83	74	53*
5	18	-8	84	106	77*	6	1	-8	0	152	75*	6	3	-11	0	23	68*	6	5	-12	93	51	55*	6	7	-11	139	35	30*
5	18	-7	0	34	68*	6	1	-7	0	64	70*	6	3	-10	294	355	20	6	5	-11	0	1	49*	6	7	-10	351	397	16
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5	18	-5	149	83	79*	6	1	-5	190	164	28	6	3	-8	176	215	29	6	5	-9	0	3	69*	6	7	-8	227	242	22
5	18	-4	0	63	86*	6	1	-4	710	680	18	6	3	-7	0	75	74*	6	5	-8	269	264	19	6	7	-7	0	81	60*
5	18	-3	0	22	90*	6	1	-3	257	284	23	6	3	-6	227	234	24	6	5	-7	38	162	55*	6	7	-6	309	359	19
5	18	-2	156	146	81*	6	1	-2	160	29	30*	6	3	-5	0	139	74*	6	5	-6	239	246	22	6	7	-5	93	1	73*
5	18	-1	43	19	68*	6	1	-1	110	18	72*	6	3	-4	420	402	15	6	5	-5	0	26	68*	6	7	-4	471	461	14
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5	18	1	0	14	86*	6	1	1	151	80	29*	6	3	-2	54	32	72*	6	5	-3	0	110	75*	6	7	-2	0	133	71*
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5	18	3	163	14	41*	6	1	3	117	73	62*	6	3	0	489	501	14	6	5	-1	227	239	24	6	7	0	503	536	14
5	18	4	212	115	34	6	1	4	137	135	37*	6	3	1	0	69	70*	6	5	0	384	407	17	6	7	1	183	190	27
5	18	5	113	17	83*	6	1	5	137	34	69*	6	3	2	64	45	67*	6	5	1	73	65	70*	6	7	2	422	392	14
5	19	-7	118	68	80*	6	1	6	580	593	14	6	3	3	114	108	57*	6	5	2	311	343	18	6	7	3	60	56	60*
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5	19	-4	193	132	35*	6	1	9	73	36	69*	6	3	6	339	401	18	6	5	5	64	14	57*	6	7	6	254	314	23
5	19	-3	106	10	81*	6	1	10	0	92	74*	6	3	7	0	30	74*	6	5	6	310	367	19	6	7	7	104	91	67*
5	19	-2	243	210	32	6	1	11	124	157	41*	6	3	8	59	6	66*	6	5	7	177	188	29	6	7	8	266	274	20
5	19	-1	52	76	79*	6	1	12	185	230	27	6	3	9	74	40	59*	6	5	8	116	86	43*	6	7	9	134	143	74*
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6	8	-14	0	120	62*	6	10	-8	254	290	22	6	12	1	82	113	71*	6	15	0	262	287	24	7	1	-4	264	227	23
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6	8	-8	316	360	19	6	10	-2	211	231	25	6	12	7	0	38	65*	6	15	6	165	265	35*	7	1	2	155	205	35*
6	8	-7	133	32	36*	6	10	-1	94	20	57*	6	12	8	137	231	38*	6	16	-8	174	186	32*	7	1	3	82	32	58*
6	8	-6	379	354	16	6	10	0	176	193	31*	6	13	-11	93	55	64*	6	16	-7	0	7	73*	7	1	4	367	384	18
6	8	-5	136	61	34*	6	10	1	0	60	69*	6	13	-10	235	269	23	6	16	-6	112	223	77*	7	1	5	0	116	74*
6	8	-4	202	178	26	6	10	2	279	303	21	6	13	-9	195	105	25	6	16	-5	0	30	80*	7	1	6	211	217	24
6	8	-3	0	8	73*	6	10	3	0	21	68*	6	13	-8	145	159	34*	6	16	-4	66	68	76*	7	1	7	114	70	68*
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6	8	-1	55	15	69*	6	10	5	0	107	73*	6	13	-6	147	175	38*	6	16	-2	250	291	25	7	1	9	0	186	70*
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6	8	1	87	24	69*	6	10	7	0	11	68*	6	13	-4	333	341	20	6	16	0	111	77	76*	7	2	-12	110	153	63*
6	8	2	363	399	17	6	10	8	273	275	20	6	13	-3	140	158	39*	6	16	1	80	29	74*	7	2	-11	0	4	67*
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6	8	7	0	4	72*	6	11	-11	60	130	72*	6	13	2	181	194	31*	6	17	-5	126	17	78*	7	2	-6	225	134	22
6	8	8	269	289	19	6	11	-10	0	167	74*	6	13	3	160	86	30*	6	17	-4	205	192	32	7	2	-5	81	121	56*
6	8	9	0	83	71*	6	11	-9	0	67	73*	6	13	4	60	109	70*	6	17	-3	91	57	61*	7	2	-4	377	349	17
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6	9	-11	89	29	69*	6	11	-4	288	302	21	6	14	-10	102	3	57*	6	17	2	87	149	80*	7	2	1	0	26	69*
6	9	-10	226	265	22	6	11	-3	0	71	73*	6	14	-9	0	68	70*	6	17	3	0	4	78*	7	2	2	334	344	18
6	9	-9	83	73	71*	6	11	-2	0	23	73*	6	14	-8	221	244	24	6	18	-3	0	40	83*	7	2	3	0	37	71*
6	9	-8	0	214	73*	6	11	-1	97	96	50*	6	14	-7	0	36	76*	6	18	-2	184	190	36*	7	2	4	153	162	32*
6	9	-7	111	37	57*	6	11	0	295	303	19	6	14	-6	244	251	23	6	18	-1	98	46	75*	7	2	5	24	15	56*
6	9	-6	333	340	18	6	11	1	130	6	68*	6	14	-5	0	77	62*	7	0	-14	125	150	63*	7	2	6	189	222	27
6	9	-5	105	92	70*	6	11	2	209	219	25	6	14	-4	0	71	75*	7	0	-12	103	78	70*	7	2	7	72	9	57*
6	9	-4	149	224	77*	6	11	3	76	66	50*	6	14	-3	223	159	23	7	0	-10	82	114	70*	7	2	8	208	219	25
6	9	-3	0	77	69*	6	11	4	228	233	22	6	14	-2	389	449	18	7	0	-8	288	282	21	7	2	9	0	112	71*
6	9	-2	127	138	70*	6	11	5	0	94	73*	6	14	-1	95	183	62*	7	0	-6	0	164	78*	7	3	-13	0	25	64*
6	9	-1	105	156	69*	6	11	6	210	241	25	6	14	0	179	154	30*	7	0	-4	322	326	22	7	3	-12	160	132	24
6	9	0	307	364	20	6	11	7	139	126	75*	6	14	1	0	9	70*	7	0	-2	396	386	17	7	3	-11	175	76	23
6	9	1	26	28	71*	6	11	8	143	43	32*	6	14	2	196	250	28	7	0	0	0	62	72*	7	3	-10	120	164	66*
6	9	2	375	387	17	6	11	9	0	2	70*	6	14	3	0	37	77*	7	0	2	436	449	15	7	3	-9	132	35	36*
6	9	3	118	107	42*	6	12	-12	190	176	23	6	14	4	282	282	21	7	0	4	242	254	22	7	3	-8	69	52	69*
6	9	4	232	256	23	6	12	-11	153	101	29*	6	14	5	133	112	70*	7	0	6	203	240	27	7	3	-7	0	29	72*
6	9	5	76	108	71*	6	12	-10	126	55	71*	6	14	6	80	48	72*	7	0	8	0	192	76*	7	3	-6	200	202	28
6	9	6	276	319	21	6	12	-9	88	56	69*	6	14	7	110	21	70*	7	1	-14	72	80	60*	7	3	-5	0	20	77*
6	9	7	42	186	52*	6	12	-8	110	202	49*	6	15	-9	71	41	62*	7	1	-13	56	25	67*	7	3	-4	219	220	27
6	9	8	88	127	70*	6	12	-7	0	26	74*	6	15	-8	0	112	76*	7	1	-12	165	190	27	7	3	-3	11	123	52*
6	9	9	115	34	68*	6	12	-6	217	231	26	6	15	-7	126	25	73*	7	1	-11	148	6	27*	7	3	-2	103	201	78*
6	9	10	215	253	23	6	12	-5	114	86	61*	6	15	-6	0	148	74*	7	1	-10	207	228	25	7	3	-1	131	86	68*
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7	4	-3	185	152	28	7	6	7	0	184	74*	7	9	1	0	30	69*	7	13	-8	0	4	69*	8	2	-1	95	23	71*
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7	4	-1	0	144	76*	7	7	-12	108	154	65*	7	9	3	0	22	66*	7	13	-6	205	204	24	8	2	1	0	17	70*
7	4	0	0	25	69*	7	7	-11	0	15	64*	7	9	4	181	227	29	7	13	-5	96	23	57*	8	2	2	98	207	74*
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7	4	4	60	123	51*	7	7	-7	133	30	35*	7	10	-11	0	11	62*	7	13	-1	0	72	73*	8	3	-10	88	49	66*
7	4	5	126	21	68*	7	7	-6	289	287	20	7	10	-10	63	75	55*	7	13	0	176	242	31*	8	3	-9	102	12	47*
7	4	6	197	200	24	7	7	-5	104	52	71*	7	10	-9	105	36	65*	7	13	1	80	57	68*	8	3	-8	113	122	70*
7	4	7	121	19	62*	7	7	-4	283	278	20	7	10	-8	128	233	68*	7	13	2	0	65	67*	8	3	-7	160	40	32*
7	4	8	191	232	25	7	7	-3	185	138	28	7	10	-7	0	26	67*	7	13	3	95	118	57*	8	3	-6	178	154	29
7	4	9	0	9	69*	7	7	-2	220	195	24	7	10	-6	47	34	68*	7	14	-6	97	82	56*	8	3	-5	179	87	27
7	5	-13	61	9	63*	7	7	-1	116	19	41*	7	10	-5	82	8	68*	7	14	-5	122	140	69*	8	3	-4	0	70	73*
7	5	-12	0	84	63*	7	7	0	370	398	17	7	10	-4	110	134	75*	7	14	-4	163	221	33*	8	3	-3	134	42	42*
7	5	-11	0	20	54*	7	7	1	73	60	67*	7	10	-3	82	30	68*	7	14	-3	91	69	70*	8	3	-2	159	157	34*
7	5	-10	119	253	75*	7	7	2	152	138	32*	7	10	-2	262	247	20	7	14	-2	0	200	75*	8	3	-1	20	37	70*
7	5	-9	0	62	72*	7	7	3	0	39	68*	7	10	-1	0	18	72*	7	14	-1	107	19	56*	8	3	0	186	116	28

7	5	-8	0	5	71*	7	7	4	52	191	72*	7	10	0	100	5	66*	7	14	0	41	67	66*	8	3	1	0	20	71*				
7	5	-7	0	49	72*	7	7	5	73	76	57*	7	10	1	0	58	70*	7	14	1	0	75	72*	8	3	2	147	151	33*				
7	5	-6	305	309	19	7	7	6	285	340	18	7	10	2	250	290	22	7	14	2	146	187	33*	8	3	3	103	10	69*				
7	5	-5	69	29	71*	7	7	7	114	109	67*	7	10	3	59	56	69*	7	15	-2	123	107	68*	8	3	4	128	146	70*				
7	5	-4	91	108	71*	7	7	8	0	10	66*	7	10	4	0	84	70*	8	0	-10	95	158	69*	8	3	5	112	52	36*				
7	5	-3	157	119	34*	7	8	-12	0	131	65*	7	10	5	117	83	35*	8	0	-8	143	171	39*	8	4	-10	161	138	26				
7	5	-2	214	196	25	7	8	-11	52	38	52*	7	10	6	142	149	30*	8	0	-6	198	148	28	8	4	-9	113	50	67*				
7	5	-1	0	72	71*	7	8	-10	0	95	70*	7	11	-10	85	203	70*	8	0	-4	135	205	79*	8	4	-8	0	108	71*				
7	5	0	317	325	19	7	8	-9	0	45	58*	7	11	-9	74	36	53*	8	0	-2	180	108	31*	8	4	-7	97	26	72*				
7	5	1	120	108	68*	7	8	-8	277	303	20	7	11	-8	0	26	66*	8	0	0	150	219	76*	8	4	-6	119	98	43*				
7	5	2	0	17	71*	7	8	-7	0	5	69*	7	11	-7	0	45	73*	8	0	2	260	244	21	8	4	-5	182	25	27				
7	5	3	152	17	27*	7	8	-6	0	34	70*	7	11	-6	200	198	27	8	0	4	90	67	51*	8	4	-4	108	154	76*				
7	5	4	213	220	24	7	8	-5	0	10	71*	7	11	-5	70	10	66*	8	1	-10	49	36	65*	8	4	-3	0	25	72*				
7	5	5	0	141	72*	7	8	-4	247	248	22	7	11	-4	0	55	70*	8	1	-9	171	41	28	8	4	-2	0	25	75*				
7	5	6	204	216	25	7	8	-3	109	38	72*	7	11	-3	0	97	69*	8	1	-8	66	145	62*	8	4	-1	92	52	73*				
7	5	7	75	24	49*	7	8	-2	345	342	18	7	11	-2	127	110	66*	8	1	-7	104	15	75*	8	4	0	164	160	31*				
7	5	8	131	53	66*	7	8	-1	0	8	72*	7	11	-1	116	3	71*	8	1	-6	76	218	82*	8	4	1	0	48	78*				
7	6	-13	0	15	52*	7	8	0	0	117	75*	7	11	0	204	223	25	8	1	-5	216	39	27	8	4	2	194	169	27				
7	6	-12	46	81	48*	7	8	1	109	9	65*	7	11	1	74	50	72*	8	1	-4	0	63	78*	8	4	3	168	47	25				
7	6	-11	0	12	65*	7	8	2	241	268	23	7	11	2	117	52	65*	8	1	-3	155	19	34*	8	4	4	156	86	27*				
7	6	-10	58	78	67*	7	8	3	0	49	67*	7	11	3	165	128	27	8	1	-2	224	212	25	8	4	5	69	31	46*				
7	6	-9	0	78	67*	7	8	4	207	214	23	7	11	4	30	158	72*	8	1	-1	0	20	73*	8	5	-9	46	29	58*				
8	5	-8	137	124	70*	8	9	0	123	68	37*																						
8	5	-7	44	37	69*	8	9	1	137	5	31*																						
8	5	-6	124	124	72*	8	10	-4	116	154	68*																						
8	5	-5	60	50	49*	8	10	-3	125	9	34*																						
8	5	-4	0	9	77*	8	10	-2	13	52	68*																						
8	5	-3	221	69	23	8	10	-1	132	17	67*																						
8	5	-2	196	212	29																												
8	5	-1	116	57	69*																												
8	5	0	102	70	53*																												
8	5	1	0	4	71*																												
8	5	2	81	69	52*																												
8	5	3	127	63	35*																												
8	5	4	180	160	25																												
8	6	-9	122	14	33*																												
8	6	-8	78	106	70*																												
8	6	-7	127	29	36*																												
8	6	-6	61	75	50*																												
8	6	-5	167	51	29*																												
8	6	-4	235	221	23																												
8	6	-3	81	68	68*																												
8	6	-2	0	56	74*																												
8	6	-1	134	18	70*																												
8	6	0	205	215	26																												
8	6	1	0	9	67*																												
8	6	2	0	124	69*																												
8	6	3	0	49	68*																												
8	6	4	144	4	27*																												
8	7	-8	55	138	67*																												
8	7	-7	0	1	67*																												
8	7	-6	251	222	20																												
8	7	-5	111	25	58*																												
8	7	-4	0	57	75*																												
8	7	-3	119	10	73*																												
8	7	-2	241	243	21																												
8	7	-1	133	61	67*																												
8	7	0	157	166	32*																												
8	7	1	71	40	59*																												
8	7	2	139	67	30*																												
8	7	3	113	52	63*																												
8	8	-7	78	6	57*																												
8	8	-6	0	44	70*																												
8	8	-5	0	6	70*																												
8	8	-4	200	221	26																												
8	8	-3	0	8	72*																												
8	8	-2	0	36	67*																												
8	8	-1	99	6	58*																												
8	8	0	104	128	72*																												
8	8	1	0	18	68*																												
8	8	2	189	171	23																												
8	9	-6	0	93	65*																												
8	9	-5	79	80	58*																												
8	9	-4	0	42	55*																												
8	9	-3	109	10	62*																												
8	9	-2	223	241	23																												
8	9	-1	85	22	46*																												

C. $[Cy_2Sn(S_2CNEt_2)Cl]$

Crystallographic Data and Refinement details for $[Cy_2Sn(S_2CNEt_2)Cl]$.

Formula	$C_{17}H_{32}ClNS_2Sn$
Formula weight	468.7
Crystal morphology	colourless block
Crystal dimensions (mm)	0.06 x 0.13 x 0.15
Crystal system	monoclinic
Space group	$P2_1/c$ (C_{2h}^5, No. 14)
Temperature (°C)	20.0
a (Å)	17.107(6)
b (Å)	11.134(2)
c (Å)	11.953(6)
β (°)	104.00(3)
V (Å^3)	2209(2)
Z	4
D_{calc} (g cm^{-3})	1.409
F(000)	960
Radiation	CuKα (λ = 1.5412Å)
μ (cm^{-1})	120.55
θ limits, data (°)	3.0 to 60.0
hkl range	0 to 13, 0 to 13, -19 to 19
Range of transmission factors	0.921 to 1.000
Scan technique	ω:2θ
Scan width (°)	1.10
No. of data measured	3683
No. of unique data	3496
R_{amal}	0.096
Program for structure solution	Direct Methods (SHELXS86)
No. of unique data used	1914
No. of parameters	200
R	0.042
R_w	0.034
G.O.F.	1.97
Min./Max. residual electron density (e Å^{-3})	-0.47 to +0.40

Fractional atomic coordinates ($Å^2$) for the non-hydrogen atoms in $[Cy_2Sn(S_2CNEt_2)Cl]$.

Atom	*x*	*y*	*z*
Sn	0.23043(4)	0.14696(5)	0.41736(5)
Cl(1)	0.2128(2)	0.3567(2)	0.4712(2)
S(1)	0.2473(2)	0.0951(2)	0.6228(2)
S(2)	0.2576(2)	-0.0963(2)	0.4566(2)
N(1)	0.2699(4)	-0.1339(6)	0.6789(6)
C(1)	0.3392(5)	0.1750(8)	0.3666(8)
C(2)	0.4108(7)	0.1908(14)	0.4592(11)
C(3)	0.4863(9)	0.2135(17)	0.4182(15)
C(4)	0.5023(8)	0.1200(16)	0.3400(13)
C(5)	0.4333(9)	0.1053(12)	0.2428(10)
C(6)	0.3560(7)	0.0849(11)	0.2811(10)
C(7)	0.1115(6)	0.1154(11)	0.3102(10)
C(8)	0.0514(8)	0.0892(14)	0.3708(10)
C(9)	-0.0307(8)	0.0645(16)	0.2943(14)
C(10)	-0.0525(9)	0.1292(20)	0.1941(15)
C(11)	0.0067(8)	0.1567(15)	0.1341(11)
C(12)	0.0908(7)	0.1791(14)	0.2104(10)
C(13)	0.2510(5)	-0.0547(7)	0.5939(7)
C(14)	0.2721(6)	-0.0986(7)	0.7975(8)
C(15)	0.3558(6)	-0.0760(10)	0.8714(9)
C(16)	0.2802(6)	-0.2621(8)	0.6598(8)
C(17)	0.2024(7)	-0.3269(8)	0.6272(9)

Anisotropic thermal parameters ($Å^2$) for the non-hydrogen atoms in $[Cy_2Sn(S_2CNEt_2)Cl]$.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Sn(1)	0.0798(4)	0.0618(4)	0.0712(4)	-0.0002(4)	-0.0005(3)	0.0089(4)
Cl(1)	0.146(2)	0.060(1)	0.126(2)	0.015(2)	0.040(2)	0.017(2)
S(1)	0.118(2)	0.049(1)	0.068(2)	0.005(1)	0.006(1)	-0.001(1)
S(2)	0.135(2)	0.058(1)	0.067(2)	0.002(1)	0.016(2)	-0.005(1)
N(1)	0.083(5)	0.049(5)	0.069(5)	-0.002(4)	0.006(4)	-0.004(5)
C(1)	0.074(6)	0.094(8)	0.086(7)	0.008(6)	0.019(6)	0.006(6)
C(2)	0.093(9)	0.27(2)	0.16(1)	-0.06(1)	0.016(9)	-0.12(1)
C(3)	0.11(1)	0.31(2)	0.28(2)	-0.08(1)	0.08(1)	-0.17(2)
C(4)	0.087(9)	0.28(2)	0.16(1)	0.02(1)	0.031(9)	-0.03(1)
C(5)	0.13(1)	0.18(1)	0.11(1)	-0.01(1)	0.042(9)	-0.005(9)
C(6)	0.104(9)	0.17(1)	0.110(9)	-0.025(9)	0.033(7)	-0.028(9)
C(7)	0.083(8)	0.16(1)	0.106(9)	-0.018(7)	-0.017(7)	0.052(8)
C(8)	0.092(9)	0.25(2)	0.11(1)	-0.03(1)	0.006(8)	0.05(1)
C(9)	0.10(1)	0.29(2)	0.19(2)	-0.05(1)	-0.02(1)	0.12(2)
C(10)	0.10(1)	0.40(1)	0.19(2)	-0.06(2)	-0.03(1)	0.11(2)
C(11)	0.10(1)	0.27(2)	0.11(1)	-0.03(1)	-0.021(8)	0.05(1)
C(12)	0.099(9)	0.27(2)	0.091(9)	-0.05(1)	-0.005(7)	0.04(1)
C(13)	0.076(6)	0.056(5)	0.066(6)	-0.005(5)	0.011(5)	-0.003(5)
C(14)	0.123(9)	0.056(5)	0.070(7)	0.004(6)	0.019(6)	0.010(5)
C(15)	0.119(9)	0.122(9)	0.090(8)	0.019(7)	-0.004(7)	-0.017(7)
C(16)	0.132(9)	0.049(6)	0.089(8)	0.017(6)	0.014(7)	0.014(5)
C(17)	0.17(1)	0.059(7)	0.119(9)	-0.008(7)	0.019(8)	-0.004(6)

Fractional atomic coordinates and B_{eq} values ($Å^2$) for the hydrogen atoms in $[Cy_2Sn(S_2CNEt_2)Cl]$.

Atom	*x*	*y*	*z*	B_{eq}
H(1a)	0.3321	0.2492	0.3261	10.8
H(2a)	0.4018	0.2587	0.5056	14.6
H(2b)	0.4185	0.1188	0.5063	14.6
H(3a)	0.5313	0.2170	0.4859	17.7
H(3b)	0.4805	0.2902	0.3791	17.7
H(4a)	0.5138	0.0451	0.3816	14.5
H(4b)	0.5488	0.1442	0.3120	14.5
H(5a)	0.4429	0.0364	0.1981	12.4
H(5b)	0.4273	0.1768	0.1955	12.4
H(6a)	0.3591	0.0056	0.3162	9.9
H(6b)	0.3116	0.0867	0.2130	9.9
H(7a)	0.1187	0.0379	0.2810	10.8
H(8a)	0.0680	0.0180	0.4181	12.4
H(8b)	0.0470	0.1564	0.4200	8.9
H(9a)	-0.0702	0.0812	0.3385	16.7
H(9b)	-0.0331	-0.0198	0.2736	16.7
H(10a)	-0.0743	0.2051	0.2125	18.7
H(10b)	-0.0942	0.0843	0.1413	18.7
H(11a)	-0.0100	0.2288	0.0887	13.5
H(11b)	0.0101	0.0904	0.0829	13.5
H(12a)	0.0947	0.2635	0.2305	12.3
H(12b)	0.1295	0.1597	0.1658	12.3
H(14a)	0.2408	-0.0256	0.7951	6.6
H(14b)	0.2477	-0.1624	0.8326	7.2
H(15a)	0.3880	-0.1483	0.8748	8.8
H(15b)	0.3809	-0.0113	0.8382	8.8
H(15c)	0.3526	-0.0539	0.9486	11.0
H(16a)	0.3083	-0.2713	0.5987	7.2
H(16b)	0.3128	-0.2968	0.7305	7.2
H(17a)	0.1747	-0.3194	0.6884	7.6
H(17b)	0.1697	-0.2925	0.5567	7.6
H(17c)	0.2124	-0.4110	0.6146	6.6

Bond distances (Å) for $[Cy_2Sn(S_2CNEt_2)Cl]$.

Atom-Atom	Distance	Atom-Atom	Distance
Sn-Cl(1)	2.459(3)	C(2)-C(3)	1.51(2)
Sn-S(1)	2.470(2)	C(3)-C(4)	1.47(2)
Sn-S(2)	2.768(3)	C(4)-C(5)	1.45(2)
Sn-C(1)	2.11(1)	C(5)-C(6)	1.52(1)
Sn-C(7)	2.15(1)	C(7)-C(8)	1.42(1)
S(1)-C(13)	1.727(9)	C(7)-C(12)	1.36(1)
S(2)-C(13)	1.696(9)	C(8)-C(9)	1.50(2)
N(1)-C(13)	1.32(1)	C(9)-C(10)	1.37(2)
N(1)-C(14)	1.46(1)	C(10)-C(11)	1.41(2)
N(1)-C(16)	1.464(9)	C(11)-C(12)	1.53(1)
C(1)-C(2)	1.53(1)	C(14)-C(15)	1.51(1)
C(1)-C(6)	1.50(1)	C(16)-C(17)	1.48(1)

Bond angles (°) for [$Cy_2Sn(S_2CNEt_2)Cl$].

Atom-Atom-Atom	Angle	Atom-Atom-Atom	Angle
Cl(1)-Sn-S(1)	87.37(9)	C(1)-C(2)-C(3)	114(1)
Cl(1)-Sn-S(2)	155.54(8)	C(2)-C(3)-C(4)	113(1)
Cl(1)-Sn-C(1)	96.1(3)	C(3)-C(4)-C(5)	110(1)
Cl(1)-Sn-C(7)	98.8(3)	C(4)-C(5)-C(6)	112(1)
S(1)-Sn-S(2)	68.17(8)	C(1)-C(6)-C(5)	115(1)
S(1)-Sn-C(1)	114.8(2)	Sn-C(7)-C(8)	115.2(8)
S(1)-Sn-C(7)	114.8(3)	Sn-C(7)-C(12)	116.4(9)
S(2)-Sn-C(1)	94.0(3)	C(8)-C(7)-C(12)	119(1)
S(2)-Sn-C(7)	92.1(3)	C(7)-C(8)-C(9)	114(1)
C(1)-Sn-C(7)	128.5(4)	C(8)-C(9)-C(10)	117(1)
Sn-S(1)-C(13)	91.0(3)	C(9)-C(10)-C(11)	119(1)
Sn-S(2)-C(13)	82.0(3)	C(10)-C(11)-C(12)	115(1)
C(13)-N(1)-C(14)	122.2(7)	C(7)-C(12)-C(11)	117(1)
C(13)-N(1)-C(16)	121.9(7)	S(1)-C(13)-S(2)	118.8(5)
C(14)-N(1)-C(16)	115.9(7)	S(1)-C(13)-N(1)	119.2(7)
Sn-C(1)-C(2)	116.0(8)	S(2)-C(13)-N(1)	122.0(6)
Sn-C(1)-C(6)	114.9(7)	N(1)-C(14)-C(15)	114.1(8)
C(2)-C(1)-C(6)	109.5(9)	N(1)-C(16)-C(17)	112.4(8)

Observed and calculated structure factors for $[Cy_2Sn(S_2CNEt_2)Cl]$.

h	k	l	Fo	Fc	sigF
0	-1	1	1730	1736	11
0	-1	2	1799	1789	11
0	-1	3	307	304	7
0	-1	4	1013	1004	9
0	-1	5	874	858	9
0	-1	6	83	86	17*
0	-1	7	449	448	11
0	-1	8	324	334	8
0	-1	9	76	26	45*
0	-1	10	351	387	9
0	-1	11	0	89	52*
0	-1	12	0	7	48*
0	-2	12	65	103	33*
0	-2	11	233	216	11
0	-2	10	0	9	51*
0	-2	9	718	771	14
0	-2	8	158	149	13
0	-2	7	439	449	9
0	-2	6	159	138	9
0	-2	5	119	123	10
0	-2	4	107	137	10
0	-2	3	461	482	7
0	-2	2	422	414	7
0	0	2	569	579	6
0	0	4	1136	1141	9
0	0	6	747	785	10
0	0	8	285	272	9
0	0	10	108	125	23*
0	0	12	0	61	47*
0	-2	1	2262	2291	14
0	-2	0	520	501	9
0	-3	12	0	38	48*
0	-3	11	184	216	14
0	-3	10	234	244	12
0	-3	9	108	102	22*
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4	-10	6	238	248	11
4	-9	0	325	315	8
4	-9	1	18	14	46*
4	-9	2	677	690	13
4	-9	3	118	90	19
4	-9	4	256	262	11
4	-4	8	64	29	54*
4	-4	9	114	90	24*
4	-4	10	94	184	59*
5	-10	1	0	13

4	-9	5	97	88	52*	4	-4	11	81	3	41*	5	-10	4	186	167	12	5	-4	3	24	30	38*	6	-10	0	128	97	12
4	-9	6	82	61	48*	4	-3	0	563	559	7	5	-10	5	0	39	49*	5	-4	4	565	512	11	6	-10	1	0	39	43*
4	-9	7	70	120	36*	4	-3	1	519	517	8	5	-10	6	208	230	11	5	-4	5	265	247	9	6	-10	2	190	187	11
4	-8	0	396	400	10	4	-3	2	108	138	10	5	-9	0	336	328	8	5	-4	6	0	70	49*	6	-10	3	58	40	31*
4	-8	1	514	516	10	4	-3	3	474	458	9	5	-9	1	161	151	13	5	-4	7	230	247	13	6	-10	4	224	239	11
4	-8	2	0	78	47*	4	-3	4	268	278	6	5	-9	2	49	99	49*	5	-4	8	195	202	16	6	-10	5	19	50	44*
4	-8	3	493	498	11	4	-3	5	748	733	11	5	-9	3	145	151	17	5	-4	9	25	25	55*	6	-9	0	356	354	8
4	-8	4	177	155	15	4	-3	6	207	201	11	5	-9	4	221	217	12	5	-4	10	93	121	55*	6	-9	1	83	36	42*
4	-8	5	0	18	50*	4	-3	7	334	364	10	5	-9	5	76	36	30*	5	-4	11	98	114	50*	6	-9	2	531	566	14
4	-8	6	100	44	51*	4	-3	8	228	233	14	5	-9	6	188	215	15	5	-3	0	273	281	6	6	-9	3	131	102	17
4	-8	7	237	247	13	4	-3	9	201	180	15	5	-9	7	78	134	48*	5	-3	1	435	463	8	6	-9	4	165	143	15
4	-8	8	0	8	52*	4	-3	10	89	149	58*	5	-8	0	144	132	14	5	-3	2	61	57	33*	6	-9	5	0	91	50*
4	-7	0	120	108	14	4	-3	11	234	241	13	5	-8	1	209	211	10	5	-3	3	839	847	9	6	-9	6	137	124	16
4	-7	1	100	106	17*	4	-2	0	157	154	6	5	-8	2	377	367	9	5	-3	4	812	785	10	6	-9	7	83	77	45*
4	-7	2	427	411	10	4	-2	1	670	673	7	5	-8	3	132	58	17	5	-3	5	43	67	41*	6	-8	0	270	285	8
4	-7	3	340	334	8	4	-2	2	250	248	6	5	-8	4	0	196	53*	5	-3	6	255	251	10	6	-8	1	469	475	9
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4	-7	6	0	0	51*	4	-2	5	234	235	8	5	-8	7	149	157	18	5	-3	9	273	288	13	6	-8	4	162	174	16
4	-7	7	192	205	15	4	-2	6	203	188	11	5	-8	8	0	99	49*	5	-3	10	71	113	56*	6	-8	5	43	47	50*
4	-7	8	115	72	23*	4	-2	7	610	608	14	5	-7	0	80	79	41*	5	-3	11	94	2	50*	6	-8	6	84	54	30*
4	-7	9	102	100	53*	4	-2	8	94	79	29*	5	-7	1	421	435	9	5	-2	0	174	182	5	6	-8	7	237	237	12
4	-6	0	222	201	8	4	-2	9	598	598	13	5	-7	2	72	9	41*	5	-2	1	616	613	7	6	-8	8	0	24	48*
4	-6	1	353	364	9	4	-2	10	0	51	58*	5	-7	3	483	472	10	5	-2	2	785	767	8	6	-7	0	37	46	34*
4	-6	2	106	72	15	4	-2	11	108	82	55*	5	-7	4	214	192	11	5	-2	3	842	849	9	6	-7	1	0	24	41*
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4	-6	6	482	468	12	4	-1	3	328	297	6	5	-7	8	155	194	19	5	-2	7	113	51	22*	6	-7	5	272	269	10
4	-6	7	240	238	13	4	-1	4	670	663	9	5	-7	9	100	196	54*	5	-2	8	227	240	15	6	-7	6	101	46	25*
4	-6	8	100	110	28*	4	-1	5	872	860	11	5	-6	0	610	632	11	5	-2	9	302	310	13	6	-7	7	0	83	55*
4	-6	9	219	233	15	4	-1	6	200	211	11	5	-6	1	274	283	7	5	-2	10	13	36	56*	6	-7	8	0	42	50*
4	-6	10	0	125	53*	4	-1	7	153	124	15	5	-6	2	815	821	11	5	-2	11	251	271	13	6	-7	9	140	133	17
4	-5	0	571	560	9	4	-1	8	530	526	12	5	-6	3	470	443	9	5	-1	0	802	788	7	6	-6	0	0	58	40*
4	-5	1	419	440	10	4	-1	9	55	178	58*	5	-6	4	212	204	11	5	-1	1	256	254	6	6	-6	1	349	339	9
4	-5	2	1151	1167	11	4	-1	10	282	263	13	5	-6	5	562	525	14	5	-1	2	309	308	6	6	-6	2	240	237	8
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4	-5	4	705	700	12	4	-1	12	57	82	50*	5	-6	7	64	14	51*	5	-1	4	1123	1137	11	6	-6	4	346	343	8
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4	-5	6	97	100	25*	4	0	2	848	870	8	5	-6	9	197	209	15	5	-1	6	862	834	12	6	-6	6	377	362	9
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4	-4	5	84	68	42*	5	-11	3	103	111	17	5	-5	8	40	40	54*	5	0	8	240	256	14	6	-5	6	272	269	11
4	-4	6	537	528	10	5	-11	4	0	107	45*	5	-5	9	0	55	55*	5	0	10	239	226	15	6	-5	7	144	109	18
4	-4	7	232	244	12	5	-10	0	285	283	8	5	-5	10	164	192	18	6	-11	0	135	147	10	6	-5	8	305	316	12
6	-5	9	51	91	55*	7	-11	1	137	161	10	7	-4	3	32	65	40*	8	-9	1	0	48	43*	8	-3	4	44	32	42*
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6	-4	2	36	80	36*	7	-10	2	322	351	7	7	-4	7	89	63	30*	8	-9	5	102	84	19*	8	-3	8	205	227	17
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6	-4	4	694	698	12	7	-10	4	0	72	46*	7	-4	9	0	59	57*	8	-8	1	396	416	10	8	-3	10	110	61	23*
6	-4	5	43	78	44*	7	-10	5	0	19	43*	7	-4	10	97	64	51*	8	-8	2	132	142	15	8	-2	0	130	148	8
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6	-3	3	503	523	10	7	-8	1	119	117	16	7	-3	8	156	152	20	8	-7	3	371	362	8	8	-2	9	224	265	15
6	-3	4	39	28	39*	7	-8	2	291	289	9	7	-3	9	177	211	18	8	-7	4	75	93	31*	8	-2	10	0	61	55*
6	-3	5	548	560	13	7	-8	3	27	40	46*	7	-3	10	0	123	57*	8	-7	5	176	195	15	8	-1	0	1191	1211	10
6	-3	6	264	241	10	7	-8	4	106	106	22*	7	-2	0	264	258	7	8	-7	6	66	87	36*	8	-1	1	184	198	6
6	-3	7	0	72	51*	7	-8	5	152	174	17	7	-2	1	155	140	7	8	-7	7	31	13	48*	8	-1	2	374	401	7
6	-3	8	228	215	14	7	-8	6	129	131	19	7	-2	2	357	344	7	8	-7	8	0	28	48*	8	-1	3	272	283	7
6	-3	9	175	191	20	7	-8	7	72	69	47*	7	-2	3	856	853	10	8	-6	0	69	80	39*	8	-1	4	58	47	42*
6	-3	10	36	95	56*	7	-7	0	0	35	40*	7	-2	4	222	229	9	8	-6	1	321	301	8	8	-1	5	325	308	9
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6	-2	1	1023	1031	9	7	-7	2	58	21	43*	7	-2	6	307	310	10	8	-6	3	0	25	45*	8	-1	7	68	49	53*
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6	-2	3	164	93	9	7	-7	4	0	117	51*	7	-2	8	21	148	58*	8	-6	5	143	171	18	8	-1	9	222	243	16
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6	-2	8	79	61	46*	7	-6	0	598	578	11	7	-1	2	604	581	9	8	-5	1	208	203	8	8	0	6	317	302	11
6	-2	9	413	436	11	7	-6	1	198	187	9	7	-1	3	108	50	13	8	-5	2	668	669	11	8	0	8	148	150	22
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6	-1	9	187	200	19	7	-5	3	0	57	43*	7	0	8	227	254	16	8	-4	4	629	642	12	9	-8	0	155	154	10
6	-1	10	190	187	18	7	-5	4	714	703	13	7	0	10	41	94	57*	8	-4	5	159	140	14	9	-8	1	46	8	40*
6	-1	11	0	100	54*	7	-5	5	125	114	19	8	-11	0	104	137	10	8	-4	6	237	225	12	9	-8	2	182	177	11
6	0	0	1925	1891	13	7	-5	6	334	313	10	8	-11	1	76	56	14*	8	-4	7	57	153	54*	9	-8	3	143	98	14
6	0	2	395	396	9	7	-5	7	0	58	53*	8	-10	0	0	19	36*	8	-4	8	126	120	23*	9	-8	4	56	41	43*
6	0	4	842	843	11	7	-5	8	78	44	44*	8	-10	1	0	15	39*	8	-4	9	80	38	34*	9	-8	5	126	105	17
6	0	6	615	600	13	7	-5	9	0	23	51*	8	-10	2	214	229	9	8	-3	0	497	511	9	9	-8	6	122	109	17
6	0	8	0	19	54*	7	-4	0	772	763	9	8	-10	3	13	12	39*	8	-3	1	114	104	10	9	-7	0	0	10	39*
6	0	10	296	285	12	7	-4	1	150	155	9	8	-10	4	226	215	8	8	-3	2	0	78	36*	9	-7	1	437	420	9
7	-11	0	0	82	36*	7	-4	2	760	747	10	8	-9	0	293	324	7	8	-3	3	529	516	11	9	-7	2	63	24	37*
9	-7	3	247	239	10	9	-1	2	362	374	8	10	-4	3	124	135	16	-1	-4	10	252	257	11	-1	-9	7	52	109	51*
9	-7	4	0	45	39*	9	-1	3	126	113	13	10	-4	4	449	461	11	-1	-4	9	208	211	13	-1	-9	6	309	285	10
9	-7	5	212	248	13	9	-1	4	780	795	12	10	-4	5	0	89	49*	-1	-4	8	149	175	16	-1	-9	5	93	36	26*
9	-7	6	90	28	45*	9	-1	5	0	27	50*	10	-4	6	121	141	21*	-1	-4	7	482	480	10	-1	-9	4	152	111	17
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9	-6	0	519	515	11	9	-1	7	186	166	16	10	-4	8	92	157	52*	-1	-4	5	482	478	11	-1	-9	2	522	515	11
9	-6	1	0	52	40*	9	-1	8	217	222	15	10	-3	0	492	481	9	-1	-4	4	1306	1329	11	-1	-9	1	193	159	13
9	-6	2	438	420	9	9	-1	9	0	51	53*	10	-3	1	89	81	14	-1	-4	3	195	178	7	-1	-10	7	31	93	49*
9	-6	3	328	321	8	9	0	0	789	784	10	10	-3	2	79	68	18*	-1	-4	2	812	824	9	-1	-10	6	71	84	35*
9	-6	4	48	62	46*	9	0	2	687	701	10	10	-3	3	494	483	12	-1	-4	1	773	770	9	-1	-10	5	73	106	52*
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-11	-1	6	0	20	42*	-11	-6	7	163	137	14	-12	-2	8	61	49	34*	-12	-7	4	0	45	54*	-13	-4	9	105	120	14		
-11	-1	5	520	530	13	-11	-6	6	0	60	50*	-12	-2	7	263	284	8	-12	-7	3	313	295	11	-13	-4	8	37	45	41*		
-11	-1	4	288	285	8	-11	-6	5	78	15	49*	-12	-2	6	65	51	42*	-12	-7	2	105	86	53*	-13	-4	7	49	96	45*		
-11	-1	3	144	141	14	-11	-6	4	0	48	54*	-12	-2	5	384	408	9	-12	-7	1	171	171	16	-13	-4	6	249	269	10		
-11	-1	2	401	429	10	-11	-6	3	271	264	12	-12	-2	4	118	129	19	-12	-8	7	133	141	14	-13	-4	5	0	95	51*		
-11	-1	1	319	322	13	-11	-6	2	84	89	34*	-12	-2	3	57	44	48*	-12	-8	6	19	29	43*	-13	-4	4	143	148	19		
-11	-2	12	0	20	41*	-11	-6	1	223	219	14	-12	-2	2	97	105	51*	-12	-8	5	144	145	16	-13	-4	3	205	209	15		
-11	-2	11	72	91	24*	-11	-7	9	40	8	34*	-12	-2	1	451	488	11	-12	-8	4	76	53	49*	-13	-4	2	279	284	12		
-11	-2	10	37	25	40*	-11	-7	8	61	57	33*	-12	-3	11	116	88	11	-12	-8	3	175	141	15	-13	-4	1	190	216	16		
-11	-2	9	86	113	43*	-11	-7	7	174	151	12	-12	-3	10	62	107	39*	-12	-8	2	101	100	52*	-13	-5	10	88	77	13		
-11	-2	8	47	36	41*	-11	-7	6	0	12	48*	-12	-3	9	220	215	9	-12	-8	1	0	92	51*	-13	-5	9	0	46	37*		
-11	-2	7	91	99	22*	-11	-7	5	299	286	10	-12	-3	8	33	6	40*	-12	-9	5	0	57	45*	-13	-5	8	137	167	13		
-11	-2	6	56	53	43*	-11	-7	4	0	74	53*	-12	-3	7	66	85	28*	-12	-9	4	87	81	44*	-13	-5	7	0	78	45*		
-11	-2	5	146	117	13	-11	-7	3	154	99	18	-12	-3	6	0	77	46*	-12	-9	3	102	107	21*	-13	-5	6	0	12	48*		
-11	-2	4	0	11	45*	-11	-7	2	76	76	52*	-12	-3	5	187	179	11	-12	-9	2	49	30	45*	-13	-5	5	151	118	16		
-11	-2	3	534	524	13	-11	-7	1	166	185	18	-12	-3	4	0	47	48*	-12	-9	1	0	42	47*	-13	-5	4	232	247	14		
-11	-2	2	85	96	48*	-11	-8	8	0	31	39*	-12	-3	3	444	464	11	-13	0	10	132	121	11	-13	-5	3	0	20	54*		
-11	-2	1	428	449	11	-11	-8	7	169	163	13	-12	-3	2	257	248	12	-13	0	8	94	120	15	-13	-5	2	189	187	16		
-11	-3	12	18	13	35*	-11	-8	6	114	98	19	-12	-3	1	300	339	12	-13	0	6	326	380	7	-13	-5	1	100	46	26*		
-11	-3	11	112	102	14	-11	-8	5	109	123	24*	-12	-4	11	18	28	36*	-13	0	4	207	205	10	-13	-6	9	71	51	19*		
-11	-3	10	35	9	28*	-11	-8	4	76	83	39*	-12	-4	10	127	129	12	-13	0	2	388	400	12	-13	-6	8	8	52	41*		
-11	-3	9	23	4	42*	-11	-8	3	302	303	11	-12	-4	9	0	65	40*	-13	-1	11	72	58	16*	-13	-6	7	82	70	22*		
-11	-3	8	88	82	19*	-11	-8	2	137	88	19	-12	-4	8	150	135	12	-13	-1	10	84	77	14*	-13	-6	6	0	56	48*		
-11	-3	7	293	300	8	-11	-8	1	208	198	14	-12	-4	7	186	186	10	-13	-1	9	0	1	37*	-13	-6	5	90	95	27*		
-11	-3	6	0	60	45*	-11	-9	6	0	67	45*	-12	-4	6	82	38	44*	-13	-1	8	86	119	18*	-13	-6	4	78	10	51*		
-11	-3	5	534	536	14	-11	-9	5	41	20	35*	-12	-4	5	123	109	19	-13	-1	7	212	248	8	-13	-6	3	232	207	14		
-11	-3	4	61	45	38*	-11	-9	4	206	184	12	-12	-4	4	160	164	16	-13	-1	6	0	53	29*	-13	-6	2	0	67	56*		
-11	-3	3	208	212	12	-11	-9	3	71	10	48*	-12	-4	3	107	103	24*	-13	-1	5	278	298	8	-13	-6	1	73	91	53*		
-11	-3	2	149	144	17	-11	-9	2	188	170	13	-12	-4	2	285	297	11	-13	-1	4	225	229	10	-13	-7	8	25	30	39*		
-11	-3	1	401	445	9	-11	-9	1	143	65	15	-12	-4	1	0	35	54*	-13	-1	3	65	30	47*	-13	-7	7	74	151	45*		
-11	-4	11	0	36	29*	-11	-10	4	24	17	35*	-12	-5	10	76	76	18*	-13	-1	2	115	111	27*	-13	-7	6	62	8	43*		
-11	-4	10	134	112	12	-11	-10	3	77	58	42*	-12	-5	9	49	36	33*	-13	-1	1	196	196	19	-13	-7	5	158	170	16		
-11	-4	9	171	177	11	-11	-10	2	83	68	23*	-12	-5	8	0	90	43*	-13	-2	11	47	64	25*	-13	-7	4	0	61	50*		
-11	-4	8	82	9	41*	-11	-10	1	0	27	43*	-12	-5	7	46	28	43*	-13	-2	10	23	14	34*	-13	-7	3	71	16	36*		
-11	-4	7	169	170	12	-12	0	12	0	17	36*	-12	-5	6	211	210	12	-13	-2	9	58	120	25*	-13	-7	2	24	31	51*		
-11	-4	6	290	299	9	-12	0	10	202	197	9	-12	-5	5	123	101	19	-13	-2	8	60	30	36*	-13	-7	1	187	175	15		
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-11	-4	4	340	318	9	-12	0	6	0	99	42*	-12	-5	3	91	19	51*	-13	-2	6	0	38	44*	-13	-8	5	113	119	18		
-11	-4	3	392	393	9	-12	0	4	237	254	9	-12	-5	2	190	185	16	-13	-2	5	190	218	12	-13	-8	4	49	41	47*		
-11	-4	2	207	218	13	-12	0	2	574	582	14	-12	-5	1	6	119	54*	-13	-2	4	46	5	48*	-13	-8	3	193	213	14		

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-11	-5	11	52	49	37*	-12	-1	11	91	69	16*	-12	-6	9	74	9	38*	-13	-2	2	75	53	40*	-13	-8	1	126	112	18
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-14	0	10	134	150	7	-14	-5	1	128	109	21	-15	-3	1	224	286	13	-16	-3	7	19	8	26*	-17	-4	7	0	23	28*
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-14	0	4	191	213	10	-14	-6	6	59	46	42*	-15	-4	7	0	52	37*	-16	-3	4	0	10	46*	-17	-4	4	63	15	38*
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-14	-1	11	17	57	25*	-14	-6	4	148	155	19	-15	-4	5	112	112	18	-16	-3	2	0	65	51*	-17	-4	2	61	135	43*
-14	-1	10	66	61	14*	-14	-6	3	67	21	50*	-15	-4	4	48	61	48*	-16	-3	1	0	32	48*	-17	-4	1	52	2	40*
-14	-1	9	83	113	13	-14	-6	2	88	93	30*	-15	-4	3	155	162	17	-16	-4	8	45	51	17*	-17	-5	5	0	33	39*
-14	-1	8	0	73	36*	-14	-6	1	150	180	18	-15	-4	2	101	145	52*	-16	-4	7	0	82	34*	-17	-5	4	0	131	36*
-14	-1	7	0	32	38*	-14	-7	7	35	18	39*	-15	-4	1	0	17	52*	-16	-4	6	50	23	38*	-17	-5	3	76	4	18*
-14	-1	6	115	159	15	-14	-7	6	75	25	42*	-15	-5	8	0	99	34*	-16	-4	5	58	31	41*	-17	-5	2	78	65	19*
-14	-1	5	46	72	40*	-14	-7	5	132	120	16	-15	-5	7	50	46	27*	-16	-4	4	65	92	37*	-17	-5	1	38	4	36*
-14	-1	4	47	30	43*	-14	-7	4	0	24	48*	-15	-5	6	86	9	20*	-16	-4	3	62	60	45*	-18	0	6	0	25	18*
-14	-1	3	144	175	17	-14	-7	3	235	231	12	-15	-5	5	83	52	24*	-16	-4	2	0	104	48*	-18	0	4	117	116	9
-14	-1	2	177	189	18	-14	-7	2	116	30	20*	-15	-5	4	174	189	14	-16	-4	1	72	82	44*	-18	0	2	131	87	13
-14	-1	1	171	203	23	-14	-7	1	0	90	48*	-15	-5	3	93	40	25*	-16	-5	7	38	4	33*	-18	-1	7	0	3	15*
-14	-2	11	51	71	17*	-14	-8	5	102	91	17*	-15	-5	2	86	141	53*	-16	-5	6	0	101	38*	-18	-1	6	69	69	7
-14	-2	10	0	27	23*	-14	-8	4	29	30	43*	-15	-5	1	95	7	48*	-16	-5	5	71	30	40*	-18	-1	5	33	61	29*
-14	-2	9	0	31	33*	-14	-8	3	23	33	45*	-15	-6	7	59	16	36*	-16	-5	4	0	3	46*	-18	-1	4	0	9	34*
-14	-2	8	60	14	33*	-14	-8	2	42	62	32*	-15	-6	6	23	66	42*	-16	-5	3	61	21	42*	-18	-1	3	117	87	12
-14	-2	7	174	229	9	-14	-8	1	77	102	45*	-15	-6	5	9	74	44*	-16	-5	2	65	141	36*	-18	-1	2	193	139	9
-14	-2	6	0	24	41*	-15	0	10	35	57	25*	-15	-6	4	0	21	45*	-16	-5	1	54	72	38*	-18	-1	1	0	13	40*
-14	-2	5	229	234	10	-15	0	8	65	113	33*	-15	-6	3	128	133	19	-16	-6	6	66	51	36*	-18	-2	7	84	86	4
-14	-2	4	60	71	45*	-15	0	6	173	245	8	-15	-6	2	0	104	50*	-16	-6	5	83	52	19*	-18	-2	6	0	20	24*
-14	-2	3	38	128	52*	-15	0	4	56	23	28*	-15	-6	1	91	72	24*	-16	-6	4	84	117	42*	-18	-2	5	78	61	12
-14	-2	2	78	35	52*	-15	0	2	98	189	61*	-15	-7	6	0	7	41*	-16	-6	3	0	44	44*	-18	-2	4	62	37	34*
-14	-2	1	320	387	12	-15	-1	10	0	73	26*	-15	-7	5	92	106	20*	-16	-6	2	75	46	24*	-18	-2	3	111	97	13
-14	-3	10	38	58	32*	-15	-1	9	0	22	26*	-15	-7	4	0	61	44*	-16	-6	1	135	126	13	-18	-2	2	0	15	37*
-14	-3	9	129	136	9	-15	-1	8	69	65	14*	-15	-7	3	0	53	48*	-17	0	8	39	70	6	-18	-2	1	56	214	35*
-14	-3	8	39	16	30*	-15	-1	7	90	157	12	-15	-7	2	0	10	44*	-17	0	6	163	163	5	-18	-3	6	0	50	28*
-14	-3	7	0	14	39*	-15	-1	6	50	87	36*	-15	-7	1	120	159	18	-17	0	4	0	23	33*	-18	-3	5	118	91	9
-14	-3	6	60	84	42*	-15	-1	5	94	121	15	-16	0	8	85	92	6	-17	-1	8	39	48	7*	-18	-3	4	0	4	35*
-14	-3	5	154	179	15	-15	-1	4	74	142	42*	-16	0	6	0	27	33*	-17	-1	7	86	102	7	-18	-3	3	32	120	29*
-14	-3	4	0	15	49*	-15	-1	3	65	35	36*	-16	0	4	79	133	19*	-17	-1	6	67	63	13*	-18	-3	2	0	72	35*
-14	-3	3	261	251	11	-15	-1	2	110	99	55*	-16	0	2	158	195	18	-17	-1	5	63	73	35*	-18	-3	1	26	11	33*
-14	-3	2	121	161	23*	-15	-1	1	130	181	25*	-16	-1	9	76	72	6	-17	-1	4	173	132	10	-18	-4	4	0	68	29*
-14	-3	1	194	183	15	-15	-2	10	0	9	25*	-16	-1	8	50	64	25*	-17	-1	3	85	81	45*	-18	-4	3	0	36	34*
-14	-4	10	49	103	32*	-15	-2	9	53	69	14*	-16	-1	7	0	1	29*	-17	-1	2	96	43	23*	-18	-4	2	30	55	24*
-14	-4	9	28	65	24*	-15	-2	8	45	33	25*	-16	-1	6	9	135	30*	-17	-1	1	192	120	13	-19	0	4	0	17	23*
-14	-4	8	0	108	40*	-15	-2	7	0	28	34*	-16	-1	5	0	85	36*	-17	-2	8	29	20	15*	-19	0	2	131	111	10
-14	-4	7	107	105	14	-15	-2	6	41	49	35*	-16	-1	4	87	5	17*	-17	-2	7	0	21	25*	-19	-1	4	67	74	9
-14	-4	6	58	12	33*	-15	-2	5	101	214	18*	-16	-1	3	0	111	47*	-17	-2	6	0	29	32*	-19	-1	3	0	54	29*
-14	-4	5	70	59	46*	-15	-2	4	0	26	46*	-16	-1	2	163	202	15	-17	-2	5	210	155	7	-19	-1	2	41	18	21*
-14	-4	4	106	138	25*	-15	-2	3	185	198	14	-16	-1	1	0	100	56*	-17	-2	4	0	2	41*						
-14	-4	3	70	4	51*	-15	-2	2	49	73	49*	-16	-2	9	37	41	21*	-17	-2	3	264	171	9						
-14	-4	2	36	161	54*	-15	-2	1	0	107	45*	-16	-2	8	0	19	25*	-17	-2	2	0	48	38*						
-14	-4	1	0	77	54*	-15	-3	10	17	11	26*	-16	-2	7	169	151	7	-17	-2	1	19	8	43*						
-14	-5	9	62	18	33*	-15	-3	9	0	35	28*	-16	-2	6	48	27	31*	-17	-3	8	23	4	20*						
-14	-5	8	65	91	36*	-15	-3	8	0	13	30*	-16	-2	5	69	108	35*	-17	-3	7	54	117	12*						
-14	-5	7	46	18	40*	-15	-3	7	127	176	11	-16	-2	4	55	86	34*	-17	-3	6	0	40	32*						
-14	-5	6	131	136	16	-15	-3	6	0	47	40*	-16	-2	3	67	89	45*	-17	-3	5	43	87	30*						
-14	-5	5	71	49	40*	-15	-3	5	30	173	42*	-16	-2	2	0	13	48*	-17	-3	4	60	42	23*						
-14	-5	4	0	39	51*	-15	-3	4	14	14	47*	-16	-2	1	202	325	14	-17	-3	3	105	99	15						

D. $[Cy_2Sn(S_2CNCy_2)Cl]$

Crystallographic Data and Refinement details for $[Cy_2Sn(S_2CNCy_2)Cl]$.

Formula	$C_{25}H_{44}ClNS_2Sn$
Formula weight	576.5
Crystal morphology	colourless block
Crystal dimensions (mm)	0.06 x 0.10 x 0.26
Crystal system	monoclinic
Space group	$P2_1/n$ (C_{2h}^5, No. 14)
Temperature (°C)	20.0
a (Å)	11.411(7)
b (Å)	16.942(5)
c (Å)	14.712(5)
β (°)	100.45(3)
V (Å^3)	2797(1)
Z	4
D_{calc} (g cm^{-3})	1.370
$F(000)$	1200
Radiation	MoKα (λ = 0.7107Å)
μ (cm^{-1})	11.70
θ limits, data (°)	3.0 to 27.5
hkl range	0 to 15, 0 to 22, -19 to 19
Range of transmission factors	0.986 to 1.000
Scan technique	ω:2θ
Scan width (°)	1.15
No. of data measured	6998
No. of unique data	6681
R_{amal}	0.069
Program for structure solution	Direct Methods (SHELXS86)
No. of unique data used	2550
No. of parameters	271
R	0.045
R_w	0.038
G.O.F.	1.42
Min./Max. residual electron density (e Å^{-3})	-0.49 to +0.54

Fractional atomic coordinates ($Å^2$) for the non-hydrogen atoms in $[Cy_2Sn(S_2CNCy_2)Cl]$.

Atom	*x*	*y*	*z*
Sn(1)	-0.06177(5)	0.27637(3)	0.19807(4)
Cl(1)	0.0094(2)	0.3925(1)	0.1192(2)
S(1)	0.1481(2)	0.2321(1)	0.2243(2)
S(2)	-0.0335(2)	0.1422(1)	0.2959(2)
N(1)	0.1903(6)	0.0904(4)	0.3091(5)
C(1)	-0.1376(6)	0.3450(4)	0.2973(5)
C(2)	-0.1927(8)	0.2955(5)	0.3629(6)
C(3)	-0.2456(9)	0.3460(6)	0.4317(7)
C(4)	-0.3351(9)	0.4041(6)	0.3815(8)
C(5)	-0.2789(9)	0.4540(6)	0.3164(8)
C(6)	-0.2256(8)	0.4044(5)	0.2473(7)
C(7)	-0.1638(7)	0.2274(5)	0.0743(6)
C(8)	-0.2853(8)	0.2041(6)	0.0821(8)
C(9)	-0.3576(8)	0.1740(7)	-0.0099(7)
C(10)	-0.2916(13)	0.1105(7)	-0.0506(9)
C(11)	-0.1731(12)	0.1295(7)	-0.0554(9)
C(12)	-0.0987(8)	0.1627(6)	0.0340(7)
C(13)	0.1112(7)	0.1474(5)	0.2799(6)
C(14)	0.3151(8)	0.0932(6)	0.2954(6)
C(15)	0.3973(9)	0.1441(5)	0.3567(7)
C(16)	0.5246(9)	0.1366(6)	0.3502(8)
C(17)	0.5464(11)	0.1234(7)	0.2548(10)
C(18)	0.4641(10)	0.0728(7)	0.1939(7)
C(19)	0.3345(9)	0.0818(5)	0.1999(7)
C(20)	0.1540(9)	0.0187(6)	0.3571(8)
C(21)	0.2095(9)	0.0133(7)	0.4546(8)
C(22)	0.1688(10)	-0.0574(7)	0.5008(8)
C(23)	0.1575(13)	-0.1314(8)	0.4457(11)
C(24)	0.1019(10)	-0.1229(6)	0.3468(9)
C(25)	0.1398(8)	-0.0518(6)	0.2991(7)

Anisotropic thermal parameters ($Å^2$) for the non-hydrogen atoms in $[Cy_2Sn(S_2CNCy_2)Cl]$.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Sn	0.0436(3)	0.0431(3)	0.0427(3)	0.0025(4)	0.0065(2)	-0.0008(4)
Cl(1)	0.082(2)	0.059(1)	0.068(2)	-0.005(1)	0.022(2)	0.012(1)
S(1)	0.044(1)	0.057(1)	0.070(2)	0.001(1)	0.016(1)	0.007(1)
S(2)	0.056(2)	0.051(1)	0.082(2)	0.007(1)	0.028(1)	0.017(1)
N(1)	0.062(5)	0.064(5)	0.045(5)	0.021(4)	0.012(4)	-0.001(4)
C(1)	0.048(5)	0.041(4)	0.034(5)	0.002(4)	0.001(4)	-0.003(4)
C(2)	0.082(6)	0.067(6)	0.072(7)	0.014(5)	0.040(6)	0.014(5)
C(3)	0.100(8)	0.094(8)	0.060(8)	0.012(6)	0.040(6)	-0.004(6)
C(4)	0.082(8)	0.094(8)	0.10(1)	0.015(6)	0.045(7)	-0.028(7)
C(5)	0.101(9)	0.076(7)	0.12(1)	0.044(6)	0.040(8)	-0.001(7)
C(6)	0.067(7)	0.074(6)	0.082(8)	0.020(5)	0.020(6)	0.004(6)
C(7)	0.055(5)	0.068(6)	0.062(6)	-0.005(5)	0.011(5)	-0.014(6)
C(8)	0.066(7)	0.13(1)	0.096(9)	-0.021(7)	0.013(6)	-0.027(8)
C(9)	0.068(7)	0.126(9)	0.071(9)	-0.022(7)	-0.009(6)	-0.030(7)
C(10)	0.14(1)	0.13(1)	0.09(1)	-0.03(1)	-0.019(9)	-0.052(8)
C(11)	0.12(1)	0.14(1)	0.10(1)	0.004(9)	0.009(9)	-0.080(9)
C(12)	0.066(7)	0.105(8)	0.069(8)	0.014(6)	0.003(6)	-0.041(7)
C(13)	0.045(5)	0.052(5)	0.044(6)	0.001(4)	0.004(4)	-0.004(4)
C(14)	0.058(6)	0.118(9)	0.048(7)	0.040(6)	0.005(5)	-0.011(6)
C(15)	0.082(7)	0.072(6)	0.074(8)	-0.027(6)	0.035(6)	-0.031(6)
C(16)	0.066(7)	0.098(8)	0.10(1)	0.032(6)	0.007(7)	0.005(7)
C(17)	0.10(1)	0.113(9)	0.15(1)	-0.041(8)	0.08(1)	-0.022(9)
C(18)	0.089(9)	0.115(9)	0.064(8)	0.054(7)	0.03(7)	0.025(7)
C(19)	0.097(8)	0.068(6)	0.061(8)	-0.017(6)	0.043(7)	-0.009(6)
C(20)	0.115(9)	0.057(6)	0.072(9)	0.026(6)	0.020(7)	0.020(6)
C(21)	0.094(9)	0.13(1)	0.056(8)	-0.030(7)	0.021(7)	0.018(7)
C(22)	0.094(8)	0.111(9)	0.077(9)	0.044(7)	0.034(7)	0.040(8)
C(23)	0.15(1)	0.14(1)	0.13(1)	-0.05(1)	0.04(1)	0.05(1)
C(24)	0.097(9)	0.070(7)	0.12(1)	0.017(6)	0.018(8)	0.026(7)
C(25)	0.061(6)	0.091(7)	0.079(9)	-0.032(6)	0.011(6)	-0.013(7)

Fractional atomic coordinates and B_{eq} values (Å^2) for the hydrogen atoms in [$Cy_2Sn(S_2CNCy_2)Cl$].

Atom	x	y	z	B_{eq}
H(1a)	-0.0730	0.3745	0.3339	4.1
H(2a)	-0.1321	0.2612	0.3969	5.5
H(2b)	-0.2557	0.2636	0.3276	5.5
H(3a)	-0.1821	0.3747	0.4705	6.7
H(3b)	-0.2850	0.3119	0.4698	6.7
H(4a)	-0.3635	0.4380	0.4262	7.5
H(4b)	-0.4022	0.3754	0.3463	7.5
H(5a)	-0.2159	0.4856	0.3524	7.6
H(5b)	-0.3390	0.4888	0.2825	7.6
H(6a)	-0.2891	0.3766	0.2073	6.2
H(6b)	-0.1848	0.4388	0.2105	5.6
H(7a)	-0.1728	0.2697	0.0292	5.6
H(8a)	-0.3257	0.2496	0.1021	9.2
H(8b)	-0.2811	0.1626	0.1279	7.5
H(9a)	-0.4330	0.1531	0.0012	7.7
H(9b)	-0.3727	0.2177	-0.0530	7.7
H(10a)	-0.3342	0.0999	-0.1128	7.3
H(10b)	-0.2917	0.0635	-0.0131	10.2
H(11a)	-0.1350	0.0818	-0.0718	9.8
H(11b)	-0.1747	0.1685	-0.1039	9.8
H(12a)	-0.0815	0.1204	0.0789	7.4
H(12b)	-0.0249	0.1837	0.0204	7.4
H(14a)	0.3421	0.0422	0.3211	4.1
H(15a)	0.3894	0.1321	0.4198	6.3
H(15b)	0.3736	0.1984	0.3426	6.9
H(16a)	0.5650	0.1847	0.3737	8.6
H(16b)	0.5575	0.0923	0.3880	8.6
H(17a)	0.5460	0.1747	0.2254	8.7
H(17b)	0.6253	0.1001	0.2602	8.7

Fractional atomic coordinates and B_{eq} values (Å^2) for the hydrogen atoms in $[Cy_2Sn(S_2CNCy_2)Cl]$.

Atom	x	y	z	B_{eq}
H(18a)	0.4720	0.0843	0.1308	7.4
H(18b)	0.4861	0.0185	0.2084	7.4
H(19a)	0.3028	0.1271	0.1634	6.8
H(19b)	0.2925	0.0346	0.1749	6.8
H(20a)	0.0721	0.0309	0.3611	7.5
H(21a)	0.1894	0.0607	0.4858	8.4
H(21b)	0.2951	0.0105	0.4588	7.8
H(22a)	0.2264	-0.0653	0.5580	6.9
H(22b)	0.0921	-0.0445	0.5164	6.9
H(23a)	0.2373	-0.1534	0.4528	9.8
H(23b)	0.1082	-0.1664	0.4754	9.8
H(24a)	0.1303	-0.1689	0.3165	8.6
H(24b)	0.0166	-0.1201	0.3434	8.6
H(25a)	0.2149	-0.0617	0.2787	6.9
H(25b)	0.0784	-0.0412	0.2455	8.6

Bond distances (Å)for [$Cy_2Sn(S_2CNCy_2)Cl$].

Atom - Atom	Distance	Atom - Atom	Distance
Sn - Cl(1)	2.493(2)	C(7) - C(12)	1.51(1)
Sn - S(1)	2.472(2)	C(8) - C(9)	1.54(1)
Sn - S(2)	2.680(2)	C(9) - C(10)	1.50(1)
Sn - C(1)	2.166(7)	C(10) - C(11)	1.40(1)
Sn - C(7)	2.143(8)	C(11) - C(12)	1.54(1)
S(1) - C(13)	1.740(8)	C(14) - C(15)	1.46(1)
S(2) - C(13)	1.712(8)	C(14) - C(19)	1.48(1)
N(1) - C(13)	1.339(9)	C(15) - C(16)	1.48(1)
N(1) - C(14)	1.47(1)	C(16) - C(17)	1.49(1)
N(1) - C(20)	1.50(1)	C(17) - C(18)	1.45(1)
C(1) - C(2)	1.50(1)	C(18) - C(19)	1.51(1)
C(1) - C(6)	1.51(1)	C(20) - C(21)	1.46(1)
C(2) - C(3)	1.53(1)	C(20) - C(25)	1.46(1)
C(3) - C(4)	1.51(1)	C(21) - C(22)	1.49(1)
C(4) - C(5)	1.51(1)	C(22) - C(23)	1.49(2)
C(5) - C(6)	1.53(1)	C(23) - C(24)	1.48(2)
C(7) - C(8)	1.47(1)	C(24) - C(25)	1.50(1)

Bond angles (°) for $[Cy_2Sn(S_2CNCy_2)Cl]$.

Atom - Atom - Atom	Angle	Atom - Atom - Atom	Angle
Cl(1) - Sn - S(1)	85.67(8)	C(8) - C(7) - C(12)	112.0(8)
Cl(1) - Sn - S(2)	154.42(8)	C(7) - C(8) - C(9)	112.6(8)
Cl(1) - Sn - C(1)	95.4(2)	C(8) - C(9) - C(10)	111.1(9)
Cl(1) - Sn - C(7)	94.7(2)	C(9) - C(10) - C(11)	114(1)
S(1) - Sn - S(2)	68.86(7)	C(10) - C(11) - C(12)	115(1)
S(1) - Sn - C(1)	123.5(2)	C(7) - C(12) - C(11)	111.6(8)
S(1) - Sn - C(7)	112.1(2)	S(1) - C(13) - S(2)	115.4(5)
S(2) - Sn - C(1)	96.7(2)	S(1) - C(13) - N(1)	122.6(6)
S(2) - Sn - C(7)	97.0(2)	S(2) - C(13) - N(1)	122.0(6)
C(1) - Sn - C(7)	124.0(3)	N(1) - C(14) - C(15)	117.6(7)
Sn - S(1) - C(13)	90.8(3)	N(1) - C(14) - C(19)	116.2(8)
Sn - S(2) - C(13)	84.7(3)	C(15) - C(14) - C(19)	118.4(8)
C(13) - N(1) - C(14)	123.0(7)	C(14) - C(15) - C(16)	116.0(8)
C(13) - N(1) - C(20)	120.5(7)	C(15) - C(16) - C(17)	114(1)
C(14) - N(1) - C(20)	116.5(7)	C(16) - C(17) - C(18)	118.1(9)
Sn - C(1) - C(2)	113.5(5)	C(17) - C(18) - C(19)	115.8(9)
Sn - C(1) - C(6)	109.9(5)	C(14) - C(19) - C(18)	112.9(9)
C(2) - C(1) - C(6)	111.4(7)	N(1) - C(20) - C(21)	113.9(9)
C(1) - C(2) - C(3)	111.9(7)	N(1) - C(20) - C(25)	113.4(9)
C(2) - C(3) - C(4)	110.8(8)	C(21) - C(20) - C(25)	120.3(9)
C(3) - C(4) - C(5)	110.4(8)	C(20) - C(21) - C(22)	112(1)
C(4) - C(5) - C(6)	112.4(8)	C(21) - C(22) - C(23)	116(1)
C(1) - C(6) - C(5)	110.6(8)	C(22) - C(23) - C(24)	116(1)
Sn - C(7) - C(8)	114.4(6)	C(23) - C(24) - C(25)	115(1)
Sn - C(7) - C(12)	112.7(6)	C(20) - C(25) - C(24)	113.3(9)

Observed and calculated structure factors for $[Cy_2Sn(S_2CNCy_2)Cl]$.

h	k	l	Fo	Fc	sigF
0	0	4	772	783	16
0	0	6	576	584	15
0	0	8	1130	1130	19
0	0	10	1107	1099	23
0	0	12	913	885	20
0	0	14	244	248	39
0	0	16	232	214	42*
0	0	18	0	231	98*
0	1	3	1015	1013	12
0	1	4	1013	1050	14
0	1	5	469	473	12
0	1	6	1070	1089	16
0	1	7	44	41	77*
0	1	8	729	745	16
0	1	9	252	273	30
0	1	10	0	35	93*
0	1	11	0	71	98*
0	1	12	437	399	24
0	1	13	0	142	99*
0	1	14	341	353	29
0	1	15	0	107	99*
0	1	16	241	184	40*
0	1	17	0	27	94*
0	1	18	152	45	78*
0	2	2	1223	1211	11
0	2	3	1269	1247	12
0	2	4	556	549	14
0	2	5	134	41	68*
0	2	6	109	41	71*
0	2	7	123	90	48*
0	2	8	810	821	16
0	2	9	0	43	73*
0	2	10	771	753	19
0	2	11	117	109	81*
0	2	12	448	364	23
0	2	13	0	26	99*
0	2	14	189	181	99*
0	2	15	205	162	48*
0	2	16	0	75	74*
0	2	17	0	88	97*
0	2	18	0	177	96*
0	3	1	566	577	10
0	3	2	1326	1336	12
0	3	3	1810	1840	14
0	3	4	1315	1325	14
0	3	5	807	825	16
0	3	6	1846	1859	17
0	3	7	371	387	18
0	3	8	743	739	17
0	3	9	233	216	34
0	3	10	49	85	79*
0	3	11	80	173	99*
0	3	12	198	211	99*
0	3	13	305	302	34
0	3	14	0	311	99*
0	4	0	933	907	10
0	4	1	483	497	9
0	4	2	642	647	13
0	4	3	485	478	13
0	4	4	572	575	13
0	4	5	201	205	23
0	4	6	299	273	18
0	4	7	767	788	15
0	4	8	601	628	14
0	4	9	669	687	17
0	4	10	432	428	22
0	4	11	327	369	32
0	4	12	136	100	77*
0	4	13	0	143	99*
0	4	14	0	64	99*
0	4	15	0	61	99*
0	4	16	162	43	98*
0	4	17	191	183	98*
0	4	18	0	146	94*
0	5	1	279	260	10
0	5	2	1145	1152	12
0	5	3	253	245	14
0	5	4	1607	1611	15
0	5	5	812	836	17
0	5	6	1469	1468	17
0	5	7	523	503	14
0	5	8	914	907	21
0	5	9	114	283	94*
0	5	10	0	32	80*
0	5	11	118	255	99*
0	5	12	0	110	99*
0	5	13	300	341	35
0	5	14	299	302	35
0	5	15	231	218	45*
0	5	16	18	275	99*
0	5	17	0	140	82*
0	5	18	56	73	93*
0	6	0	1186	1185	12
0	6	1	1087	1127	12
0	6	2	1138	1168	13
0	6	3	1503	1507	15
0	6	4	231	194	18
0	6	5	278	276	18
0	6	6	0	10	74*
0	6	7	806	761	20
0	6	8	269	249	27
0	6	9	807	782	19
0	6	10	479	500	22
0	6	11	543	531	21
0	6	12	275	269	38
0	6	13	95	198	99*
0	6	14	129	29	99*
0	6	15	0	10	99*
0	6	16	0	134	99*
0	6	17	167	166	97*
0	6	18	114	96	79*
0	7	1	0	36	52*
0	7	2	891	862	13
0	7	3	178	201	20
0	7	4	538	547	11
0	7	5	828	839	18
0	7	6	205	177	27
0	7	7	450	440	16
0	7	8	231	249	34
0	7	9	0	12	92*
0	7	10	142	172	98*
0	7	11	459	422	23
0	7	12	155	74	99*
0	7	13	466	429	23
0	7	14	177	151	99*
0	7	15	297	322	35
0	7	16	132	91	99*
0	7	17	154	108	97*
0	8	0	1092	1101	14
0	8	1	1219	1202	14
0	8	2	547	551	12
0	8	3	179	205	21
0	8	4	0	66	66*
0	8	5	419	418	14
0	8	6	271	242	21
0	8	7	453	440	17
0	8	8	0	116	89*
0	8	9	173	222	96*
0	8	10	0	9	99*
0	8	11	583	572	19
0	8	12	178	229	99*
0	8	13	136	179	85*
0	8	14	195	57	99*
0	8	15	0	116	99*
0	8	16	82	3	95*
0	8	17	73	135	94*
0	9	1	517	517	13
0	9	2	272	276	14
0	9	3	1013	978	16
0	9	4	87	161	68*
0	9	5	728	736	15
0	9	6	47	64	64*
0	9	7	332	358	22
0	9	8	0	39	88*
0	9	9	101	137	94*
0	9	10	0	13	96*
0	9	11	279	257	33
0	9	12	0	25	95*
0	9	13	483	497	23
0	9	14	136	38	97*
0	9	15	165	318	85*
0	9	16	0	59	98*
0	9	17	180	137	91*
0	10	0	72	122	49*
0	10	1	726	731	16
0	10	2	213	213	18
0	10	3	248	241	17
0	10	4	427	419	13
0	10	5	280	275	20
0	10	6	0	35	79*
0	10	7	607	601	14
0	10	8	80	231	91*
0	10	9	594	636	18
0	10	10	0	53	92*
0	10	11	450	453	22
0	10	12	76	52	95*
0	10	13	0	105	98*
0	10	14	202	119	48*
0	10	15	214	155	44*
0	10	16	143	56	63*
0	11	1	290	309	15
0	11	2	300	307	15
0	11	3	718	679	18
0	11	4	176	247	31*
0	11	5	900	895	19
0	11	6	0	31	81*
0	11	7	345	386	23
0	11	8	213	210	37*
0	11	9	133	159	61*
0	11	10	143	49	91*
0	11	11	115	231	80*
0	11	12	0	134	99*
0	11	13	329	332	29
0	11	14	0	110	97*
0	11	15	115	252	98*
0	11	16	0	66	92*
0	12	0	391	391	12
0	12	1	188	204	24
0	12	2	242	203	20
0	12	3	285	299	19
0	12	4	0	88	74*
0	12	5	0	87	78*
0	12	6	23	67	81*
0	12	7	487	524	17
0	12	8	0	145	86*
0	12	9	517	521	18
0	12	10	145	134	91*
0	12	11	0	198	98*
0	12	12	0	97	94*
0	12	13	0	57	95*
0	12	14	0	26	95*
0	12	15	0	34	92*
0	13	1	0	66	71*
0	13	2	0	127	72*
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3	10	-2	59	134	66*	3	12	-11	153	93	37*	3	13	14	0	133	91*	3	16	-13	0	17	72*	3	18	-3	0	6	69*
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4	19	-8	130	163	66*	5	1	-14	0	103	91*	5	2	6	265	253	29	5	4	-9	198	180	28	5	5	11	181	157	53*
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5	7	-8	249	242	21	5	8	14	133	55	96*	5	10	5	211	112	34	5	12	0	384	366	16	5	14	0	135	175	76*
5	7	-7	486	475	12	5	8	15	0	20	93*	5	10	6	476	462	18	5	12	1	280	268	22	5	14	1	262	253	23
5	7	-6	503	470	12	5	9	-17	0	8	80*	5	10	7	174	156	46*	5	12	2	93	92	77*	5	14	2	100	62	76*
5	7	-5	408	386	12	5	9	-16	236	209	29	5	10	8	510	525	19	5	12	3	109	142	79*	5	14	3	0	16	78*
5	7	-4	267	264	16	5	9	-15	0	14	85*	5	10	9	0	42	94*	5	12	4	219	199	31	5	14	4	107	67	79*
5	7	-3	0	64	61*	5	9	-14	216	261	35	5	10	10	257	254	37	5	12	5	0	25	83*	5	14	5	106	85	79*
5	7	-2	206	233	19	5	9	-13	0	14	87*	5	10	11	0	15	96*	5	12	6	221	220	33	5	14	6	94	144	60*
5	7	-1	175	201	23	5	9	-12	93	198	81*	5	10	12	0	94	96*	5	12	7	202	187	38*	5	14	7	0	194	88*
5	14	8	191	241	41*	5	17	-8	132	3	68*	5	20	-1	245	238	20	6	1	15	60	33	71*	6	3	2	73	166	73*
5	14	9	252	262	32	5	17	-7	356	346	15	5	20	0	0	97	72*	6	2	-18	160	210	47*	6	3	3	383	365	17
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5	15	-13	0	117	74*	5	17	-4	0	80	70*	5	20	3	44	48	53*	6	2	-15	140	51	76*	6	3	6	404	412	21
5	15	-12	160	143	34*	5	17	-3	137	199	74*	6	0	-18	143	202	56*	6	2	-14	91	207	93*	6	3	7	287	298	32
5	15	-11	69	32	60*	5	17	-2	0	52	75*	6	0	-16	0	157	94*	6	2	-13	0	90	88*	6	3	8	404	408	25
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5	15	-5	292	269	18	5	17	4	137	49	76*	6	0	-4	555	566	12	6	2	-7	943	954	17	6	3	14	0	177	93*
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5	16	-7	168	120	30*	5	18	6	0	79	79*	6	1	-6	385	357	12	6	2	15	126	74	66*	6	4	2	788	778	18
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5	16	4	167	57	36*	5	19	1	154	189	34*	6	1	5	0	61	89*	6	3	-8	170	180	30*	6	4	13	240	253	38
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6	14	-5	82	89	72*	6	16	4	306	301	22	6	20	0	0	137	69*	7	2	-13	563	576	18	7	3	9	228	269	40*
6	14	-4	240	200	22	6	16	5	124	75	52*	7	0	-17	65	189	91*	7	2	-12	0	111	87*	7	3	10	177	86	94*
6	14	-3	66	7	71*	6	16	6	0	128	82*	7	0	-15	394	436	25	7	2	-11	520	506	16	7	3	11	368	362	26
6	14	-2	70	18	62*	6	16	7	0	64	83*	7	0	-13	542	512	19	7	2	-10	280	245	24	7	3	12	0	91	95*
6	14	-1	265	286	22	6	16	8	115	26	83*	7	0	-11	620	609	16	7	2	-9	367	339	18	7	3	13	191	178	44*
6	14	0	183	218	32*	6	16	9	0	119	84*	7	0	-9	249	240	28	7	2	-8	0	24	75*	7	3	14	162	60	88*
6	14	1	414	440	17	6	17	-10	77	146	70*	7	0	-7	366	370	15	7	2	-7	164	13	27	7	4	-17	119	25	86*
6	14	2	238	215	26	6	17	-9	118	107	68*	7	0	-5	932	963	16	7	2	-6	331	320	14	7	4	-16	123	127	87*
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6	14	5	0	213	87*	6	17	-6	106	155	70*	7	0	1	411	388	16	7	2	-3	668	639	17	7	4	-13	377	402	21
6	14	6	52	33	85*	6	17	-5	0	142	74*	7	0	3	289	241	26	7	2	-2	128	19	30*	7	4	-12	127	150	84*
6	14	7	0	8	87*	6	17	-4	255	242	21	7	0	5	989	980	23	7	2	-1	763	770	17	7	4	-11	328	355	21
6	14	8	91	11	64*	6	17	-3	0	158	73*	7	0	7	436	469	22	7	2	0	176	175	28	7	4	-10	0	50	77*
6	14	9	175	157	88*	6	17	-2	72	182	75*	7	0	9	180	239	92*	7	2	1	278	276	21	7	4	-9	197	161	29
6	14	10	0	97	89*	6	17	-1	97	69	51*	7	0	11	87	141	68*	7	2	2	146	62	77*	7	4	-8	453	445	14
6	14	11	231	155	31	6	17	0	101	147	75*	7	0	13	122	185	62*	7	2	3	311	259	23	7	4	-7	152	78	29*
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7	6	-15	144	122	85*	7	7	8	238	268	39	7	9	3	228	228	31	7	11	1	213	202	29	7	13	4	291	286	25
7	6	-14	304	317	25	7	7	9	179	213	52*	7	9	4	516	513	16	7	11	2	688	706	17	7	13	5	128	58	84*
7	6	-13	0	158	85*	7	7	10	337	362	29	7	9	5	113	166	87*	7	11	3	261	292	26	7	13	6	83	75	82*
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7	6	-9	0	129	74*	7	8	-16	144	98	82*	7	9	9	0	81	98*	7	11	7	0	42	91*	7	13	10	80	143	87*

7	6	-8	226	236	24	7	8	-15	157	111	80*	7	9	10	268	272	34	7	11	8	96	137	91*	7	14	-13	171	227	30*
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7	6	-3	112	51	66*	7	8	-10	404	414	15	7	10	-14	34	213	68*	7	12	-14	128	116	69*	7	14	-8	146	141	34*
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7	6	-1	210	210	25	7	8	-8	127	22	71*	7	10	-12	0	155	78*	7	12	-12	178	153	31*	7	14	-6	239	260	22
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7	6	1	87	156	76*	7	8	-6	500	510	13	7	10	-10	105	85	70*	7	12	-10	99	47	54*	7	14	-4	357	359	17
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7	6	10	186	158	50*	7	8	3	149	71	47*	7	10	-1	320	305	20	7	12	-1	200	221	28	7	14	5	55	209	85*
7	6	11	102	128	97*	7	8	4	405	388	19	7	10	0	121	47	76*	7	12	0	0	23	76*	7	14	6	291	268	26
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7	6	14	135	127	86*	7	8	7	133	111	69*	7	10	3	130	41	67*	7	12	3	0	6	80*	7	14	9	59	115	88*
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7	7	-15	0	56	88*	7	8	10	151	167	97*	7	10	6	541	564	17	7	12	6	145	322	90*	7	15	-10	165	91	29*
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7	15	-5	145	63	36*	7	18	-1	56	79	61*	8	1	10	0	2	92*	8	3	3	315	279	24	8	5	-4	158	130	30*
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7	15	-2	268	269	22	7	18	2	0	3	74*	8	1	13	126	39	86*	8	3	6	416	408	22	8	5	-1	547	558	14
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7	15	3	145	124	41*	7	19	-3	0	8	68*	8	2	-13	134	20	71*	8	3	11	86	117	91*	8	5	4	423	427	20
7	15	4	0	153	83*	7	19	-2	87	28	68*	8	2	-12	234	229	30	8	3	12	209	260	41*	8	5	5	336	368	26
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7	15	7	0	47	84*	7	19	1	93	197	71*	8	2	-9	198	211	31	8	4	-16	183	191	39*	8	5	8	104	64	95*
7	15	8	99	110	84*	8	0	-16	162	207	92*	8	2	-8	285	292	20	8	4	-15	0	71	85*	8	5	9	0	101	98*
7	16	-11	77	157	68*	8	0	-14	133	21	63*	8	2	-7	414	394	14	8	4	-14	40	52	85*	8	5	10	136	113	93*
7	16	-10	87	69	68*	8	0	-12	198	233	39*	8	2	-6	0	72	67*	8	4	-13	73	83	82*	8	5	11	0	6	94*
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9	1	11	0	199	93*	9	3	8	211	150	42*	9	5	5	67	63	86*	9	7	4	127	97	58*	9	9	6	128	205	91*
9	1	12	0	27	84*	9	3	9	269	317	33	9	5	6	115	247	93*	9	7	5	159	63	85*	9	9	7	115	79	75*
9	2	-16	80	144	72*	9	3	10	0	90	93*	9	5	7	247	216	35	9	7	6	280	247	30	9	9	8	204	231	42*
9	2	-15	188	223	40*	9	3	11	85	208	89*	9	5	8	210	210	41*	9	7	7	141	163	71*	9	9	9	123	27	64*
9	2	-14	159	98	83*	9	3	12	0	48	87*	9	5	9	270	254	33	9	7	8	248	258	35	9	9	10	160	191	51*
9	2	-13	130	140	71*	9	4	-16	145	120	83*	9	5	10	101	122	93*	9	7	9	276	181	31	9	10	-14	203	177	27
9	2	-12	186	43	35*	9	4	-15	104	115	63*	9	5	11	0	125	94*	9	7	10	0	193	93*	9	10	-13	100	17	51*
9	2	-11	0	46	78*	9	4	-14	138	159	83*	9	5	12	145	78	73*	9	7	11	136	60	75*	9	10	-12	121	55	61*
9	2	-10	0	72	77*	9	4	-13	121	86	67*	9	6	-16	136	161	79*	9	8	-15	0	64	77*	9	10	-11	0	22	72*
9	2	-9	283	252	20	9	4	-12	0	148	80*	9	6	-15	0	79	83*	9	8	-14	201	221	30	9	10	-10	86	40	71*
9	2	-8	0	45	70*	9	4	-11	143	95	76*	9	6	-14	219	250	30	9	8	-13	90	29	74*	9	10	-9	114	44	69*
9	2	-7	565	559	14	9	4	-10	119	38	71*	9	6	-13	0	33	79*	9	8	-12	0	175	77*	9	10	-8	214	230	26
9	2	-6	384	381	14	9	4	-9	366	377	16	9	6	-12	241	231	26	9	8	-11	110	31	73*	9	10	-7	0	40	72*
9	2	-5	496	512	13	9	4	-8	69	110	71*	9	6	-11	0	88	76*	9	8	-10	0	10	74*	9	10	-6	363	370	16
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9	2	-1	101	32	64*	9	4	-4	357	352	16	9	6	-7	279	264	18	9	8	-6	513	503	13	9	10	-2	213	141	25
9	2	0	276	304	25	9	4	-3	89	65	71*	9	6	-6	396	374	15	9	8	-5	217	210	25	9	10	-1	74	30	73*
9	2	1	559	549	15	9	4	-2	201	169	28	9	6	-5	246	230	21	9	8	-4	580	547	12	9	10	0	0	124	77*
9	2	2	160	248	91*	9	4	-1	288	263	22	9	6	-4	435	453	14	9	8	-3	128	69	73*	9	10	1	0	97	81*
9	2	3	678	675	17	9	4	0	0	34	79*	9	6	-3	91	25	71*	9	8	-2	193	188	28	9	10	2	268	278	25
9	2	4	158	156	52*	9	4	1	765	752	17	9	6	-2	276	295	22	9	8	-1	72	64	74*	9	10	3	93	41	58*
9	2	5	564	558	17	9	4	2	0	204	87*	9	6	-1	182	247	33*	9	8	0	0	85	77*	9	10	4	290	298	27
9	2	6	134	77	91*	9	4	3	656	677	15	9	6	0	121	42	66*	9	8	1	0	48	79*	9	10	5	0	15	88*
9	2	7	303	287	30	9	4	4	275	279	29	9	6	1	377	414	19	9	8	2	0	186	82*	9	10	6	209	186	38*
9	2	8	0	37	95*	9	4	5	397	393	23	9	6	2	151	201	45*	9	8	3	124	105	63*	9	10	7	24	5	85*
9	2	9	175	31	93*	9	4	6	125	124	70*	9	6	3	348	346	22	9	8	4	279	329	28	9	10	8	0	6	90*
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9	3	-16	0	44	85*	9	4	10	156	53	91*	9	6	7	154	131	93*	9	8	8	0	15	91*	9	11	-12	257	267	21

9	11	-11	0	36	54*	9	13	0	240	223	25	9	17	-4	0	50	67*	10	2	-9	0	68	74*	10	4	-9	206	185	26
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9	11	-9	50	116	72*	9	13	2	184	141	34*	9	17	-2	0	104	72*	10	2	-7	225	229	23	10	4	-7	0	22	70*
9	11	-8	177	214	30*	9	13	3	96	21	80*	9	17	-1	183	180	28	10	2	-6	366	385	15	10	4	-6	117	132	70*
9	11	-7	0	189	73*	9	13	4	0	9	81*	9	17	0	0	43	69*	10	2	-5	0	15	71*	10	4	-5	214	190	23
9	11	-6	93	86	71*	9	13	5	0	80	84*	9	17	1	96	119	54*	10	2	-4	607	600	14	10	4	-4	214	235	24
9	11	-5	106	109	50*	9	13	6	130	86	84*	10	0	-16	0	106	85*	10	2	-3	0	117	76*	10	4	-3	102	216	75*
9	11	-4	126	65	71*	9	13	7	0	105	86*	10	0	-14	352	355	23	10	2	-2	725	704	16	10	4	-2	406	449	16
9	11	-3	0	9	61*	9	14	-11	107	59	68*	10	0	-12	387	356	20	10	2	-1	136	100	78*	10	4	-1	171	177	35*
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9	11	0	313	321	21	9	14	-8	61	138	67*	10	0	-6	360	336	15	10	2	2	135	142	56*	10	4	2	139	205	87*
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9	11	3	0	115	82*	9	14	-5	0	129	74*	10	0	0	548	532	16	10	2	5	138	11	92*	10	4	5	229	197	36
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9	12	-7	122	142	74*	9	15	-8	135	154	35*	10	1	-9	156	54	32*	10	3	-10	357	373	18	10	5	-9	198	191	27
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9	12	2	261	297	27	9	15	1	0	147	80*	10	1	0	414	408	18	10	3	-1	193	161	31	10	5	0	298	300	22
9	12	3	0	96	69*	9	15	2	0	18	81*	10	1	1	0	24	85*	10	3	0	338	385	21	10	5	1	359	325	19
9	12	4	241	258	31	9	15	3	0	11	79*	10	1	2	393	406	21	10	3	1	143	203	85*	10	5	2	454	464	17
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9	12	8	25	1	86*	9	16	-7	131	159	36*	10	1	6	286	267	31	10	3	5	142	114	91*	10	5	6	235	222	35
9	13	-12	96	176	69*	9	16	-6	103	104	52*	10	1	7	136	9	69*	10	3	6	245	157	35	10	5	7	0	29	94*
9	13	-11	135	167	35*	9	16	-5	213	211	23	10	1	8	0	32	92*	10	3	7	0	5	93*	10	5	8	136	25	88*
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9	13	-4	118	24	73*	9	16	2	128	28	71*	10	2	-13	94	67	83*	10	4	-13	206	133	29	10	6	-11	307	319	20				
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9	13	-2	154	123	36*	9	16	4	0	14	77*	10	2	-11	0	24	77*	10	4	-11	265	189	20	10	6	-9	235	207	23				
9	13	-1	253	247	23	9	17	-5	118	64	64*	10	2	-10	347	352	18	10	4	-10	257	264	22	10	6	-8	109	29	73*				
10	6	-7	64	34	68*	10	8	-2	288	247	20	10	10	7	178	206	42*	10	13	4	0	103	82*	11	1	-7	67	63	71*				
10	6	-6	136	85	69*	10	8	-1	326	278	19	10	10	8	133	2	85*	10	13	5	0	51	82*	11	1	-6	0	42	70*				
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10	6	0	122	216	67*	10	8	5	242	301	33	10	11	-7	307	295	18	10	14	-5	120	101	72*	11	1	0	0	15	84*				
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10	7	-2	128	76	43*	10	9	5	189	199	40*	10	12	-3	115	100	72*	10	16	-3	159	116	30*	11	2	-3	145	90	74*				
10	7	-1	158	106	36*	10	9	6	0	10	90*	10	12	-2	101	127	54*	10	16	-2	203	205	23	11	2	-2	0	129	76*				
10	7	0	178	169	34*	10	9	7	0	19	89*	10	12	-1	188	171	31	10	16	-1	0	53	69*	11	2	-1	85	210	80*				
10	7	1	274	299	25	10	9	8	0	13	90*	10	12	0	0	87	77*	10	16	0	141	124	36*	11	2	0	249	228	28				
10	7	2	198	181	35*	10	9	9	89	128	73*	10	12	1	0	76	78*	11	0	-15	133	102	84*	11	2	1	327	300	24				
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12	3	-4	0	19	74*	12	6	-12	0	38	70*	12	8	5	229	227	30	13	0	-7	125	55	71*	13	3	0	0	93	81*
12	3	-3	0	88	76*	12	6	-11	0	104	69*	12	9	-10	0	15	66*	13	0	-5	120	121	43*	13	3	1	159	195	42*
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12	4	4	281	237	27	12	7	-2	19	51	65*	12	10	4	0	3	66*	13	2	-8	43	130	67*	13	5	-4	0	189	75*
12	4	5	175	170	89*	12	7	-1	324	324	20	12	11	-8	113	53	37*	13	2	-7	0	23	70*	13	5	-3	27	40	74*
12	4	6	86	163	88*	12	7	0	70	109	68*	12	11	-7	226	196	21	13	2	-6	95	174	73*	13	5	-2	72	104	52*
12	4	7	120	106	71*	12	7	1	229	262	29	12	11	-6	111	68	41*	13	2	-5	0	108	71*	13	5	-1	0	131	78*
12	5	-13	0	43	70*	12	7	2	0	17	83*	12	11	-5	151	20	31*	13	2	-4	122	40	71*	13	5	0	107	26	59*
12	5	-12	102	73	47*	12	7	3	119	182	71*	12	11	-4	26	38	60*	13	2	-3	119	234	80*	13	5	1	202	190	31
12	5	-11	101	146	73*	12	7	4	0	21	85*	12	11	-3	117	141	72*	13	2	-2	0	98	79*	13	5	2	55	83	81*
12	5	-10	138	220	39*	12	7	5	0	2	86*	12	11	-2	98	22	73*	13	2	-1	271	254	24	13	5	3	42	190	84*
12	5	-9	80	216	72*	12	7	6	0	58	83*	12	11	-1	136	245	77*	13	2	0	95	137	83*	13	5	4	120	164	69*
12	5	-8	275	263	19	12	8	-11	76	46	67*	12	11	0	5	76	77*	13	2	1	179	159	39*	13	5	5	164	162	40*
12	5	-7	0	169	72*	12	8	-10	0	30	68*	12	11	1	245	262	25	13	2	2	130	78	83*	13	6	-10	0	172	71*
12	5	-6	224	212	25	12	8	-9	53	55	69*	12	11	2	102	58	77*	13	2	3	47	9	87*	13	6	-9	0	81	66*
12	5	-5	0	20	73*	12	8	-8	0	6	67*	12	11	3	0	180	80*	13	2	4	163	44	84*	13	6	-8	155	122	30*
12	5	-4	0	86	75*	12	8	-7	151	194	32*	12	12	-7	198	210	23	13	2	5	164	133	83*	13	6	-7	37	82	69*
12	5	-3	172	161	32*	12	8	-6	68	12	70*	12	12	-6	101	97	57*	13	3	-11	0	13	66*	13	6	-6	0	33	70*
12	5	-2	0	59	76*	12	8	-5	397	382	15	12	12	-5	210	211	23	13	3	-10	114	118	66*	13	6	-5	101	10	68*
12	5	-1	241	213	27	12	8	-4	68	71	72*	12	12	-4	71	123	70*	13	3	-9	0	107	58*	13	6	-4	224	198	24
12	5	0	0	181	81*	12	8	-3	414	382	16	12	12	-3	46	114	72*	13	3	-8	77	124	53*	13	6	-3	0	119	77*

13	6	-2	204	210	29	14	1	-9	119	54	63*	14	5	0	109	129	77*														
13	6	-1	202	171	30	14	1	-8	0	80	67*	14	5	1	127	81	45*														
13	6	0	189	189	32*	14	1	-7	101	45	43*	14	6	-7	224	198	19														
13	6	1	0	72	80*	14	1	-6	96	157	70*	14	6	-6	61	64	67*														
13	6	2	0	123	84*	14	1	-5	115	62	42*	14	6	-5	175	179	27														
13	6	3	0	3	82*	14	1	-4	238	264	24	14	6	-4	105	28	69*														
13	6	4	130	3	67*	14	1	-3	0	9	75*	14	6	-3	154	91	32*														
13	7	-9	0	31	67*	14	1	-2	305	329	21	14	6	-2	129	77	40*														
13	7	-8	142	143	31*	14	1	-1	129	53	79*	14	6	-1	0	20	76*														
13	7	-7	0	11	67*	14	1	0	168	182	39*	14	6	0	0	141	75*														
13	7	-6	239	271	22	14	1	1	0	44	81*	14	7	-5	92	120	67*														
13	7	-5	0	30	70*	14	1	2	70	17	80*	14	7	-4	0	90	71*														
13	7	-4	307	301	19	14	1	3	0	16	80*	14	7	-3	139	179	36*														
13	7	-3	57	51	73*	14	2	-9	0	83	67*	14	7	-2	119	95	60*														
13	7	-2	167	184	34*	14	2	-8	159	199	29*																				
13	7	-1	0	67	77*	14	2	-7	0	86	70*																				
13	7	0	0	51	77*	14	2	-6	185	197	27																				
13	7	1	144	123	77*	14	2	-5	0	26	72*																				
13	7	2	146	112	79*	14	2	-4	150	105	33*																				
13	7	3	167	127	37*	14	2	-3	0	44	76*																				
13	8	-9	0	66	68*	14	2	-2	115	64	75*																				
13	8	-8	119	78	37*	14	2	-1	0	117	78*																				
13	8	-7	0	79	68*	14	2	0	0	181	82*																				
13	8	-6	0	5	69*	14	2	1	125	151	51*																				
13	8	-5	91	66	58*	14	2	2	215	223	31																				
13	8	-4	0	120	74*	14	3	-9	0	111	67*																				
13	8	-3	0	84	74*	14	3	-8	85	40	55*																				
13	8	-2	244	227	22	14	3	-7	88	81	68*																				
13	8	-1	0	72	62*	14	3	-6	0	98	70*																				
13	8	0	194	202	30	14	3	-5	116	42	69*																				
13	8	1	0	2	76*	14	3	-4	206	235	26																				
13	8	2	77	112	79*	14	3	-3	119	25	73*																				
13	8	3	0	42	76*	14	3	-2	249	231	23																				
13	9	-7	0	22	68*	14	3	-1	0	90	79*																				
13	9	-6	203	261	25	14	3	0	115	161	60*																				
13	9	-5	0	22	70*	14	3	1	0	95	80*																				
13	9	-4	219	284	25	14	3	2	0	79	82*																				
13	9	-3	0	11	74*	14	4	-8	88	194	51*																				
13	9	-2	38	138	62*	14	4	-7	88	127	68*																				
13	9	-1	0	7	78*	14	4	-6	102	163	58*																				
13	9	0	116	36	74*	14	4	-5	121	104	41*																				
13	9	1	0	7	74*	14	4	-4	0	37	71*																				
13	10	-6	0	68	68*	14	4	-3	124	15	72*																				
13	10	-5	0	68	67*	14	4	-2	131	133	74*																				
13	10	-4	27	80	68*	14	4	-1	0	22	78*																				
13	10	-3	0	5	73*	14	4	0	202	222	31																				
13	10	-2	143	192	37*	14	4	1	0	92	76*																				
13	10	-1	88	69	71*	14	4	2	242	224	25																				
13	10	0	215	226	26	14	5	-7	63	32	66*																				
14	0	-8	209	178	21	14	5	-6	111	61	40*																				
14	0	-6	139	188	35*	14	5	-5	58	111	58*																				
14	0	-4	112	145	50*	14	5	-4	44	146	71*																				
14	0	-2	0	14	66*	14	5	-3	174	144	30*																				
14	0	0	157	165	81*	14	5	-2	209	173	26																				
14	0	2	207	217	33	14	5	-1	0	118	76*																				

E. $[^tBu_2Sn(S_2CN(Et)Cy)Cl]$

Crystallographic Data and Refinement details for [$^{t}Bu_2Sn(S_2CNCyEt)Cl$].

Formula	$C_{17}H_{34}ClNS_2Sn$
Formula weight	470.7
Crystal morphology	colourless plate
Crystal dimensions (mm)	0.08 x 0.32 x 0.37
Crystal system	monoclinic
Space group	$P2_1/n$ (C_{2h}^5, No. 14)
Temperature (°C)	20.0
a (Å)	13.481(5)
b (Å)	11.466(5)
c (Å)	15.351(8)
β (°)	107.51(4)
V (Å^3)	2262(1)
Z	4
D_{calc} (g cm^{-3})	1.382
F(000)	968
Radiation	MoKα (λ = 0.7107Å)
μ (cm^{-1})	14.29
θ limits, data (°)	3.0 to 27.5
hkl range	0 to 18, 0 to 15, -20 to 20
Range of transmission factors	0.955 to 1.000
Scan technique	ω:2θ
Scan width (°)	1.00
No. of data measured	5699
No. of unique data	5478
R_{amal}	0.107
Program for structure solution	Direct Methods (SIR92)
No. of unique data used	2707
No. of parameters	199
R	0.049
R_w	0.053
G.O.F.	1.57
Min./Max. residual electron density (e Å^{-3})	-1.24 to +0.73

Fractional atomic coordinates ($Å^2$) for the non-hydrogen atoms in [$^tBu_2Sn(S_2CNCyEt)Cl$].

Atom	*x*	*y*	*z*
Sn(1)	-0.09221(4)	0.30436(4)	0.68721(3)
Cl(1)	-0.2270(2)	0.1510(2)	0.6604(2)
S(1)	0.0115(2)	0.1532(2)	0.6386(2)
S(2)	0.1011(2)	0.3858(2)	0.6901(2)
N(1)	0.2086(4)	0.2055(5)	0.6543(4)
C(1)	-0.0631(7)	0.3257(8)	0.8341(6)
C(2)	0.0080(11)	0.2268(14)	0.8829(8)
C(3)	-0.1640(8)	0.3202(10)	0.8562(6)
C(4)	-0.0137(10)	0.4458(12)	0.8622(7)
C(5)	-0.1784(6)	0.4272(7)	0.5822(5)
C(6)	-0.2870(7)	0.4389(9)	0.5909(6)
C(7)	-0.1256(8)	0.5450(8)	0.5969(7)
C(8)	-0.1827(9)	0.3784(10)	-0.4105(6)
C(9)	0.1190(6)	0.2450(6)	0.6607(5)
C(10)	0.2193(6)	0.0828(6)	0.6295(6)
C(11)	0.1807(8)	0.0596(8)	0.5282(6)
C(12)	0.3043(5)	0.2774(5)	0.6831(5)
C(13)	0.3620(6)	0.2800(7)	0.6128(5)
C(14)	0.4533(7)	0.3634(9)	0.6448(7)
C(15)	0.5253(7)	0.3278(8)	0.7374(8)
C(16)	0.4685(7)	0.3180(8)	0.8070(7)
C(17)	0.3728(7)	0.2394(8)	0.7751(5)

Anisotropic thermal parameters (Å^2) for the non-hydrogen atoms in [^{t}Bu$_2$Sn(S$_2$CNCyEt)Cl].

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Sn	0.0403(3)	0.0413(3)	0.0378(3)	0.0040(3)	0.0097(2)	0.0057(3)
Cl(1)	0.066(1)	0.066(1)	0.119(2)	0.029(1)	0.036(1)	0.020(1)
S(1)	0.050(1)	0.043(1)	0.086(2)	0.010(1)	0.024(1)	0.022(1)
S(2)	0.047(1)	0.040(1)	0.079(2)	0.006(1)	0.022(1)	0.019(1)
N(1)	0.040(3)	0.039(3)	0.036(3)	-0.005(3)	0.009(2)	0.004(3)
C(1)	0.070(6)	0.078(6)	0.044(5)	-0.009(5)	0.022(4)	-0.005(5)
C(2)	0.17(1)	0.22(2)	0.066(8)	-0.12(1)	0.027(8)	-0.060(9)
C(3)	0.102(8)	0.119(8)	0.057(6)	-0.008(7)	0.044(6)	-0.015(6)
C(4)	0.15(1)	0.17(1)	0.064(8)	0.06(1)	0.055(7)	0.066(8)
C(5)	0.048(5)	0.055(5)	0.037(5)	-0.003(4)	-0.002(3)	0.000(4)
C(6)	0.066(6)	0.100(8)	0.074(7)	-0.016(6)	0.010(5)	-0.018(6)
C(7)	0.070(6)	0.069(6)	0.105(8)	-0.001(6)	-0.015(6)	-0.026(6)
C(8)	0.13(1)	0.125(9)	0.038(6)	-0.009(8)	0.014(6)	-0.005(6)
C(9)	0.052(5)	0.033(3)	0.031(4)	0.001(4)	0.006(3)	0.005(3)
C(10)	0.051(5)	0.042(4)	0.070(6)	-0.004(4)	0.010(4)	0.015(4)
C(11)	0.082(7)	0.091(7)	0.067(7)	-0.001(6)	0.013(5)	0.047(6)
C(12)	0.037(4)	0.032(4)	0.046(5)	-0.003(3)	0.008(3)	-0.001(3)
C(13)	0.048(4)	0.084(6)	0.043(5)	0.001(5)	0.015(4)	-0.012(4)
C(14)	0.061(6)	0.105(8)	0.090(8)	0.007(6)	0.033(6)	-0.022(6)
C(15)	0.048(5)	0.080(7)	0.113(9)	0.012(5)	0.012(6)	0.014(6)
C(16)	0.063(6)	0.073(6)	0.067(6)	-0.002(5)	-0.014(5)	0.014(5)
C(17)	0.067(6)	0.071(5)	0.036(5)	0.007(5)	0.000(4)	0.006(4)

Fractional atomic coordinates and B_{eq} values ($Å^2$) for the hydrogen atoms in [$^tBu_2Sn(S_2CNCyEt)Cl$].

Atom	x	y	z	B_{eq}
H(2a)	0.0221	0.2352	0.9470	14.8
H(2b)	-0.0714	0.2297	0.8678	14.8
H(2c)	-0.0252	0.1541	0.8640	14.8
H(3a)	-0.1940	0.2450	0.8413	8.4
H(3b)	-0.2130	0.3775	0.8218	8.4
H(3c)	-0.1517	0.3344	0.9195	8.4
H(4a)	-0.0590	0.5047	0.8289	11.7
H(4b)	0.0508	0.4499	0.8492	11.7
H(4c)	-0.0024	0.4571	0.9257	11.7
H(6a)	-0.3217	0.3659	0.5783	7.8
H(6b)	-0.3248	0.4955	0.5486	7.8
H(6c)	-0.2827	0.4627	0.6512	7.8
H(7a)	-0.1191	0.5716	0.6569	8.6
H(7b)	-0.1659	0.5990	0.5537	8.6
H(7c)	-0.0584	0.5383	0.5892	8.6
H(8a)	-0.1139	0.3671	0.4865	9.4
H(8b)	-0.2181	0.4319	0.4432	9.4
H(8c)	-0.2186	0.3061	0.4804	9.4
H(10a)	0.1809	0.0353	0.6585	5.3
H(10b)	0.2908	0.0622	0.6511	5.3
H(11a)	0.1874	-0.0211	0.5172	7.8
H(11b)	0.2207	0.1036	0.4984	7.8
H(11c)	0.1097	0.0818	0.5052	7.8

Atom	x	y	z	B_{eq}
H(12a)	0.2832	0.3551	0.6897	3.8
H(13a)	0.3167	0.3059	0.5559	5.5
H(13b)	0.3867	0.2041	0.6058	5.5
H(14a)	0.4277	0.4396	0.6491	7.9
H(14b)	0.4912	0.3631	0.6017	7.9
H(15a)	0.5555	0.2544	0.7318	7.9
H(15b)	0.5786	0.3846	0.7572	7.9
H(16a)	0.4469	0.3937	0.8188	7.1
H(16b)	0.5144	0.2867	0.8615	7.1
H(17a)	0.3946	0.1612	0.7712	5.8
H(17b)	0.3347	0.2435	0.8180	5.8

Bond distances (Å) for [$^{t}Bu_2Sn(S_2CNCyEt)Cl$].

Atom - Atom	Distance	Atom - Atom	Distance
Sn(1) - Cl(1)	2.472(2)	C(1) - C(4)	1.53(1)
Sn(1) - S(1)	2.479(2)	C(5) - C(6)	1.52(1)
Sn(1) - S(2)	2.756(2)	C(5) - C(7)	1.51(1)
Sn(1) - C(1)	2.182(8)	C(5) - C(8)	1.51(1)
Sn(1) - C(5)	2.192(7)	C(10) - C(11)	1.51(1)
S(1) - C(9)	1.739(7)	C(12) - C(13)	1.51(1)
S(2) - C(9)	1.713(7)	C(12) - C(17)	1.50(1)
N(1) - C(9)	1.320(8)	C(13) - C(14)	1.52(1)
N(1) - C(10)	1.476(9)	C(14) - C(15)	1.52(1)
N(1) - C(12)	1.482(8)	C(15) - C(16)	1.49(1)
C(1) - C(2)	1.53(1)	C(16) - C(17)	1.53(1)
C(1) - C(3)	1.50(1)		

Bond angles (°) for [$^{t}Bu_2Sn(S_2CNCyEt)Cl$].

Atom - Atom - Atom	Angle	Atom - Atom - Atom	Angle
Cl(1) - Sn(1) - S(1)	84.57(8)	C(3) - C(1) - C(4)	108.7(9)
Cl(1) - Sn(1) - S(2)	152.57(7)	Sn(1) - C(5) - C(6)	107.7(6)
Cl(1) - Sn(1) - C(1)	98.4(3)	Sn(1) - C(5) - C(7)	110.0(5)
Cl(1) - Sn(1) - C(5)	97.7(2)	Sn(1) - C(5) - C(8)	108.4(6)
S(1) - Sn(1) - S(2)	68.01(6)	C(6) - C(5) - C(7)	109.4(8)
S(1) - Sn(1) - C(1)	116.6(2)	C(6) - C(5) - C(8)	110.6(7)
S(1) - Sn(1) - C(5)	116.8(2)	C(7) - C(5) - C(8)	110.7(8)
S(2) - Sn(1) - C(1)	94.0(2)	S(1) - C(9) - S(2)	116.5(4)
S(2) - Sn(1) - C(5)	94.8(2)	S(1) - C(9) - N(1)	120.4(5)
C(1) - Sn(1) - C(5)	125.3(3)	S(2) - C(9) - N(1)	123.1(5)
Sn(1) - S(1) - C(9)	91.7(2)	N(1) - C(10) - C(11)	113.8(7)
Sn(1) - S(2) - C(9)	83.3(3)	N(1) - C(12) - C(13)	112.8(6)
C(9) - N(1) - C(10)	120.6(6)	N(1) - C(12) - C(17)	110.7(6)
C(9) - N(1) - C(12)	121.4(6)	C(13) - C(12) - C(17)	112.0(6)
C(10) - N(1) - C(12)	117.5(5)	C(12) - C(13) - C(14)	108.8(7)
Sn(1) - C(1) - C(2)	108.3(7)	C(13) - C(14) - C(15)	111.2(7)
Sn(1) - C(1) - C(3)	109.7(6)	C(14) - C(15) - C(16)	111.7(8)
Sn(1) - C(1) - C(4)	108.6(6)	C(15) - C(16) - C(17)	112.3(7)
C(2) - C(1) - C(3)	109.6(9)	C(12) - C(17) - C(16)	110.5(7)
C(2) - C(1) - C(4)	112(1)		

Observed and calculated structure factors for [^{t}Bu$_2$Sn(S$_2$CNCyEt)Cl].

h	k	l	Fo	Fc	sigF
0	0	4	1736	1820	30
0	0	6	2095	2153	36
0	0	8	936	995	20
0	0	10	470	486	13
0	0	12	0	126	62*
0	0	14	302	329	18
0	0	16	378	362	19
0	0	18	158	211	87*
0	1	2	2542	2595	43
0	1	3	24	21	29*
0	1	4	2200	2175	38
0	1	5	370	370	9
0	1	6	607	598	14
0	1	7	861	856	17
0	1	8	341	355	10
0	1	9	95	44	23*
0	1	10	751	770	19
0	1	11	560	565	15
0	1	12	632	630	17
0	1	13	268	236	16
0	1	14	341	343	16
0	1	15	109	54	69*
0	1	16	146	10	74*
0	1	17	125	76	80*
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4	5	-10	0	211	72*	4	6	10	378	387	13	4	8	1	72	28	50*	4	10	-2	79	12	52*	4	12	5	120	103	61*
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7	9	-7	58	77	50*	7	11	1	206	210	21	8	1	-17	64	84	54*	8	2	4	610	612	17	8	4	-7	231	247	22
7	9	-6	57	51	49*	7	11	2	84	4	46*	8	1	-16	299	341	16	8	2	5	490	512	14	8	4	-6	230	209	19
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7	9	3	237	229	18	7	12	-8	71	95	57*	8	1	-7	51	48	51*	8	2	14	123	186	87*	8	4	3	655	629	19
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9	3	12	108	191	80*	9	5	5	55	44	58*	9	7	3	321	324	15	9	9	8	71	36	65*	10	0	-8	803	835	21
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13	4	-11	87	69	47*	13	6	0	273	262	18	14	0	-14	111	147	35*	14	2	6	115	97	27*	14	5	-3	190	143	22
13	4	-10	192	142	25	13	6	1	217	173	21	14	0	-12	301	279	15	14	3	-15	194	133	20	14	5	-2	0	28	66*
13	4	-9	160	114	29*	13	6	2	273	311	19	14	0	-10	140	144	28*	14	3	-14	0	69	63*	14	5	-1	281	257	18
13	4	-8	385	372	17	13	6	3	95	168	56*	14	0	-8	216	200	18	14	3	-13	35	8	65*	14	5	0	0	3	65*
13	4	-7	295	317	20	13	6	4	110	183	68*	14	0	-6	385	370	14	14	3	-12	54	24	56*	14	5	1	250	257	19
13	4	-6	406	413	16	13	6	5	60	19	65*	14	0	-4	231	213	17	14	3	-11	170	181	27	14	5	2	0	24	63*
13	4	-5	253	271	20	13	7	-13	184	132	31*	14	0	-2	87	71	36*	14	3	-10	87	89	67*	14	5	3	0	102	66*
13	4	-4	128	141	66*	13	7	-12	205	217	31	14	0	0	0	94	54*	14	3	-9	304	288	18	14	5	4	0	9	60*
13	4	-3	0	81	66*	13	7	-11	257	233	26	14	0	2	253	249	15	14	3	-8	220	218	22	14	6	-13	143	199	73*
13	4	-2	281	287	18	13	7	-10	0	146	81*	14	0	4	281	352	14	14	3	-7	238	219	21	14	6	-12	86	127	78*
13	4	-1	297	286	16	13	7	-9	165	171	38*	14	0	6	82	137	58*	14	3	-6	251	229	19	14	6	-11	246	240	25
13	4	0	404	409	15	13	7	-8	0	9	77*	14	1	-16	160	148	22	14	3	-5	114	35	66*	14	6	-10	0	123	80*
13	4	1	196	193	19	13	7	-7	100	38	75*	14	1	-15	73	20	49*	14	3	-4	63	28	65*	14	6	-9	39	79	74*
13	4	2	282	288	16	13	7	-6	52	79	73*	14	1	-14	70	109	62*	14	3	-3	306	271	16	14	6	-8	134	12	71*
14	6	-7	164	132	32*	15	1	-6	105	87	63*	15	4	-7	76	42	68*	16	0	2	181	186	18	16	4	-1	127	140	33*
14	6	-6	0	108	55*	15	1	-5	387	372	15	15	4	-6	132	32	30*	16	1	-13	115	98	35*	16	4	0	0	36	63*
14	6	-5	238	239	24	15	1	-4	153	110	24	15	4	-5	0	86	68*	16	1	-12	234	231	20	16	5	-9	74	68	69*
14	6	-4	107	141	45*	15	1	-3	50	83	61*	15	4	-4	201	202	23	16	1	-11	95	99	56*	16	5	-8	0	77	72*
14	6	-3	232	211	22	15	1	-2	0	1	60*	15	4	-3	0	40	67*	16	1	-10	354	327	16	16	5	-7	0	35	75*
14	6	-2	0	70	67*	15	1	-1	200	205	19	15	4	-2	322	304	16	16	1	-9	122	37	33*	16	5	-6	123	130	71*
14	6	-1	171	110	25	15	1	0	136	126	25*	15	4	-1	130	43	29*	16	1	-8	0	119	71*	16	5	-5	59	113	69*
14	6	0	0	11	65*	15	1	1	276	286	15	15	4	0	212	219	21	16	1	-7	0	6	64*	16	5	-4	185	151	26
14	6	1	0	58	68*	15	1	2	65	142	57*	15	4	1	98	66	39*	16	1	-6	258	222	18	16	5	-3	175	161	26
14	6	2	85	121	55*	15	1	3	193	222	18	15	4	2	113	19	60*	16	1	-5	58	49	64*	16	5	-2	105	9	55*
14	6	3	170	182	27	15	1	4	0	69	47*	15	4	3	0	22	59*	16	1	-4	393	375	15	16	5	-1	160	128	26
14	7	-11	0	85	78*	15	2	-14	126	96	64*	15	5	-12	0	127	75*	16	1	-3	45	108	62*	16	6	-7	0	140	76*
14	7	-10	0	149	78*	15	2	-13	107	94	39*	15	5	-11	74	45	52*	16	1	-2	138	228	70*	16	6	-6	130	99	37*
14	7	-9	223	191	29	15	2	-12	264	229	18	15	5	-10	0	49	69*	16	1	-1	114	96	30*	16	6	-5	0	75	74*
14	7	-8	252	234	25	15	2	-11	239	224	20	15	5	-9	101	37	53*	16	1	0	81	3	38*	16	6	-4	32	94	69*
14	7	-7	122	137	46*	15	2	-10	143	164	34*	15	5	-8	97	97	69*	16	1	1	0	27	58*	17	0	-9	62	82	62*
14	7	-6	186	164	31	15	2	-9	146	250	73*	15	5	-7	187	133	28	16	1	2	122	128	27*	17	0	-7	179	145	23
14	7	-5	0	35	74*	15	2	-8	156	31	24	15	5	-6	230	258	24	16	2	-12	81	68	45*	17	0	-5	308	304	18
14	7	-4	0	14	70*	15	2	-7	118	94	34*	15	5	-5	65	76	68*	16	2	-11	120	88	38*	17	0	-3	126	186	69*
14	7	-3	0	69	69*	15	2	-6	50	45	65*	15	5	-4	274	247	19	16	2	-10	0	89	67*	17	1	-10	114	37	65*
14	7	-2	187	160	26	15	2	-5	114	131	67*	15	5	-3	0	33	68*	16	2	-9	132	129	34*	17	1	-9	267	232	19
14	7	-1	166	125	27	15	2	-4	62	161	68*	15	5	-2	126	57	67*	16	2	-8	246	240	20	17	1	-8	0	33	56*
14	7	0	299	236	17	15	2	-3	298	273	15	15	5	-1	105	46	39*	16	2	-7	0	113	66*	17	1	-7	232	208	20
14	7	1	126	150	67*	15	2	-2	307	309	16	15	5	0	124	146	65*	16	2	-6	0	166	70*	17	1	-6	90	69	62*
14	7	2	66	138	68*	15	2	-1	249	233	16	15	5	1	0	12	64*	16	2	-5	62	110	54*	17	1	-5	0	7	52*
14	8	-10	151	146	79*	15	2	0	207	187	18	15	5	2	204	209	20	16	2	-4	0	11	63*	17	1	-4	0	35	61*
14	8	-9	0	23	81*	15	2	1	67	87	58*	15	6	-11	61	95	55*	16	2	-3	121	50	31*	17	1	-3	186	194	23
14	8	-8	0	13	78*	15	2	2	0	62	61*	15	6	-10	124	193	78*	16	2	-2	134	111	30*	17	1	-2	88	17	46*
14	8	-7	0	90	78*	15	2	3	109	75	29*	15	6	-9	209	150	26	16	2	-1	97	122	52*	17	2	-9	33	4	62*
14	8	-6	136	174	44*	15	2	4	170	204	21	15	6	-8	215	195	26	16	2	0	169	160	22	17	2	-8	150	9	27*
14	8	-5	109	71	62*	15	3	-14	187	186	23	15	6	-7	90	21	70*	16	2	1	180	214	22	17	2	-7	166	139	27
14	8	-4	231	234	27	15	3	-13	0	93	64*	15	6	-6	111	68	70*	16	3	-12	58	55	63*	17	2	-6	131	40	29*
14	8	-3	115	32	59*	15	3	-12	86	46	65*	15	6	-5	0	115	72*	16	3	-11	165	170	28*	17	2	-5	197	197	23
14	8	-2	153	154	34*	15	3	-11	0	41	56*	15	6	-4	104	130	69*	16	3	-10	117	46	64*	17	2	-4	126	124	64*
14	8	-1	0	8	69*	15	3	-10	101	97	57*	15	6	-3	105	109	70*	16	3	-9	64	68	64*	17	2	-3	76	104	48*
14	8	0	54	35	51*	15	3	-9	0	13	63*	15	6	-2	221	237	23	16	3	-8	117	24	35*	17	2	-2	78	127	62*
14	9	-5	0	78	74*	15	3	-8	156	158	30*	15	6	-1	83	56	65*	16	3	-7	0	20	65*	17	3	-8	68	114	65*
14	9	-4	0	38	77*	15	3	-7	121	80	65*	15	6	0	0	150	71*	16	3	-6	0	83	68*	17	3	-7	71	33	63*
15	0	-13	145	130	27*	15	3	-6	234	234	19	15	6	1	100	25	53*	16	3	-5	136	95	32*	17	3	-6	0	55	63*
15	0	-11	423	380	15	15	3	-5	183	112	22	15	7	-9	83	48	72*	16	3	-4	0	29	63*	17	3	-5	92	57	48*
15	0	-9	421	387	15	15	3	-4	248	234	19	15	7	-8	0	110	75*	16	3	-3	217	195	20	17	3	-4	109	12	63*
15	0	-7	187	125	21	15	3	-3	137	80	29*	15	7	-7	109	165	64*	16	3	-2	0	27	60*	17	3	-3	106	100	63*
15	0	-5	328	305	15	15	3	-2	77	48	60*	15	7	-6	200	204	29	16	3	-1	252	201	16						
15	0	-3	517	503	15	15	3	-1	0	3	60*	15	7	-5	154	126	33*	16	3	0	37	49	63*						
15	0	-1	328	337	14	15	3	0	226	222	18	15	7	-4	0	164	76*	16	3	1	0	22	60*						
15	0	1	0	47	56*	15	3	1	116	90	62*	15	7	-3	162	33	29*	16	4	-11	129	79	36*						
15	0	3	113	124	29*	15	3	2	282	281	16	15	7	-2	0	12	67*	16	4	-10	107	24	68*						
15	1	-14	135	98	28*	15	3	3	115	130	62*	15	7	-1	0	24	70*	16	4	-9	147	137	33*						
15	1	-13	223	239	21	15	3	4	75	121	62*	16	0	-12	171	163	27	16	4	-8	119	67	38*						
15	1	-12	109	10	61*	15	4	-13	0	33	66*	16	0	-10	0	129	57*	16	4	-7	77	122	68*						
15	1	-11	125	113	63*	15	4	-12	134	172	68*	16	0	-8	445	399	15	16	4	-6	0	88	68*						
15	1	-10	120	93	34*	15	4	-11	31	4	64*	16	0	-6	426	379	15	16	4	-5	109	97	55*						
15	1	-9	91	161	69*	15	4	-10	178	193	29	16	0	-4	0	46	62*	16	4	-4	0	12	66*						
15	1	-8	0	110	63*	15	4	-9	81	12	53*	16	0	-2	296	274	16	16	4	-3	62	18	64*						
15	1	-7	401	397	15	15	4	-8	165	174	30*	16	0	0	280	288	15	16	4	-2	46	96	55*						

Chapter 6

Conclusion

6.1 Conclusion

A combined crystallographic and theoretical study into the influence of crystal packing on molecular geometry in certain diorganotin compounds is reported.

Firstly, an array diorganotin systems including polymorphs, solvated molecules and systems with multiple molecules in the asymmetric unit were investigated. Polymorphs of particular compounds converged to the same yet more symmetric gas phase structure (as determined by *ab initio* geometry optimisations). Generally, while bond angles subtended at tin did not change significantly beyond that required to effect symmetrisation of the structure, Sn-ligand separations tended to elongate in the gas phase. For systems with multiple molecules in the asymmetric unit and/or with solvent trapped in the lattice similar observations were made. In terms of energy differences it may be concluded that the energy difference between molecules in two distinct crystalline environments (i.e. polymorphs) are greater than energy differences between two molecules that crystallise in the one lattice. Further, the presence of solvent in the lattice does not markedly alter the energy differences calculated between the condensed (solid state) and gas phases, allowing for different sizes of the molecules.

A series of diimine adducts, R_2SnCl_2(2,2'-bipyridyl) and R_2SnCl_2(1,10-phenanthroline), all adopting a common structural motif, i.e. a distorted octahedral in the solid state, were systematically investigated by combined crystallographic and theoretical methods. Correlations between the structural and electronic parameters associated with the tin centre were investigated without the influence of significant changes in molecular geometry. An examination of the experimental Sn-N and Sn-Cl bond lengths with the moderated (i.e. the changing the nature of R) Lewis acidities of the tin atoms shows a general correlation i.e. longer distances with decreasing Lewis acidities. Deviations from these correlations could be explained in terms of *intra*molecular Cl...H interactions. Generally the gas phase structures, as generated by the *ab initio* geometry optimisations,

displayed no significant differences between the chemically equivalent geometric parameters about the tin centre. In addition a better correlation between the Sn-Cl and the Sn-N bond distances and the Lewis acidity of the tin atom is apparent when compared to the solid state structures.

A similar investigation of a series of structures with increased flexibility in the coordination environments was undertaken. The $R_2Sn(S_2CNR'_2)Cl$ series of compounds chosen, consistently adopted a common structural motif in which the tin atom exists in a distorted trigonal bipyramid geometry. Attempts to correlate the experimental Sn-ligand parameters in the solid state structures with systematic variations in the Lewis acidity of the tin centre (i.e. by moderating R) and the Lewis basicity of the dithiocarbamate ligand (i.e. by moderating R') were unsuccessful across the series. There was no correlation found between the Sn-ligand parameters and the systematic variations in the Lewis acidity of the tin center or the Lewis basicity of the dithiocarbamate ligand in the solid state. Gas phase structures were more symmetric and systematic variations in the Sn-ligand parameters could be correlated with the Lewis basicity of the dithiocarbamate ligands. Trends were also found upon variation of the Lewis acidity of the tin center but these could not be correlated with the electronic structures of the tin-bound substituents alone, indicating that the steric profiles of the substituents may influence the Lewis acidity of the tin center.

These key results are attributed to the influence of crystal packing forces on the geometric parameters about the tin centre in the solid state. These results indicate that there is no inherent chemical reason for the adoption of non-symmetric structures in the solid state and thus, indicate that intermolecular forces, i.e. crystal packing effects over and above electronic and steric effects do exert a significant influence on the molecular geometry in these systems.