Synthesis and characterisation of a range of antimony(I/III) *N*'-bis(2,6-diisopropylphenyl)formamidinate complexes

Authors

Areej Al-Dabbagh[a], Zhifang Guo[a], Peter Junk[a]* and Jun Wang[a]

[a]College of Science and Engineering, James Cook University, Townsville, QLD, 4811, Australia

Correspondence email: peter.junk@jcu.edu.au

Abstract Formamidinatoantimony(I/III) complexes have been successfully synthesised as monomers or dimers in the solid state featuring a variety of coordination geometries and have also been comprehensively characterized. The antimony(I) formamidinate complex, $[Sb_2(DippForm)_2]\cdot 7thf$ (**1**) was obtained by a metathesis reaction between sodium bis(trimethylsilyl)amide ($NaN(SiMe_3)_2$) and *N,N´*-bis(2,6-diisopropylphenyl)formamidine (DippFormH) followed by $SbCl_3$. A range of trivalent haloformamidinatoantimony(III) complexes, $[Sb(DippForm)_2X]$ (X = Cl, **2**; Br, **3**; I, **4**) and $[Sb(DippForm)X_2]$ **(**X = Br, **5**; I, **6)** were also synthesized by adding DippFormH and $MN(SiMe_3)_2$ (M = Li or Na) to the corresponding antimony halides SbX_3(X = Cl, Br, I) in differing ratios. The complexes were all stable to rearrangement.

Keywords:Antimony (I)/(III) complexes; *N,N'*-bis(2,6-diisopropylphenyl)formamidine; Crystal structures; Formamidinates.

1. Introduction

Nitrogen-based ligand systems, in particular guanidinates and amidinates are of major importance and there are limited examples of mono and trivalent antimony complexes cited in the literature where the molecular structures are crystallographically authenticated. [CSD Version 5.42, Feb. 2021] The first guanidinatoantimony(III) complex, $[Sb\{(iPrN)_2CN\text{-}(H)iPr\}\{(iPrN)_2CNiPr\}]$ was obtained by the reaction between 1,2,3-triisopropylguanidine $[(iPrNH)_2C{=}NiPr]$ with antimony tris(dimethylamide) $[Sb(NMe_2)_3]$ in toluene, and features helices through N–H···N hydrogen bonding (Bailey et al., 1997), and two more guanidinatoantimony (III) complexes $[X_2Sb\{\kappa^2\text{-}N,N´\text{-}(ArN)_2CR\}]$ [X = Cl, I; Ar = 2,6-iPr$_2$C$_6$H$_3$(Dipp); R = $N(Cy)_2$] were reported in 2007 (Green et al., 2007). The first structurally characterized mononuclear amidinatoantimony(III) complex $[Ph_2Cl_2Sb(N_2Me_2CPh)]$ was reported in 1982 (Weller et al., 1982), and in 1986 the crystal structure of $[C_6H_5C(NCH_3)_2SbCl_4]$ was reported by

the reaction of N-chlor-*N*,*N*'-dimethylbenzamidine and $SbCl_3$ in CH_2C1_2 solution (Honeise et al., 1986). Later, a number of amidinatoantimony(III) complexes, $[Cl_2Sb\{(Me_3SiN)_2CPh\}]$ (Ergezinger et al., 1988), $Sb[\{2\text{-}(6\text{-}Me)C_5H_3N\}NSiMe_3]_2Cl$ (Raston et al., 1998), $ClSb[PhC(NSiMe_3)_2]_2$ (Pata-Siebel et al., 1990), $[RC(NR')_2]SbCl_2$ [R = *t*Bu, R´ = *i*Pr, Cy, 2,6-$iPr_2C_6H_3$(Dipp); R = *n*Bu, R´ = *i*Pr] (Lyhs et al., 2009), [*t*Bu$(NR)_2$] (R =iPr or Dipp) (Lyhs et al., 2011), and $Sb(hpp)_nCl_{3-n}$ (n = 1 or 2) (Day et al., 2012), were obtained by the metathesis reactions of the alkali metal complexes and SbX_3 (X = F, Cl, Br, I).

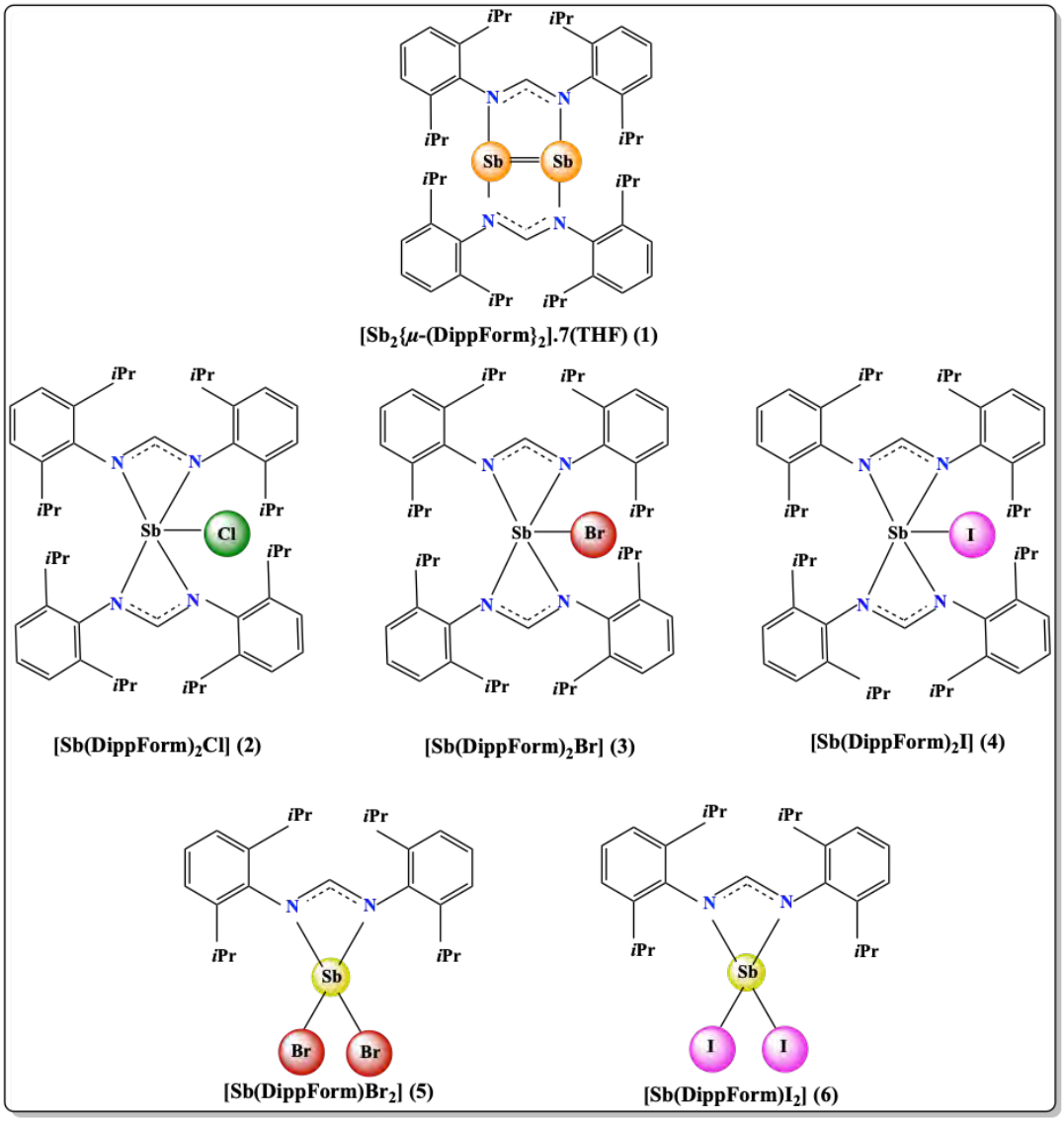
N,*N*´-Bis(aryl)formamidinate (RNC(H)NR) ligands are a very distinct class of nitrogen based ligands. That distinction belongs to the ability of their phenyl substituents to be readily adjusted in order to achieve synthetic requirements, such as modifying the steric bulk at the ortho position (H→iPr). Utilising amidinate ligands of high steric demand can result in complexes with uncommon low coordination numbers. A number of bismuth(III) formamidinate complexes $[Bi(L)X_2]_2$ [LH = *N*,*N*′-bis(2,6-diisopropylphenyl)formamidine (DippFormH) or *N*,*N*′-bis(2,6-dimethylphenyl)formamidine (XylFormH); X = Br, Cl], $Bi(L)_2X$ [LH = XylFormH, *N*,*N*′-bis(2-phenylphenyl)formamidine (2-PhPhFormH); X = Br, Cl)] and $Bi(L)_3$ (LH = *N*,*N*′-bis(2,6-diethylphenyl)formamidine (EtFormH) or *N*,*N*′-bis(2,4,6-trimethylphenyl)formamidine (MesFormH)] have been synthesized through metathesis reactions of the alkali metal formamidinates ML (M = Li or K) with BiX_3 (X = Cl, Br or Bu^n) (Brym et al., 2007). The bulky isopropyl groups affect the ligand flexibility, and as a consequence different coordination modes of DippForm can be adopted (Deacon et al., 2017). Extension of this chemistry to antimony (III) enabled an exploration of the formamidinatoantimony chemistry.

The trivalent state is common for the heavier pnictogen (As, Sb, Bi) analogues, and some interesting divalent complexes have been developed (Zhao et al., 2017). The kinetic stabilization of low-coordination group 15 chemistry was established by Yoshifuji etal in 1981 when they reported the first stable diphosphene, Mes*P=PMes* (Mes* = $C_6H_2tBu_3$-2,4,6) (Yoshifuji et al., 1981), followed by products of base coordinated heavier dipnictenes, RE=ER (E = P, As, Sb, or Bi) ((Jones, 2001; Tokitoh, 2000). The lowest unoccupied molecular orbitals (LUMOs) of dipnictenes including antimony have the ability to accept electrons from reducing agents (Sasamori et al., 2006). Consequently, the doubly bonded systems of the heavier group 15 elements (dipnictenes) have become accessible and ArSb=SbAr (Ar = 2,4,6-$[CH(SiMe_3)_2]_3C_6H_2$) was successfully obtained (Sasamori et al., 2005). A study reported on a different synthetic approach, showing that initial treatment of $SbCl_3$ with $K[(TerN)_2P]$ (Ter = 2,6-dimesityl-phenyl) led to a diazadipnictane, $[Ter_2N_2P(III)Sb(III)Cl_2]$, which was transformed to a cyclic diazastibaphosphenium cation $[P(\mu\text{-}NTer)2SbCl]^+$ by a halide abstraction step using $SbCl_3$. A donor-stabilised $[Sb_2]^{2+}$ ion of a dimerised biradical $[Sb_2\text{-}\{\mu\text{-}(TerN)_2P\}_2]$ was obtained from a subsequent reduction of $[Ter_2N_2PSbCl_2]$ with KC_8 in a non-polar solvent (Hinz et al., 2016).

We now report the successful syntheses of a range of formamidinatoantimony(I/III) complexes by metathesis reactions of the alkali bis(trimethylsilyl)amide, *N*,*N*′-bis(2,6-diisopropylphenyl)formamidine (DippFormH) and SbX_3 (X = Cl, Br, I). The interesting monovalent $[Sb_2(DippForm)_2]$ was also obtained by the reduction of Sb^{3+} to Sb^{+}.

2. Results and discussion

The synthesis of a variety of antimony(I/III) formamidinate complexes was achieved by the reactions of M[DippForm] (prepared by treatment of $MN(SiMe_3)_2$ (M = Li, Na) with DippFormH) and SbX_3 (X = Cl, Br, I) in different ratios (**Scheme 1**).

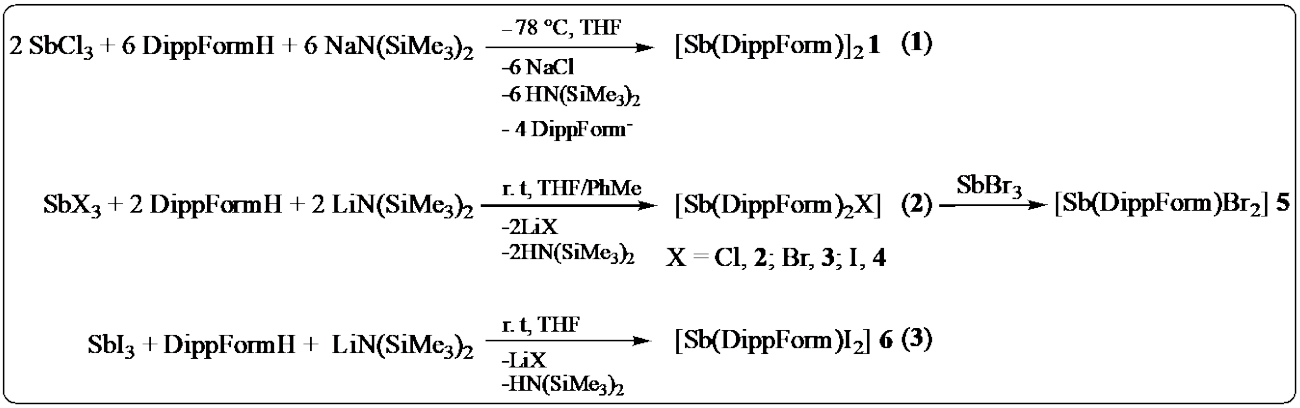


Scheme 1

The antimony(I) formamidinate complex $[Sb_2(DippForm)_2]\cdot 7thf$ (**1**) was prepared by the reaction between $NaN(SiMe_3)_2$, DippFormH, followed by adding $SbCl_3$ in THF from a 3 : 3 : 1 reaction stoichiometry [eq.1]. The dimeric crystalline complex **1** was isolated instead of an expected Sb^{3+}

complex $[SbL_{3-n}Cl_n]$ (n = 2, 1, 0) due to an unanticipated reduction reaction, reducing Sb^{3+} to Sb^{+}. NaCl precipitated from the reaction mixture and Sb(I) was trapped in the C–N pocket forming a bridged Sb^{+} compound. Reduction reactions of SbX_3 (X = Cl, Br, I) with DippFormH and several reducing agents (Na, K, Mg) were also attempted, as well as the reactions with hydride transfer reagents (NaH, KH, $LiAlH_4$) in different solvents (THF, PhMe, hexane), with the aim of forming low valent Sb species. However, all reduction reactions were unsuccessful. The low valent Sb complex presumably formed by reductive elimination, as found in some reported Bi and Sb complexes. (Zhao et al., 2017; Jones, 1991; Waterman & Tilley, 2006).

The bis-substituted antimony(III) formamidinate complexes $[Sb(DippForm)_2Cl]$ (**2**), $[Sb(DippForm)_2Br]$ (**3**), $[Sb(DippForm)_2I]$ (**4**), and the unisubstituted $[Sb(DippForm)I_2]$ (**6**) were obtained in good yields by the reaction of $LiN(SiMe_3)_2$, DippFormH with corresponding SbX_3 (X = Cl, Br, I) in 2 : 2 : 1 and 1 : 1 : 1 ratios, respectively [eq.2 and eq.3]. $[Sb(DippForm)Br_2]$ (**5**) was prepared by the reaction of $[Sb(DippForm)_2Br]$ (**3**) with $SbBr_3$ in THF in 1 : 1 stoichiometry.



It was worth noting that the attempted reactions to synthesise the tris-substituted complex $[Sb(DippForm)_3]$ by treating $LiN(SiMe_3)_2$, DippFormH with SbX_3 (X = Cl, Br, I) in 3 : 3 : 1 all failed, in spite of comparable findings having previously been described for organobismuth complexes $[Bi(MesForm)_3]$ and $[Bi(EtForm)_3]$.[14] This outcome is attributed to the bulkiness of DippForm (steric coordination number 2.54, *cf* $C_6H_3(tBu)_2$-2,6, 2.42 $(Me_3Si)_2N$, 2.17) (Marcalo & Pires de Matos, 1989; Cole et al., 2005; Cole et al., 2007; Guo et al., 2020) and DippForm is more bulky compared with MesForm and EtForm.

All antimony formamidinates (**1**-**6**) were identified by X-ray crystallography, being crystallised from THF (**1**, **5**), toluene (**2, 4, 6**) or hexane (**3**). Complexes **2** and **3** gave microanalyses for the bulk products as expected for the compositions indicated by X-ray crystallography. Although satisfactory microanalyses could not be obtained for **1, 4** and **5** (the products were highly air and moisture sensitive, which led to low carbon percentage), they had IR spectra in close agreement with those of appropriate comparison (compound **3** and **6**), and the ^{1}H NMR spectra were consistent with the X-ray composition.

In the ^{1}H NMR spectra, the NCHN resonance of the free ligand DippFormH was substantially shifted to higher frequencies from its position in complexes **1-6**.

3. X-ray crystallograpuic study

Representative structures of **1-6** are shown in **Figure 1-3**, which also list important bond distances and angles. Crystal data, data collection and structure refinement details are given in **Table 1**.

[Sb$_2$(DippForm)$_2$]·7thf (**1**)

The monovalent antimony formamidinate complex [Sb$_2$(DippForm)$_2$]·7thf (**1**) crystallized in the monoclinic space group $P2_1/c$. As shown in **Figure 1**, the structure of dinuclear complex **1** has an inversion centre at the midpoint of the Sb−Sb interaction. Each Sb atom is coordinated in a unidentate fashion with two DippForm ligands and bridging Sb$_2$ unit trapped by the two DippForm ligands . The Sb atoms form two Sb-N bonds that are close to linear [N1-Sb1-N3: 171.1(2) °; N2-Sb2-N4 170.6(2) °]. The Sb1–Sb2 bond length of 2.6808(8) Å is slightly longer than the bond length of 2.6438(4) Å found in [Sb$_2$-{μ-(TerN)$_2$P}$_2$] (Hinz et al., 2016). The average Sb–N bond length is 2.300(7) Å, which is shorter than those found in [Sb$_2$-{μ-(TerN)$_2$P}$_2$] [Sb-N: 2.372(2) Å] (Hinz et al., 2016).

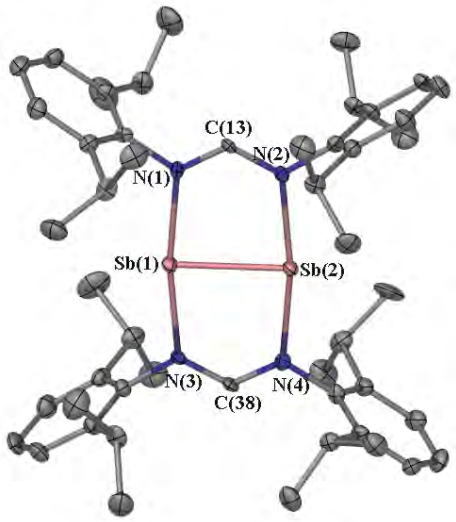


Figure 1 Molecular diagram of [Sb$_2$(DippForm)$_2$]·7thf (**1**) represented by 50% thermal ellipsoids. The lattice thf molecules and hydrogen atoms have been omitted for clarity. Selected bond lengths (Å) and angles (°): Sb(1)–N(1) 2.299(7), Sb(1)–N(3) 2.287(6), Sb(2)–N(2) 2.301(6), Sb(2)–N(4) 2.313(7), Sb(1)–Sb(2) 2.6808(8), N(1)-Sb(1)-N(3) 171.1(2); N(2)-Sb(2)-N(4) 170.6(2).

[Sb(DippForm)$_2$X] (**X = Cl, 2; Br, 3; I, 4**)

The mono-halide compounds [Sb(DippForm)$_2$X] (X = Cl, **2**; Br, **3**; I, **4**) crystallised in the monoclinic space group $P2_1/c$ with five coordinate Sb ions (**Figure 2**). The Sb atom is chelated by two bidentate DippForm ligands and one terminal halide ligand (X= Cl, Br, I). The geometry around the Sb atom is a distorted trigonal bipyramid. The antimony atom shares a plane with the halide atom X and two nitrogen

atoms (N2/N3) from the two DippForm ligands in equatorial positions, while the other two nitrogen atoms (N1/N4) from the ligands above and below the plane (axial or apical positions) [N1-Sb-N4 **2** 154.62(1), **3** 156.22(10), **4** 156.04(13)]. The coordination environment for the Sb atom in (**2-4**) is similar with the reported Bi complexes [Bi(XylForm)$_2$Br] and [Bi(2-PhPhForm)$_2$Br], where XylForm and 2-PhPhForm ligands were involved instead of the bulky DippForm ligand (Brym et al., 2007). The two *N*,*N*′-DippForm ligands have a *transoid* disposition [C(13)-Sb-C(38) **2** 129.97(6), **3** 130.85(11), **4** 130.54(13) °]. It is apparent that the Sb-N bond distances with the same *N*,*N*′-DippForm ligand are significantly different, a single Sb-N bond (Sb-N1 and Sb-N3 around 2.1-2.2 Å), and a secondary longer interaction Sb–N bond (Sb-N2 and Sb-N4 around 2.5-2.6 Å), which are similar to the reported [Ter$_2$N$_2$PSbCl$_2$] (Hinz et al., 2016) and [BiL$_2$Br] (Brym et al., 2007). The average Sb-N bond distance is 2.359(17), 2.369(3) and 2.376(4) Å for **2, 3** and **4**, respectively, which has as expected slightly shorter than the average Bi-N bond length of [Bi(XylForm)$_2$Br] and [Bi(2-PhPhForm)$_2$Br] (Brym et al., 2007). The Sb–X bond length is 2.3972(7), 2.5581(6) and 2.7722(5) for Sb–Cl**,** Sb–Br and Sb–I, respectively. The Sb-Br in [Sb(DippForm)$_2$Br] is also shorter than the Bi-Br in [Bi(XylForm)$_2$Br] [2.740(1)] and [Bi(2-PhPhForm)$_2$Br] [2.6908(5)] (Brym et al., 2007).

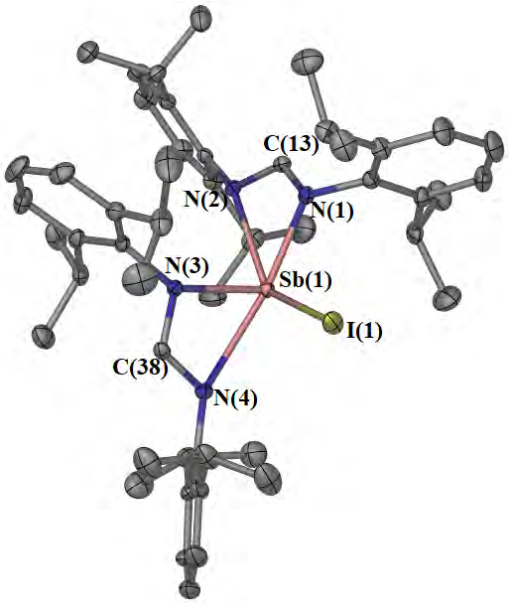


Figure 2 Molecular diagram of **[Sb(DippForm)$_2$I]** (representative of Cl, **2**, Br, **3**, I, **4**) with non-hydrogen atoms represented by 50% thermal ellipsoids. Selected bond lengths (Å) and angles (°): **Compound 2** Sb(1)–N(1) 2.1587(19), Sb(1)–N(2) 2.6044(17), Sb(1)–N(3) 2.1121(17), Sb(1)–N(4) 2.5593(19), Sb(1)–Cl(1) 2.3972(7), C(13)–Sb(1)–C(38) 129.97(6), C(13)–Sb(1)–Cl(1) 114.16(5), C(38)–Sb(1)–Cl(1) 86.29(4); **Compound 3** Sb(1)–N(1) 2.158(3), Sb(1)–N(2) 2.629(3), Sb(1)–N(3) 2.111(3), Sb(1)–N(4) 2.576(3), Sb(1)–Br(1) 2.5581(6), C(13)–Sb(1)–C(38) 130.85(11), C(13)–Sb(1)–Br(1) 114.28(7), C(38)–Sb(1)–Br(1) 87.58(8); **Compound 4** Sb(1)–N(1) 2.163(4), Sb(1)–N(2)

2.634(3), Sb(1)–N(3) 2.113(4), Sb(1)–N(4) 2.595(4), Sb(1)–I(1) 2.7722(5), C(13)–Sb(1)–C(38) 130.54(13), C(13)–Sb(1)–I(1) 114.77(10), C38(1)–Sb(1)–I(1) 88.30(9).

[Sb(DippForm)X_2] (X = Br, 5; I, 6)

The mono-formamidinatoantimony(III) complexes [Sb(DippForm)X_2] (Br, **5**; I, **6**) (**Figure 3**) are monomers, with one bidentate DippForm ligand and two terminal halide (Br, **5**; I, **6**) ligands bound to Sb giving four coordinate metal centres. Compounds **5** and **6** are isostructural and crystallize in the triclinic space group *P*-1. The coordination environment observed for the central Sb atoms in **5** and **6** can be described as a heavily distorted tetrahedral geometry. The average Sb-N bond distance is 2.263(2) and 2.273(5) Å for **5** and **6**, respectively. The Sb–X bond length is 2.558(7) and 2.774(7) for Sb–Br and Sb–I, respectively. All the bond lengths differ is as expected from ionic radii differences. In contrast, the solid state structures of Group 15 tetra-coordinated bismuth (III) formamidinate complexes of the general formula [Bi(L)Br(μ-Br)(thf)]$_2$ [L = DippForm or XylForm)] have previously observed, forming symmetrical dimers, bridged by two bromides and a coordinated thf molecule on each Bi atom (Brym et al., 2007).

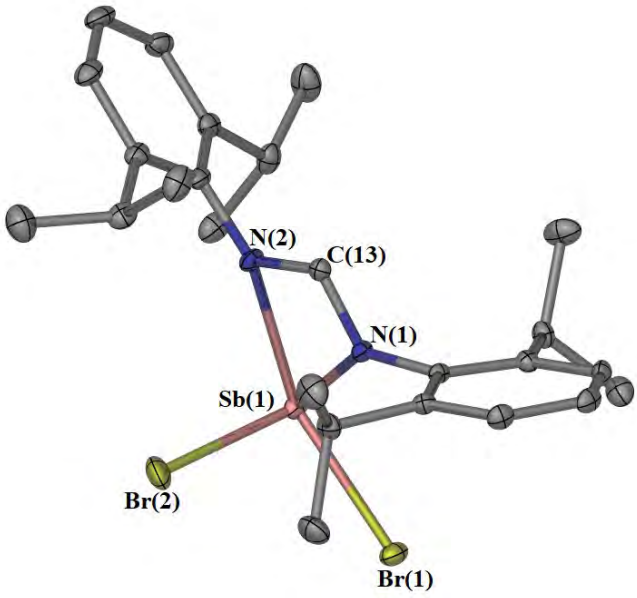


Figure 2 Molecular diagram of **[Sb(DippForm)Br_2]** (representative of Br, **5**, I, **6**) with non-hydrogen atoms represented by 50% thermal ellipsoids. Selected bond lengths (Å) and angles (°): **Compound 5** Sb(1)–N(1) 2.091(2), Sb(1)–N(2) 2.435(2), Sb(1)–Br(1) 2.5989(14), Sb(1)–Br(2) 2.5172(7), Br(1)–Sb(1)–Br(2) 94.98(3), C(13)–Sb(1)–Br(1) 119.68(4), C(13)–Sb(1)–Br(2) 95.33(6); **Compound 6** Sb(1)–N(1) 2.105(5), Sb(1)–N(2) 2.441(5), Sb(1)–I(1) 2.8190(6), Sb(1)–I(2) 2.7282(8), I(1)–Sb(1)–I(2) 95.93(3), C(13)–Sb(1)–I(1) 120.55(10), C(13)–Sb(1)–I(2) 94.87(15).

Table 1

Experimental details

Crystal	**1**	**2**	**3**
Chemical formula	$C_{50}H_{70}N_4Sb_2\cdot7(C_4H_8O)$	$C_{50}H_{70}ClN_4Sb$	$C_{50}H_{70}BrN_4Sb$
M_r	1475.32	884.30	928.76
Crystal system, space group	Monoclinic, $P2_1/c$	Monoclinic, $P2_1/c$	Monoclinic, $P2_1/c$
Temperature (K)	100	100	123
a, b, c (Å)	21.243 (4), 18.997 (4), 21.743 (4)	18.443 (4), 20.455 (4), 12.817 (3)	18.7239 (14), 20.5497 (17), 12.9785 (10)
β (°)	118.60 (3)	97.46 (3)	96.886 (4)
V (Å^3)	7704 (3)	4794.3 (17)	4957.7 (7)
Z	4	4	4
Radiation type	Synchrotron, λ = 0.71073 Å	Synchrotron, λ = 0.71073 Å	Mo $K\alpha$
μ (mm^{-1})	0.75	0.67	1.40
Crystal size (mm)	0.06 × 0.04 × 0.01	0.11 × 0.05 × 0.03	0.5 × 0.35 × 0.07
Data collection			
Diffractometer	ADSC Quantum 315r	ADSC Quantum 210r	Bruker *APEX*-II CCD
Absorption correction	Multi-scan XDS (Kabsch, 1993)	Multi-scan XDS (Kabsch, 1993)	Multi-scan *SADABS2012*/1 (Bruker,2012)
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	21388, 21388, 17952	58107, 8002, 7706	63607, 8731, 5851
R_{int}	?	0.039	0.109
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.742	0.595	0.595
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.091, 0.271, 1.19	0.029, 0.073, 1.08	0.040, 0.102, 1.01

No. of reflections	21388	8002	8731
No. of parameters	882	522	522
No. of restraints	151		
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	2.59, -3.73	1.01, −0.82	0.62, −0.74

Crystal	**4**	**5**	**6**
Chemical formula	$C_{50}H_{70}IN_4Sb$	$C_{25}H_{35}Br_2N_2Sb$	$C_{25}H_{35}I_2N_2Sb$
M_r	975.75	645.12	739.10
Crystal system, space group	Monoclinic, $P2_1/c$	Triclinic, *P*-1	Triclinic, *P*-1
Temperature (K)	123	100	123
a, *b*, *c* (Å)	18.616 (2), 20.713 (2), 12.9942 (13)	10.105 (2), 10.332 (2), 14.240 (3)	10.4137 (4), 10.5559 (4) 14.6097 (5)
β (°)	96.750 (5)	96.69 (3), 103.93 (3), 111.72 (3)	95.876 (2), 104.946 (2), 111.754 (2)
V (Å^3)	4975.8 (9)	1305.2 (5)	1405.64 (9)
Z	4	2	2
Radiation type	Mo *K*α	Synchrotron, λ = 0.71073 Å	Mo *K*α
μ (mm^{-1})	1.21	4.13	3.19
Crystal size (mm)	0.45 × 0.3 × 0.08	0.1 × 0.04 × 0.02	0.45 × 0.15 × 0.08
Data collection			
Diffractometer	Bruker *APEX*-II CCD	ADSC Quantum 210r	Bruker *APEX*-II CCD
Absorption correction	Multi-scan *SADABS2012*/1 (Bruker,2012)	Multi-scan XDS (Kabsch, 1993)	Multi-scan *SADABS2012*/1 (Bruker,2012)

No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	63063, 8728, 5504	23524, 6298, 6079	35754, 6393, 4879
R_{int}	0.089	0.032	0.077
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.595	0.744	0.650
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.045, 0.118, 1.01	0.028, 0.075, 1.07	0.071, 0.227, 1.04
No. of reflections	8728	6298	6393
No. of parameters	521	279	279
No. of restraints			
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.85, −1.17	0.50, −1.25	2.98, −2.24

Computer programs: SHELXT 2014/5 (Sheldrick, 2014), *SHELXL* 2018/3 (Sheldrick, 2015), Olex2 1.3 (Dolomanov *et al.*, 2009).

4. Conclusions

This is the first reported contribution for formamidinato-based mono and trivalent antimony chemistry. Herein we reported the results of metathesis reactions, which produced monomeric structures with the generic formula [Sb(DippForm)$_{3-n}$X$_n$] (n = 1, X = Cl **2**, Br **3**, I **4**; n = 2, X = Br **5**, I **6**, synthesised by the addition of M (DippFormH), (M = Li, Na), to the appropriate SbX_3 (X = Cl, Br, I) compounds. The sterically bulky formamidinate ligand (DippForm) highlights the ability to stabilize low-oxidation-state *p*-block compounds with unusual coordination modes. Isolation of the Sb^+ dimeric structure of [Sb$_2${μ-(DippForm}$_2$]·7thf (**1**) was the alternative to an expected Sb^{3+} monomeric complex, but the synthesis was repeatable using the method described. Overall, the results add to the large field of main group metal *N,N'*-chelated compounds by introducing new ligands to antimony chemistry. Compounds **2-6** are forming the basis of further chemistry where we intend to treat these compounds with reducing agents to form further (to **1**) low valent antimony compounds.

5. Experimental

General

The antimony compounds described here are highly air- and moisture sensitive, hence were prepared and were handled using vacuum-nitrogen line techniques and a dry box under an atmosphere of purified nitrogen. DippFormH was prepared by literature methods (Roberts, 1949). All other chemicals were purchased from Sigma and used without purification. Solvents (thf, toluene, hexane, C_6D_6) were pre-dried by distillation over sodium or sodium benzophenone ketyl before being stored under an atmosphere of nitrogen. IR spectra were recorded as Nujol mulls between NaCl plates using a Nicolet-Nexus FTIR spectrophotometer within the range 4000–400 cm^{-1}. ^1H NMR spectra were recorded on a Bruker AVANCE III HD 400MHz instrument. Microanalyses were determined by the Elemental Analysis Service, London Metropolitan University, and all the samples were sealed in tubes under nitrogen before transport. Melting points were determined in sealed glass capillaries under nitrogen and are uncalibrated. Crystals were immersed in viscous hydrocarbon oil, and were examined on the MX1 or MX2 beamlines at the Australian Synchrotron or Bruker APEX-II. Crystal data and refinement details are given in **Table S1**. CCDC 2090149-2090154 for compound **1-6**, contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

[Sb_2{μ-(DippForm}$_2$]·7thf (**1**)

A solution of Na(DippForm), prepared from DippFormH (1.08 g, 3.0 mmol) and $NaN(SiMe_3)_2$ (0.6 M solution in PhMe, 1.8 mL, 3.0 mmol) in THF (5 mL), was added dropwise to a solution of $SbCl_3$ (1.0 mmol) in THF (10 mL) at -78 °C while stirring. The solution adopted a dark green colour after 5 minutes, the suspension was stirred for 5 h and allowed to warm to ambient temperature, and continued to be stirred for 18 h. The solution was filtered by cannula and concentrated under vacuum to the point of crystallisation ca.5 mL. Light orange block crystals **1** were obtained at -30 °C overnight. The crystals were dried in vacuo after separation from the mother solution via syringe. Yield = 0.66 g (62 %), M.P. 210-212 °C. ^1H NMR (400 MHz, C_6D_6, 25 °C): δ (ppm) = 1.12 (d, J = 6.7 Hz, 48H, $CH(CH_3)_2$),1.34 (m, 28H, CH_2-thf), 3.42 (sept, 8H, $CH(CH_3)_2$), 3.64 (m, 28H, OCH_2-thf), 6.98 (m, 4H, p-ArH), 7.06 (m, 8H, m-ArH), 10.60 (s, 2H, NC(H)N). Elemental analysis calcd. (%) for $C_{78}H_{126}N_4O_7Sb_2$ (MW, 1475.32): $C_{50}H_{70}N_4Sb_2$ (MW, 970.65, loss of 7 THF in lattice): C 61.87, H 7.27, N 5.77; found: C 58.61, H 7.22, N 3.57, showing low carbon and nitrogen percentage. IR (Nujol, cm^{-1}): 2923 (s), 2728 (w), 2364 (m), 2183 (m), 1926 (s), 1861 (s), 1792 (s), 1668 (m), 1581 (m), 1462 (s), 1377 (s), 1257 (m), 1182 (m), 1093 (m), 930 (s), 823 (w), 721 (s), 672 (m).

[Sb(DippForm)$_2$Cl] (**2**)

A solution of Li(DippForm), prepared from DippFormH (0.72 g, 2.0 mmol) and $LiN(SiMe_3)_2$ (1 M solution in thf, 2.0 mL, 2.0 mmol) in THF (20 mL), was added dropwise to a solution of $SbCl_3$ (0.22 g, 1.0 mmol) in THF (10 mL) at room temperature with stirring. The colour of the solution changed within seconds. The reaction mixture continued to be stirred for two days at ambient temperature. The reaction

mixture was dried under vacuum and dissolved in PhMe (20 mL). The mixture was then filtered to remove LiCl. The filtrate was concentrated under vacuum, colourless block crystals **2** were obtained at -30 °C. Yield = 0.43 g (60 %), M.P. 198-200 °C. ^{1}H NMR (400 MHz, C_6D_6, 25 °C): δ (ppm) = 1.13 (d, J = 6.8, 48H, $CH(CH_3)_2$), 3.44 (sept, 8H, $CH(CH_3)_2$), 6.91 (m, 4H, *p*-ArH), 7.03 (m, 8H, *m*-ArH), 10.93 (s, 2H, NC(H)N). Elemental analysis calcd. (%) for $C_{50}H_{70}ClN_4Sb$ (MW, 884.32): C 67.91, H 7.98, N 6.34; found: C 67.49, H 7.83, N 6.20. IR (Nujol, cm^{-1}): 2922 (m), 2727 (w), 2166 (w), 2097 (m), 2060 (m), 2008 (vs), 1926 (s), 1862 (s), 1796 (s), 1734 (vs), 1666 (s), 1640 (w), 1586 (s), 1464 (vs), 1454 (vs), 1377 (s), 1294 (w), 1232 (m), 1184 (m), 1156 (m), 1097 (s), 1057 (s), 1011 (s), 956 (s), 934 (s), 881 (m), 821 (s), 798 (s), 721 (s), 672 (s), 474 (w).

[Sb(DippForm)$_2$Br] (**3**)

$LiN(SiMe_3)_2$ (1 M solution in thf, 6.0 mL, 6.0 mmol) was added to DippFormH (2.16 g, 6.0 mmol) in THF (20 mL) and the solution stirred at room temperature for 2 h, and then added dropwise to $SbBr_3$ (3.0 mmol) in PhMe (10 mL). After warming to room temperature, the mixture was stirred for 36 h to yield a yellow-brown solution with a white precipitate. Volatiles were removed under reduced pressure, and the residue extracted with hexane (30 mL). The filtrate was concentrated under vacuum, large yellow crystals of **3** were obtained at -30 °C one week. Yield = 1.73 g (80 %), M.P. 168-170 °C. ^{1}H NMR (400 MHz, C_6D_6, 25 °C): δ (ppm) = 1.15 (d, J = 6.8 Hz, 48H, $CH(CH_3)_2$), 3.45 (sept, 8H, $CH(CH_3)_2$), 6.99 (m, 4H, *p*-ArH), 7.03 (m, 8H, *m*-ArH), 8.04 (s, 2H, NC(H)N); Elemental analysis calcd. (%) for $C_{50}H_{70}BrN_4Sb$ (MW, 928.80): C 64.60, H 7.64, N 6.02; found: C 64.85, H 7.79, N 5.97. IR (Nujol, cm^{-1}): 2922 (m), 2722 (vs), 2665 (m), 2599 (vs), 2482 (vs), 2359 (s), 2290 (s), 2193 (s), 2122 (vs), 2060 (vs), 2001 (s), 1976 (s), 1929 (s), 1864 (s), 1793 (s), 1776 (vs), 1699 (vs), 1587 (w), 1454 (m), 1380 (m), 1259 (m), 1097 (m), 1056 (s), 987 (s), 797 (s), 694 (s), 608 (s), 590 (s), 537 (s). A reaction stoichiometry of 2:1 (LiDippForm:Sb) gave **3** as the sole identifiable Sb-containing product.

[Sb(DippForm)$_2$I] (**4**)

$LiN(SiMe_3)_2$ (1 M solution in thf, 2.0 mL, 2.0 mmol) was added to DippFormH (0.72 g, 2.0 mmol) in THF (20 mL) and the solution stirred at room temperature for 2 h, and then added dropwise to a solution of SbI_3 (1.0 mmol) in THF (10 mL). After warming to room temperature, the mixture was stirred for 36 h to yield a yellow solution. The reaction mixture was dried under vacuum and dissolved in PhMe (20 mL). The mixture was then filtered to remove LiCl. The filtrate was concentrated under vacuum, small yellow-white crystals **4** were obtained at -30 °C for 12h. Yield = 0.54 g (75 %), M.P. 188-190 °C. ^{1}H NMR (400 MHz, C_6D_6, 25 °C): δ (ppm) = 1.15 (d, J = 6.6 Hz, 48H, $CH(CH_3)_2$), 3.42 (sept, 8H, $CH(CH_3)_2$), 6.98 (m, 4H, *p*-ArH), 7.06 (m, 8H, *m*-ArH), 7.86 (s, 2H, NC(H)N). Elemental analysis calcd. (%) for $C_{50}H_{70}IN_4Sb$ (MW, 975.79): C 61.56, H 7.18, N 5.74; found: C 53.03, H 6.32, N 4.94 (significantly low in the C percentage). IR (Nujol, cm^{-1}): 2915 (w), 2722 (vs), 2665 (m), 2594 (vs), 2544 (m), 2487 (m), 2460 (vs), 2398 (m), 2287 (m), 2187 (s), 2127 (w), 2082 (vs), 2001 (s), 1971 (s),

1928 (s), 1865 (s), 1793 (s), 1736 (w), 1704 (s), 1583 (w), 1462 (m), 1378 (m), 1043 (m), 987 (m), 820 (m), 723 (s), 694 (s), 607 (s), 590 (s), 537 (s), 411 (w). A reaction stoichiometry of 2:1 (Li(DippForm):Sb) gave **4** and Li(DippForm).

[Sb(DippForm)Br_2] (**5**)

3 (0.92 g, 1.0 mmol) was reacted with $SbBr_3$ (0.36 g, 1.0 mmol) in THF (20 mL) at room temperature with stirring. The reaction was continued for 8 h at room temperature. The orange solution was concentrated to ca. 10 mL, cubic shiny yellow crystals **5** were obtained at 15 °C for a day. Yield = 0.30 g (32 %), M.P. 170-172 °C. ^{1}H NMR (400 MHz, C_6D_6, 25 °C): δ (ppm) = 1.21 (d, J = 6.9 Hz, 24H, $CH(CH_3)_2$), 3.33 (sept, 4H, $CH(CH_3)_2$), 6.88 (m, 2H, *p*-ArH), 7.08 (m, 4H, *m*-ArH), 7.56 (s, 1H, NC(H)N). Elemental analysis calcd. (%) for $C_{25}H_{35}Br_2N_2Sb$ (MW, 645.12): C 46.54, H 5.43, N 4.34; found: C 43.13, H 5.19, N 4.22 (low in the C percentage only). IR (Nujol, cm^{-1}): 2962 (s), 2923 (vs), 2732 (m), 2581 (w), 2393 (s), 2253 (m), 2166 (w), 2020 (m), 1978 (s), 1949 (s), 1877 (s), 1800 (s), 1731 (m), 1644 (vs), 1593 (s), 1511 (s), 1462 (s), 1376 (s), 1311 (m), 1257 (s), 1121 (m), 1042 (s), 969 (m), 802 (m), 763 (s), 676 (w), 627 (w), 426 (w). A reaction stoichiometry of 2:1 (LiDippForm:Sb) gave **5** as the sole identifiable Sb-containing product.

[Sb(DippForm)I_2] (**6**)

$LiN(SiMe_3)_2$ (1 M solution in thf, 1.0 mL, 1.0 mmol) was added to DippFormH (0.36 g, 1.0 mmol) in THF (20 mL) and the solution stirred at room temperature for 2 h, and then added dropwise to a solution of SbI_3 (1.0 mmol) in THF (10 mL) at room temperature. The mixture was stirred for 36 h to yield a yellow brown solution. The reaction mixture was dried under vacuum and dissolved in PhMe (20 mL). The mixture was then filtered. The filtrate was concentrated under vacuum, shiny brown-orange crystals **6** were obtained at -30 °C overnight. Yield = 0.21 g (58 %), M.P. 156-158 °C. ^{1}H NMR (400 MHz, C_6D_6, 25 °C): δ (ppm) = 1.11 (d, J = 6.9 Hz, 24H, $CH(CH_3)_2$), 3.22 (sept, 4H, $CH(CH_3)_2$), 6.76 (m, 2H, *p*-ArH), 6.99 (m, 4H, *m*-ArH), 8.31 (s, 1H, NC(H)N). Elemental analysis calcd. (%) for $C_{25}H_{35}I_2N_2Sb$ (MW, 739.12): C 40.61, H 4.73, N 3.79; found: C 27.47, H 4.92, N 2.91 (low in C and N percentage). IR (Nujol, cm^{-1}): 2923 (s), 2853 (vs), 2727 (m), 2663 (w), 2411 (m), 2356 (s), 2290 (m), 1936 (s), 1870 (vs), 1632 (m), 1588 (vs), 1462 (vs), 1376 (s), 1260 (vs), 1168 (vs), 1074 (m), 911 (s), 885 (m), 849 (s), 722 (s), 666 (s).

Acknowledgements The authors acknowledge support by the Ministry of Higher Education and Scientific Research in Iraq (MHESR) for sponsorship of Areej K. Aldabbagh Ph.D. study at James Cook University. And the Australian Research Council (ARC) for funding (DP190100798). Parts of this research were undertaken on the MX1 beamline at the Australian Synchrotron, part of ANSTO (Cowieson et al., 2015), and part using the MX2 beamline at the Australian Synchrotron, part of ANSTO, and made use of the Australian Cancer Research Foundation (ACRF) detector" (Aragao et al., 2018).

References

Aragao, D., Aishima, J., Cherukuvada, H., Clarken, R., Clift, M., Cowieson, N. P., Ericsson, D. J., Gee, C. L., Macedo, S., Mudie, N., Panjikar, S., Price, J. R., Riboldi-Tunnicliffe, A., Rostan, R., Williamson, R. & Caradoc-Davies, T. T. (2018). J. Synchrotron Radiat. 25, 885-891.

Bailey, P. J., Gould, R. O., Harmer, C. N., Pace, S., Steiner, A. & Wright, D. S. (1997). Chem. Commun. 1161-1162.

Barbour, L. J. (2001). J. Supramol. Chem. 1, 189-191.

Bruker (2012). APEX2, SAINT and SHELXTL. Bruker AXS Inc., Madison, Wisconsin, USA.

Brym, M., Forsyth, C. M., Jones, C., Junk, P. C., Rose, R. P., Stascha, A. & Turner, D. R. (2007). Dalton Trans. 3282-3288.

Cole, M. L., Deacon, G. B., Forsyth, C. M., Junk, P. C., Konstas, K. & Wang, J. (2007). Chem. Eur. J. 13, 8092-8110.

Cole, M. L., Deacon, G. B., Junk, P. C. & Konstas, K. (2005). Chem. Commun. 1581-1583.

Cowieson, N. P., Aragao, D., Clift, M., Ericsson, D. J., Gee, C., Harrop, S. J., Mudie, N., Panjikar, S., Price, J. R., Riboldi-Tunnicliffe, A., Williamson, R. & Caradoc-Davies, T. (2015). J. Synchrotron Radiat. 22, 187-190.

Day, B. M., Coles, M. P. & Hitchcock, P. B. (2012). Eur. J. Inorg. Chem. 841–846.

Ergezinger, C., Weller, F. & Dehnicke, K. (1988). Z. Naturforsch., B: Anorg. Chem. Org. Chem. 43, 1119-1124.

Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). J. Appl. Crystallogr. 42, 339-341.

Green, S. P., Jones, C., Jin, G. & Stasch, A. (2007). Inorg. Chem. 46, 8-10.

Guo, Z., Blair, V., Deacon, G. B. & Junk, P. C. (2020). Dalton Trans. 49, 13588–13600.

Hinz, A., Rothe, J., Schulz, A. & Villinger, A. (2016). Dalton Trans. 45, 6044-6052.

Honeise, W., Schwarz, W., Heckmann, G. & Schmidt, A. (1986). Z. Anorg. Allg. Chem. 533, 55-64.

Jones, C. (2001). Coord. Chem. Rev. 215, 151-169.

Jones, C., Engelhardt, L. M., Junk, P. C., Hutchings, D. S., Patalinghug, W. C., Raston, C. L. & White, A. H. (1991). J. Chem. Soc., Chem. Commun. 21, 1560-1562.

Kabsch, W. (1993). J. Appl. Crystallogr. 26, 795.

Lyhs, B., Blaser, D., Wolper, C. & Schulz, S. (2011). Chem. Eur. J. 17, 4914-4920.

Lyhs, B., Schulz, S., Westphal, U., Blaser, D., Boese, R. & Bolte, M. (2009). Eur. J. Inorg. Chem. 2247–2253.

Marcalo, J. & Pires de Matos, A. (1989). Polyhedron, 8, 2431-2437.

McPhillips, T. M., McPhillips, S. E., Chiu, H. J., Cohen, A. E., Deacon, A. M., Ellis, P. J., Garman, E., Gonzalez, A., Sauter, N. K., Phizackerley, R. P., Soltis, S. M. & Kuhn, J. P. (2002). J. Synchrotron. Radiat. 9, 401-406.

Pata-Siebel, U., Miller, U., Ergezinger, C., Borgsen, B. & Dehnicke, K. (1990). Z. Anorg. Allg. Chem. 582, 30-36.

Weller, V., Pebler, J. & Dehnicke, K. (1982). Z. Anorg. Allg. Chem. 486, 61-69.

Raston, C. L., Skelton, B. W., Tolhurst, V. A. & White, A. H. (2000). J. Chem. Soc., Dalton Trans. 1279-1285.

Roberts, R. M. (1949). J. Org. Chem. 14, 277.

Sasamori, T., Mieda, E., Nagahora, N., Sato, K., Shiomi, D., Takui, T., Hosoi, Y., Furukawa, Y., Takagi, N., Nagase, S. & Tokitoh, N. (2006). J. Am. Chem. Soc. 128, 12582-12588.

Sasamori, T., Mieda, E., Nagahora, N., Takeda, N., Takagi, N., Nagase, S. & Tokitoh, N. (2005). Chem. Lett. 34, 166-167.

Sheldrick, G. M. (2015a). Acta Cryst. A71, 3-8.

Sheldrick, G. M. (2015b). Acta Cryst. C71, 3–8.

Tokitoh, N. (2000). J. Organomet. Chem. 611, 217-227.

Waterman, R. & Tilley, T. D. (2006). Inorg. Chem. 45, 9625-9627.

Yoshifuji, M., Shima, I., Inamoto, N., Hirotsu, K. & Higuchi, T. (1981) J. Am. Chem. Soc. 103, 4587-4589.

Deacon, G. B., Hossain, Md E., Junk, P. C. & Salehisaki. M. (2017). Coord. Chem. Rev. 340, 247–265.

Zhao, M., Hao, T., Zhang, X., Ma, J., Su, J. & Zheng, W. (2017). Inorg. Chem. 56, 12678-12681.

Supporting information

Synthesis and characterisation of a range of antimony(I/III) *N,N′*-bis(2,6-diisopropylphenyl)formamidinate complexes

Areej Al-Dabbagh[a], Zhifang Guo[a], Peter Junk[a]* and Jun Wang[a]

[a]College of Science and Engineering, James Cook University, Townsville, QLD, 4811, Australia

Correspondence email: peter.junk@jcu.edu.au

Computing details

Data collection: MX2 ADSC Quantum 315r ((Aragao et al., 2018) for complex **1**, MX1 ADSC Quantum 210r (Cowieson et al., 2015) for complex **2** and **5**; APEX-II (Bruker, 2012) for complexes **3**, **4**, and **6**; program(s) used to solve structure: *SHELXT* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL* 2018/3 (Sheldrick, 2015b); molecular graphics: X-seed (Barbour, 2001) and Olex2 1.3 (Dolomanov *et al.*, 2009). Software used to prepare material for publication: *SHELXL* 2018/3 (Sheldrick, 2015b).

1.

Crystal data	
$C_{50}H_{70}N_4Sb_2 \cdot 7(C_4H_8O)$	$F(000) = 3120$
$M_r = 1475.32$	$D_x = 1.272$ Mg m^{-3}
Monoclinic, $P2_1/c$	Synchrotron, λ = 0.71073 Å
$a = 21.243$ (4) Å	Cell parameters from 17952 reflections
$b = 18.997$ (4) Å	θ = 1-31°
$c = 21.743$ (4) Å	μ = 0.75 mm^{-1}
β = 118.60 (3)°	$T = 100$ K
$V = 7704$ (3) Å^3	Block, yellow
$Z = 4$	0.06 × 0.04 × 0.01
Data collection	
ADSC Quantum 315r Diffractometer	17945 observed [$I > 2\sigma(I)$] reflections
Radiation source: MX2 Beamline Australian Synchrotron	R_{int} = ?
Scan method: Phi scans	θ_{max} = 31.8°, θ_{min} = 1.1°
Absorption correction: Multi-scan, XDS (Kabsch, 1993)	h = −29→25
21388 measured reflections	k = −24→24
21388 independent reflections	l = −25→28
Refinement	
Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.091$	$w = 1/[\sigma^2(F_o^2) + (0.0266P)^2 + 120.4927P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.271$	
$S = 1.19$	
21388 reflections	$(\Delta/\sigma)_{max} = 0.001$

882 parameters	$\Delta\rho_{max} = 2.59$ e Å^{-3}
151 restraints	$\Delta\rho_{min} = -3.73$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Single crystals coated with viscous hydrocarbon oil were mounted on glass fibres or loops. Complexes (**1**, **2**, and **5**) were measured at the Australian Synchrotron on the MX1 or MX2 beamline at 100K, data integration was completed using Blue-ice (McPhillips *et al*., 2002) and XDS (Kabsch, 1993) software programs. Complexes **3**, **4** and **6** were measured on a "Bruker APEX-II CCD' diffractometer equipped with graphite-monochromated Mo-K_α radiation (λ = 0.71073 Å) at 123 K. The structures were solved by direct methods using SHELXS, or intrinsic phasing methods using SHELXT (Sheldrick, 2015a), and refined with a full-matrix least-squares procedure using SHELXL-2018/3 (Sheldrick, 2015b). All non-hydrogen atoms were refined with anisotropic atomic displacement parameters.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}^*/U_{eq}
Sb1	0.22335(3)	0.47851(3)	0.78145(3)	0.01868(12)
Sb2	0.28581(3)	0.54143(3)	0.71417(3)	0.01811(12)
N1	0.1974(4)	0.5904(4)	0.8027(4)	0.0202(13)
N3	0.2555(3)	0.3755(3)	0.7496(3)	0.0156(11)
C14	0.2720(4)	0.7104(4)	0.7264(4)	0.0185(14)
N4	0.3076(3)	0.4285(3)	0.6894(3)	0.0175(12)
C9	0.1578(4)	0.6003(4)	0.8398(4)	0.0157(13)
C34	0.2374(4)	0.3099(4)	0.7718(4)	0.0190(14)
C39	0.3418(4)	0.4185(4)	0.6474(4)	0.0198(15)
C33	0.1713(5)	0.2793(5)	0.7289(5)	0.0241(16)
C15	0.3349(4)	0.7455(5)	0.7749(4)	0.0220(15)
C22	0.2293(4)	0.7376(4)	0.6589(4)	0.0206(15)
C29	0.2863(4)	0.2806(5)	0.8366(4)	0.0221(15)
C21	0.2493(5)	0.8015(5)	0.6412(4)	0.0236(16)
H21	0.220148	0.821288	0.596162	0.028
C45	0.4096(5)	0.3971(5)	0.5667(5)	0.0296(18)
H45	0.432986	0.388743	0.539527	0.035
C13	0.2174(4)	0.6481(4)	0.7824(4)	0.0151(12)

H13	0.206342	0.69278	0.794395	0.018
C19	0.3529(5)	0.8077(5)	0.7540(5)	0.0259(17)
H19	0.395435	0.831552	0.785888	0.031
C41	0.4616(4)	0.4246(5)	0.7589(4)	0.0233(16)
H41	0.430718	0.44694	0.776499	0.028
C8	0.1940(4)	0.6005(4)	0.9135(4)	0.0204(15)
C23	0.1620(4)	0.7000(5)	0.6039(4)	0.0231(16)
H23	0.155685	0.655783	0.625307	0.028
C47	0.3007(5)	0.4116(5)	0.5746(4)	0.0224(15)
C7	0.1536(5)	0.6100(5)	0.9481(4)	0.0256(17)
H7	0.177144	0.610399	0.99781	0.031
C20	0.3109(5)	0.8364(5)	0.6884(5)	0.0277(18)
H20	0.324236	0.879596	0.675707	0.033
C40	0.4171(4)	0.4168(4)	0.6804(4)	0.0205(15)
C10	0.2746(4)	0.5922(5)	0.9556(4)	0.0251(17)
H10	0.292123	0.575666	0.922847	0.03
C4	0.0830(4)	0.6080(5)	0.8017(4)	0.0219(15)
C32	0.1547(5)	0.2162(5)	0.7524(5)	0.032(2)
H32	0.110141	0.193724	0.723584	0.039
O1	0.4989(4)	0.6227(5)	0.6569(4)	0.0424(18)
C35	0.1182(5)	0.3090(5)	0.6579(5)	0.0281(18)
H35	0.138819	0.353401	0.650319	0.034
C16	0.3830(4)	0.7169(5)	0.8481(4)	0.0231(16)
H16	0.35711	0.677258	0.8566	0.028
C44	0.4496(5)	0.4057(5)	0.6386(5)	0.0257(17)
H44	0.500413	0.404102	0.659974	0.031
C31	0.2007(6)	0.1867(5)	0.8154(6)	0.033(2)
H31	0.188287	0.144281	0.830151	0.04
C46	0.3353(5)	0.4006(5)	0.5343(5)	0.0277(18)
H46	0.307883	0.395472	0.484966	0.033
C28	0.3582(5)	0.3148(5)	0.8844(4)	0.0261(18)
H28	0.365852	0.353543	0.857654	0.031
C48	0.2193(5)	0.4177(5)	0.5370(4)	0.0279(18)
H48	0.20369	0.425308	0.57319	0.034
C12	0.2967(6)	0.5374(6)	1.0134(6)	0.039(2)
H12A	0.280538	0.552287	1.04673	0.059
H12B	0.348975	0.532489	1.037849	0.059

H12C	0.274677	0.492027	0.992802	0.059
C5	0.0457(5)	0.6177(5)	0.8394(5)	0.0279(18)
H5	-0.004898	0.623509	0.814565	0.034
C17	0.4522(5)	0.6873(6)	0.8525(5)	0.036(2)
H17A	0.44035	0.649811	0.817735	0.053
H17B	0.482633	0.668308	0.899485	0.053
H17C	0.477901	0.725041	0.843015	0.053
C43	0.4848(5)	0.3522(6)	0.7939(5)	0.032(2)
H43A	0.442169	0.324568	0.784519	0.048
H43B	0.514655	0.358327	0.844528	0.048
H43C	0.512245	0.327596	0.774902	0.048
C6	0.0802(5)	0.6190(5)	0.9116(5)	0.0274(17)
H6	0.053766	0.625921	0.93608	0.033
C36	0.1052(6)	0.2580(7)	0.5981(5)	0.042(3)
H36A	0.151	0.246744	0.59975	0.064
H36B	0.073068	0.27999	0.553053	0.064
H36C	0.083228	0.214631	0.603416	0.064
C3	0.0431(5)	0.6058(5)	0.7226(5)	0.0285(19)
H3	0.078576	0.595273	0.705942	0.034
C25	0.0950(5)	0.7447(6)	0.5807(5)	0.036(2)
H25A	0.101849	0.79018	0.563533	0.054
H25B	0.086261	0.752219	0.620573	0.054
H25C	0.053863	0.720385	0.543199	0.054
C11	0.3106(5)	0.6638(6)	0.9856(6)	0.037(2)
H11A	0.2998	0.696598	0.947067	0.056
H11B	0.36264	0.657306	1.012974	0.056
H11C	0.292325	0.68282	1.015899	0.056
C30	0.2660(5)	0.2193(5)	0.8577(5)	0.0301(19)
H30	0.297563	0.19933	0.901974	0.036
C1	0.0085(7)	0.6762(7)	0.6921(6)	0.047(3)
H1A	-0.014148	0.674137	0.640835	0.07
H1B	0.045097	0.713194	0.709415	0.07
H1C	-0.027961	0.686758	0.706174	0.07
C42	0.5270(5)	0.4717(6)	0.7801(5)	0.034(2)
H42A	0.563253	0.446344	0.773188	0.051
H42B	0.54696	0.48465	0.829613	0.051
H42C	0.512686	0.514373	0.751304	0.051

C37	0.0472(5)	0.3269(8)	0.6551(6)	0.049(3)
H37A	0.028871	0.285428	0.668242	0.074
H37B	0.012576	0.341475	0.607479	0.074
H37C	0.054307	0.365402	0.687817	0.074
C49	0.1944(6)	0.4821(6)	0.4870(6)	0.043(3)
H49A	0.202004	0.472622	0.446763	0.065
H49B	0.222084	0.523692	0.512098	0.065
H49C	0.143302	0.490736	0.470604	0.065
C51	0.4508(5)	0.6083(6)	0.5853(5)	0.037(2)
H51A	0.449746	0.557149	0.576158	0.044
H51B	0.466353	0.6332	0.554906	0.044
C18	0.4000(6)	0.7719(6)	0.9046(5)	0.036(2)
H18A	0.434299	0.806009	0.90385	0.053
H18B	0.420858	0.74897	0.950487	0.053
H18C	0.355846	0.796382	0.895757	0.053
C24	0.1718(6)	0.6796(6)	0.5413(5)	0.039(2)
H24A	0.128597	0.655643	0.50636	0.058
H24B	0.213112	0.648054	0.55675	0.058
H24C	0.180064	0.722103	0.520604	0.058
C53	0.3951(6)	0.6892(7)	0.6266(6)	0.047(3)
H53A	0.406449	0.734987	0.61253	0.057
H53B	0.355778	0.695644	0.638299	0.057
C50	0.1842(6)	0.3495(6)	0.4975(6)	0.042(3)
H50A	0.1321	0.352864	0.477864	0.064
H50B	0.202192	0.309611	0.529998	0.064
H50C	0.196092	0.342534	0.459598	0.064
C27	0.4199(5)	0.2624(7)	0.9064(6)	0.041(3)
H27A	0.465644	0.287475	0.931144	0.061
H27B	0.416783	0.239485	0.864671	0.061
H27C	0.416738	0.226825	0.937416	0.061
C26	0.3575(6)	0.3473(7)	0.9481(6)	0.045(3)
H26A	0.349618	0.310327	0.975145	0.068
H26B	0.318846	0.382097	0.932671	0.068
H26C	0.403597	0.370348	0.977515	0.068
C54	0.4604(6)	0.6570(6)	0.6868(6)	0.039(2)
H54A	0.490307	0.693977	0.720124	0.047
H54B	0.446047	0.622782	0.712169	0.047

C52	0.3763(6)	0.6337(7)	0.5701(6)	0.046(3)
H52A	0.349765	0.654438	0.522601	0.055
H52B	0.347683	0.595081	0.574773	0.055
O3	0.2151(4)	0.6908(4)	0.3398(4)	0.0374(16)
C59	0.1826(6)	0.6475(6)	0.2781(5)	0.036(2)
H59A	0.219921	0.624798	0.270002	0.043
H59B	0.151527	0.676314	0.236588	0.043
C60	0.1391(6)	0.5930(6)	0.2909(6)	0.039(2)
H60A	0.168308	0.551085	0.314685	0.047
H60B	0.097051	0.578269	0.246553	0.047
C62	0.1753(7)	0.6833(7)	0.3765(7)	0.049(3)
H62A	0.155203	0.729299	0.379676	0.059
H62B	0.206926	0.666042	0.424656	0.059
C61	0.1163(7)	0.6319(8)	0.3377(8)	0.055(3)
H61A	0.07018	0.656564	0.309579	0.066
H61B	0.111228	0.599153	0.370427	0.066
O2	0.2883(4)	0.4722(4)	0.3713(4)	0.0389(17)
C55	0.3320(5)	0.5289(5)	0.4162(5)	0.034(2)
H55A	0.339729	0.522965	0.464562	0.041
H55B	0.309041	0.57515	0.398059	0.041
C57	0.3771(6)	0.5013(6)	0.3386(6)	0.040(2)
H57A	0.359651	0.542174	0.306463	0.048
H57B	0.415627	0.477245	0.333416	0.048
C58	0.3169(7)	0.4515(8)	0.3265(6)	0.050(3)
H58A	0.279021	0.453607	0.276913	0.059
H58B	0.335088	0.402635	0.337202	0.059
C56	0.4021(5)	0.5231(6)	0.4141(5)	0.036(2)
H56A	0.433722	0.486925	0.447372	0.043
H56B	0.427658	0.568687	0.425042	0.043
O4	0.2908(5)	0.2781(4)	0.1397(5)	0.050(2)
C63	0.3139(6)	0.3279(6)	0.1976(6)	0.038(2)
H63A	0.354877	0.308858	0.240461	0.046
H63B	0.274211	0.338679	0.207783	0.046
C66	0.3421(7)	0.2863(6)	0.1152(7)	0.044(3)
H66A	0.320806	0.272459	0.06532	0.052
H66B	0.384734	0.256526	0.142892	0.052
C64	0.3354(6)	0.3919(5)	0.1723(7)	0.042(3)

H64A	0.373494	0.418118	0.21204	0.051
H64B	0.293868	0.423481	0.146531	0.051
C65	0.3628(6)	0.3641(5)	0.1243(6)	0.037(2)
H65A	0.415462	0.369741	0.145775	0.045
H65B	0.339846	0.388842	0.078675	0.045
O5	0.0665(5)	0.4351(4)	0.0876(5)	0.048(2)
C67	0.0422(6)	0.5033(6)	0.0959(6)	0.043(2)
H67A	0.039368	0.505606	0.140041	0.051
H67B	-0.005756	0.513814	0.056212	0.051
C68	0.0976(6)	0.5545(6)	0.0976(6)	0.042(2)
H68A	0.082397	0.574128	0.050412	0.05
H68B	0.104831	0.59373	0.130325	0.05
C69	0.1656(7)	0.5118(7)	0.1225(9)	0.061(4)
H69A	0.204036	0.529785	0.167598	0.073
H69B	0.182695	0.512034	0.087386	0.073
C70	0.1413(7)	0.4375(7)	0.1309(8)	0.056(3)
H70A	0.164989	0.40121	0.116388	0.067
H70B	0.15366	0.428906	0.1803	0.067
N2	0.2527(3)	0.6449(3)	0.7456(3)	0.0161(11)
C38	0.2879(4)	0.3723(4)	0.7110(4)	0.0196(14)
H38	0.297473	0.327349	0.698229	0.024
C2	-0.0137(7)	0.5483(7)	0.6954(7)	0.054(3)
H2A	-0.049917	0.558432	0.709897	0.081
H2B	0.008828	0.502801	0.714665	0.081
H2C	-0.036554	0.546744	0.644164	0.081
O6	-0.0257(5)	0.6404(6)	0.1282(5)	0.059(2)
C74	-0.0743(9)	0.6172(13)	0.1532(8)	0.091(7)
H74A	-0.062794	0.641231	0.197747	0.11
H74B	-0.069243	0.565799	0.16192	0.11
C73	-0.1476(9)	0.6338(13)	0.1003(9)	0.089(6)
H73A	-0.162626	0.680601	0.108631	0.107
H73B	-0.181883	0.597724	0.098742	0.107
C71	-0.0680(6)	0.6630(7)	0.0577(6)	0.045(3)
H71A	-0.047582	0.645377	0.028125	0.054
H71B	-0.069871	0.715066	0.05514	0.054
C72	-0.1410(8)	0.6333(10)	0.0337(8)	0.072(5)
H72A	-0.144779	0.584934	0.015402	0.086

H72B	-0.17828	0.663175	-0.003017	0.086
O7	0.4958(13)	0.4876(16)	0.9475(10)	0.078(7)
C75	0.4385(11)	0.5291(13)	0.9504(9)	0.040(5)
H75A	0.397544	0.498688	0.942555	0.048
H75B	0.42132	0.566809	0.914567	0.048
C76	0.4734(10)	0.5601(9)	1.0235(10)	0.037(4)
H76A	0.437161	0.573768	1.037618	0.045
H76B	0.503251	0.601553	1.027136	0.045
C77	0.5193(14)	0.4984(13)	1.0672(9)	0.043(4)
H77A	0.560199	0.515099	1.111464	0.052
H77B	0.490481	0.464875	1.078356	0.052
C78	0.5451(13)	0.4647(14)	1.0194(11)	0.042(5)
H78A	0.594595	0.480016	1.033167	0.05
H78B	0.54457	0.412757	1.022832	0.05
O8	0.0606(14)	0.5003(14)	0.5577(12)	0.103(9)
C79	0.0122(18)	0.5582(12)	0.5231(16)	0.060(6)
H79A	0.038749	0.602699	0.528984	0.072
H79B	-0.022426	0.564487	0.540905	0.072
C80	-0.026(2)	0.5341(15)	0.4461(15)	0.110(12)
H80A	0.005213	0.540172	0.423783	0.132
H80B	-0.071802	0.558563	0.418147	0.132
C81	-0.0360(16)	0.4557(15)	0.4580(18)	0.085(10)
H81A	-0.070443	0.449379	0.476059	0.102
H81B	-0.051411	0.427342	0.414917	0.102
C82	0.0414(14)	0.4385(10)	0.5138(12)	0.051(5)
H82A	0.043285	0.395507	0.540338	0.061
H82B	0.073067	0.432406	0.492446	0.061

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sb1	0.0235(2)	0.0152(2)	0.0198(2)	-0.00064(17)	0.0124(2)	-0.00099(18)
Sb2	0.0225(2)	0.0148(2)	0.0189(2)	0.00103(17)	0.01138(19)	0.00089(18)
N1	0.024(3)	0.020(3)	0.023(3)	0.003(2)	0.016(3)	-0.001(2)
N3	0.019(3)	0.011(3)	0.017(3)	0.001(2)	0.009(2)	0.000(2)
C14	0.018(3)	0.021(4)	0.015(3)	0.001(3)	0.007(3)	0.001(3)
N4	0.019(3)	0.019(3)	0.015(3)	-0.003(2)	0.009(2)	-0.003(2)

C9	0.013(3)	0.017(4)	0.011(3)	-0.004(2)	0.001(3)	0.001(2)
C34	0.019(3)	0.018(4)	0.019(4)	0.000(3)	0.008(3)	-0.002(3)
C39	0.017(3)	0.026(4)	0.011(3)	0.002(3)	0.003(3)	-0.002(3)
C33	0.023(4)	0.023(4)	0.029(4)	-0.004(3)	0.014(3)	-0.002(3)
C15	0.022(4)	0.023(4)	0.020(4)	0.001(3)	0.010(3)	0.002(3)
C22	0.021(4)	0.019(4)	0.018(4)	0.005(3)	0.006(3)	0.004(3)
C29	0.019(4)	0.024(4)	0.019(4)	0.003(3)	0.006(3)	0.001(3)
C21	0.025(4)	0.022(4)	0.019(4)	0.007(3)	0.007(3)	0.003(3)
C45	0.031(4)	0.040(5)	0.022(4)	-0.004(3)	0.017(4)	-0.001(4)
C13	0.016(3)	0.012(3)	0.014(3)	0.003(2)	0.005(3)	0.000(2)
C19	0.023(4)	0.022(4)	0.025(4)	0.003(3)	0.005(3)	-0.005(3)
C41	0.018(4)	0.029(5)	0.016(4)	-0.001(3)	0.003(3)	0.001(3)
C8	0.019(3)	0.022(4)	0.018(4)	-0.004(3)	0.006(3)	-0.002(3)
C23	0.022(4)	0.023(4)	0.013(3)	0.002(3)	-0.001(3)	0.001(3)
C47	0.024(4)	0.025(4)	0.017(4)	-0.001(3)	0.008(3)	0.001(3)
C7	0.027(4)	0.032(5)	0.017(4)	-0.003(3)	0.009(3)	-0.002(3)
C20	0.029(4)	0.023(4)	0.026(4)	0.005(3)	0.009(4)	-0.005(3)
C40	0.019(4)	0.023(4)	0.015(3)	0.002(3)	0.004(3)	0.004(3)
C10	0.018(4)	0.042(5)	0.007(3)	-0.004(3)	-0.001(3)	-0.002(3)
C4	0.016(3)	0.024(4)	0.020(4)	0.002(3)	0.004(3)	0.002(3)
C32	0.030(5)	0.032(5)	0.039(5)	-0.002(4)	0.019(4)	-0.006(4)
O1	0.031(4)	0.054(5)	0.030(4)	-0.003(3)	0.005(3)	0.007(3)
C35	0.018(4)	0.032(5)	0.029(4)	-0.009(3)	0.007(3)	-0.006(3)
C16	0.018(4)	0.024(4)	0.020(4)	-0.002(3)	0.004(3)	-0.002(3)
C44	0.024(4)	0.027(5)	0.030(4)	0.002(3)	0.015(4)	0.003(3)
C31	0.042(5)	0.020(5)	0.045(6)	0.006(4)	0.027(5)	-0.004(4)
C46	0.032(4)	0.031(5)	0.018(4)	-0.001(3)	0.010(4)	0.004(3)
C28	0.020(4)	0.033(5)	0.013(4)	0.005(3)	-0.002(3)	-0.001(3)
C48	0.023(4)	0.040(5)	0.017(4)	-0.004(3)	0.006(3)	0.001(3)
C12	0.038(5)	0.036(6)	0.034(5)	0.009(4)	0.009(4)	0.010(4)
C5	0.020(4)	0.035(5)	0.030(5)	0.001(4)	0.013(4)	0.002(3)
C17	0.019(4)	0.049(6)	0.028(5)	0.009(4)	0.003(4)	0.012(4)
C43	0.028(4)	0.035(5)	0.024(4)	0.009(4)	0.005(4)	-0.001(4)
C6	0.027(4)	0.032(5)	0.027(4)	-0.002(3)	0.015(4)	0.002(3)
C36	0.041(6)	0.051(7)	0.026(5)	-0.006(4)	0.008(5)	0.002(5)
C3	0.018(4)	0.039(5)	0.020(4)	0.003(3)	0.002(3)	-0.001(3)
C25	0.022(4)	0.036(6)	0.032(5)	-0.002(4)	-0.001(4)	0.005(4)

C11	0.023(4)	0.045(6)	0.033(5)	-0.012(4)	0.005(4)	-0.009(4)
C30	0.036(5)	0.024(5)	0.031(5)	0.010(3)	0.016(4)	0.005(3)
C1	0.045(6)	0.053(8)	0.028(5)	0.012(5)	0.006(5)	0.004(5)
C42	0.028(4)	0.035(6)	0.029(5)	0.002(4)	0.006(4)	-0.003(4)
C37	0.019(4)	0.081(10)	0.032(6)	-0.009(6)	-0.001(4)	0.009(5)
C49	0.041(6)	0.024(5)	0.051(7)	0.012(4)	0.011(5)	0.013(4)
C51	0.031(5)	0.040(6)	0.029(5)	-0.008(4)	0.006(4)	0.002(4)
C18	0.037(5)	0.039(6)	0.022(4)	-0.005(4)	0.007(4)	-0.002(4)
C24	0.046(6)	0.038(6)	0.027(5)	-0.011(4)	0.013(5)	0.000(4)
C53	0.040(6)	0.052(7)	0.041(6)	-0.013(5)	0.012(5)	0.003(5)
C50	0.030(5)	0.042(7)	0.043(6)	-0.006(5)	0.007(5)	-0.013(4)
C27	0.027(5)	0.052(7)	0.035(5)	0.015(5)	0.009(4)	0.011(4)
C26	0.035(5)	0.068(9)	0.027(5)	-0.010(5)	0.009(4)	-0.008(5)
C54	0.040(6)	0.038(6)	0.030(5)	-0.005(4)	0.009(4)	0.008(4)
C52	0.029(5)	0.051(7)	0.038(6)	-0.012(5)	0.000(5)	-0.001(4)
O3	0.044(4)	0.038(4)	0.033(4)	-0.006(3)	0.021(3)	-0.014(3)
C59	0.037(5)	0.042(6)	0.025(5)	-0.001(4)	0.011(4)	-0.005(4)
C60	0.037(5)	0.037(6)	0.035(5)	-0.008(4)	0.011(5)	-0.011(4)
C62	0.065(8)	0.050(7)	0.049(7)	-0.008(5)	0.041(7)	-0.014(6)
C61	0.055(7)	0.062(8)	0.066(8)	-0.018(7)	0.044(7)	-0.021(6)
O2	0.039(4)	0.039(4)	0.041(4)	-0.010(3)	0.021(3)	-0.013(3)
C55	0.038(5)	0.026(5)	0.035(5)	-0.006(4)	0.015(4)	-0.006(4)
C57	0.042(6)	0.042(6)	0.039(6)	0.008(4)	0.022(5)	0.000(5)
C58	0.057(7)	0.061(8)	0.037(6)	-0.015(5)	0.027(6)	-0.016(6)
C56	0.030(5)	0.035(6)	0.034(5)	-0.002(4)	0.009(4)	-0.002(4)
O4	0.079(6)	0.032(4)	0.057(5)	-0.011(4)	0.047(5)	-0.021(4)
C63	0.047(6)	0.038(6)	0.031(5)	0.002(4)	0.019(5)	0.005(4)
C66	0.068(8)	0.026(5)	0.052(7)	-0.002(4)	0.041(6)	-0.001(5)
C64	0.047(6)	0.024(5)	0.070(8)	-0.011(5)	0.039(6)	-0.010(4)
C65	0.051(6)	0.026(5)	0.045(6)	0.002(4)	0.030(5)	-0.001(4)
O5	0.045(5)	0.033(4)	0.065(6)	-0.007(4)	0.024(4)	0.000(3)
C67	0.043(6)	0.033(6)	0.047(6)	-0.006(5)	0.018(5)	0.000(4)
C68	0.047(6)	0.033(6)	0.042(6)	0.001(4)	0.018(5)	-0.003(5)
C69	0.048(7)	0.038(7)	0.091(11)	0.010(7)	0.029(8)	-0.005(5)
C70	0.040(6)	0.041(7)	0.079(10)	0.013(6)	0.022(7)	-0.004(5)
N2	0.020(3)	0.014(3)	0.014(3)	0.000(2)	0.008(2)	-0.001(2)
C38	0.025(4)	0.011(3)	0.025(4)	0.002(3)	0.014(3)	0.001(3)

C2	0.055(7)	0.050(8)	0.038(6)	0.000(5)	0.008(6)	-0.016(6)
O6	0.048(5)	0.079(7)	0.045(5)	0.009(5)	0.019(4)	0.012(5)
C74	0.074(11)	0.16(2)	0.048(9)	0.045(11)	0.039(9)	0.031(12)
C73	0.057(9)	0.15(2)	0.063(10)	0.025(11)	0.035(9)	-0.003(11)
C71	0.047(6)	0.047(7)	0.044(6)	0.006(5)	0.025(6)	0.001(5)
C72	0.059(9)	0.086(12)	0.061(9)	0.020(8)	0.022(8)	-0.004(8)
O7	0.076(13)	0.118(17)	0.050(9)	0.018(10)	0.037(10)	0.061(11)
C75	0.051(11)	0.031(10)	0.046(9)	0.005(8)	0.030(9)	0.011(8)
C76	0.030(7)	0.039(9)	0.054(9)	-0.018(7)	0.029(7)	-0.004(6)
C77	0.031(8)	0.053(10)	0.048(8)	-0.013(7)	0.020(7)	-0.001(7)
C78	0.047(11)	0.045(12)	0.053(10)	0.022(10)	0.041(10)	0.023(10)
O8	0.114(17)	0.063(13)	0.077(12)	-0.013(9)	0.002(12)	0.033(11)
C79	0.078(17)	0.026(10)	0.081(15)	0.004(9)	0.041(13)	0.001(9)
C80	0.16(2)	0.029(13)	0.084(14)	0.005(11)	0.009(16)	0.017(14)
C81	0.101(17)	0.029(12)	0.084(17)	-0.005(11)	0.012(13)	0.011(12)
C82	0.082(15)	0.035(10)	0.048(11)	0.008(8)	0.042(11)	0.015(10)

Geometric parameters (Å, º)

Sb1—Sb2	2.6808 (8)	C18—H18B	0.9800
Sb1—N1	2.299 (7)	C18—H18C	0.9800
Sb1—N3	2.287 (6)	C24—H24A	0.9800
Sb2—N4	2.313 (7)	C24—H24B	0.9800
Sb2—N2	2.301 (6)	C24—H24C	0.9800
N1—C9	1.428 (9)	C53—H53A	0.9900
N1—C13	1.324 (9)	C53—H53B	0.9900
N3—C34	1.453 (10)	C53—C54	1.506 (16)
N3—C38	1.318 (9)	C53—C52	1.521 (16)
C14—C15	1.413 (11)	C50—H50A	0.9800
C14—C22	1.403 (10)	C50—H50B	0.9800
C14—N2	1.433 (10)	C50—H50C	0.9800
N4—C39	1.424 (10)	C27—H27A	0.9800
N4—C38	1.312 (9)	C27—H27B	0.9800
C9—C8	1.406 (10)	C27—H27C	0.9800
C9—C4	1.405 (10)	C26—H26A	0.9800

C34—C33	1.388 (11)	C26—H26B	0.9800
C34—C29	1.403 (11)	C26—H26C	0.9800
C39—C47	1.401 (10)	C54—H54A	0.9900
C39—C40	1.407 (11)	C54—H54B	0.9900
C33—C32	1.412 (13)	C52—H52A	0.9900
C33—C35	1.520 (13)	C52—H52B	0.9900
C15—C19	1.384 (12)	O3—C59	1.437 (12)
C15—C16	1.522 (11)	O3—C62	1.421 (12)
C22—C21	1.401 (11)	C59—H59A	0.9900
C22—C23	1.533 (11)	C59—H59B	0.9900
C29—C28	1.522 (12)	C59—C60	1.501 (14)
C29—C30	1.393 (12)	C60—H60A	0.9900
C21—H21	0.9500	C60—H60B	0.9900
C21—C20	1.386 (12)	C60—C61	1.512 (16)
C45—H45	0.9500	C62—H62A	0.9900
C45—C44	1.387 (12)	C62—H62B	0.9900
C45—C46	1.388 (13)	C62—C61	1.491 (17)
C13—H13	0.9500	C61—H61A	0.9900
C13—N2	1.334 (9)	C61—H61B	0.9900
C19—H19	0.9500	O2—C55	1.451 (12)
C19—C20	1.383 (12)	O2—C58	1.429 (13)
C41—H41	1.0000	C55—H55A	0.9900
C41—C40	1.512 (11)	C55—H55B	0.9900
C41—C43	1.533 (13)	C55—C56	1.515 (14)
C41—C42	1.525 (13)	C57—H57A	0.9900
C8—C7	1.398 (11)	C57—H57B	0.9900
C8—C10	1.514 (11)	C57—C58	1.510 (16)
C23—H23	1.0000	C57—C56	1.522 (15)
C23—C25	1.520 (12)	C58—H58A	0.9900
C23—C24	1.521 (13)	C58—H58B	0.9900
C47—C46	1.401 (12)	C56—H56A	0.9900

C47—C48	1.523 (12)	C56—H56B	0.9900
C7—H7	0.9500	O4—C63	1.458 (13)
C7—C6	1.379 (12)	O4—C66	1.432 (13)
C20—H20	0.9500	C63—H63A	0.9900
C40—C44	1.394 (11)	C63—H63B	0.9900
C10—H10	1.0000	C63—C64	1.494 (15)
C10—C12	1.523 (13)	C66—H66A	0.9900
C10—C11	1.543 (14)	C66—H66B	0.9900
C4—C5	1.398 (12)	C66—C65	1.528 (14)
C4—C3	1.511 (12)	C64—H64A	0.9900
C32—H32	0.9500	C64—H64B	0.9900
C32—C31	1.366 (14)	C64—C65	1.513 (14)
O1—C51	1.421 (12)	C65—H65A	0.9900
O1—C54	1.424 (13)	C65—H65B	0.9900
C35—H35	1.0000	O5—C67	1.438 (14)
C35—C36	1.536 (14)	O5—C70	1.407 (14)
C35—C37	1.519 (14)	C67—H67A	0.9900
C16—H16	1.0000	C67—H67B	0.9900
C16—C17	1.534 (12)	C67—C68	1.514 (16)
C16—C18	1.518 (13)	C68—H68A	0.9900
C44—H44	0.9500	C68—H68B	0.9900
C31—H31	0.9500	C68—C69	1.513 (18)
C31—C30	1.390 (14)	C69—H69A	0.9900
C46—H46	0.9500	C69—H69B	0.9900
C28—H28	1.0000	C69—C70	1.544 (18)
C28—C27	1.528 (14)	C70—H70A	0.9900
C28—C26	1.522 (14)	C70—H70B	0.9900
C48—H48	1.0000	C38—H38	0.9500
C48—C49	1.551 (14)	C2—H2A	0.9800
C48—C50	1.535 (14)	C2—H2B	0.9800
C12—H12A	0.9800	C2—H2C	0.9800

C12—H12B	0.9800	O6—C74	1.446 (17)
C12—H12C	0.9800	O6—C71	1.423 (14)
C5—H5	0.9500	C74—H74A	0.9900
C5—C6	1.379 (13)	C74—H74B	0.9900
C17—H17A	0.9800	C74—C73	1.46 (2)
C17—H17B	0.9800	C73—H73A	0.9900
C17—H17C	0.9800	C73—H73B	0.9900
C43—H43A	0.9800	C73—C72	1.52 (2)
C43—H43B	0.9800	C71—H71A	0.9900
C43—H43C	0.9800	C71—H71B	0.9900
C6—H6	0.9500	C71—C72	1.491 (18)
C36—H36A	0.9800	C72—H72A	0.9900
C36—H36B	0.9800	C72—H72B	0.9900
C36—H36C	0.9800	O7—C75	1.475 (13)
C3—H3	1.0000	O7—C78	1.470 (14)
C3—C1	1.518 (15)	C75—H75A	0.9900
C3—C2	1.522 (15)	C75—H75B	0.9900
C25—H25A	0.9800	C75—C76	1.514 (13)
C25—H25B	0.9800	C76—H76A	0.9900
C25—H25C	0.9800	C76—H76B	0.9900
C11—H11A	0.9800	C76—C77	1.530 (13)
C11—H11B	0.9800	C77—H77A	0.9900
C11—H11C	0.9800	C77—H77B	0.9900
C30—H30	0.9500	C77—C78	1.529 (13)
C1—H1A	0.9800	C78—H78A	0.9900
C1—H1B	0.9800	C78—H78B	0.9900
C1—H1C	0.9800	O8—C79	1.446 (15)
C42—H42A	0.9800	O8—C82	1.444 (14)
C42—H42B	0.9800	C79—H79A	0.9900
C42—H42C	0.9800	C79—H79B	0.9900
C37—H37A	0.9800	C79—C80	1.538 (14)

C37—H37B	0.9800	C80—H80A	0.9900
C37—H37C	0.9800	C80—H80B	0.9900
C49—H49A	0.9800	C80—C81	1.546 (14)
C49—H49B	0.9800	C81—H81A	0.9900
C49—H49C	0.9800	C81—H81B	0.9900
C51—H51A	0.9900	C81—C82	1.539 (14)
C51—H51B	0.9900	C82—H82A	0.9900
C51—C52	1.531 (15)	C82—H82B	0.9900
C18—H18A	0.9800		
N1—Sb1—Sb2	85.80 (15)	C54—C53—C52	101.4 (9)
N3—Sb1—Sb2	85.34 (15)	C52—C53—H53A	111.5
N3—Sb1—N1	171.1 (2)	C52—C53—H53B	111.5
N4—Sb2—Sb1	85.44 (15)	C48—C50—H50A	109.5
N2—Sb2—Sb1	85.23 (15)	C48—C50—H50B	109.5
N2—Sb2—N4	170.6 (2)	C48—C50—H50C	109.5
C9—N1—Sb1	119.9 (5)	H50A—C50—H50B	109.5
C13—N1—Sb1	123.5 (5)	H50A—C50—H50C	109.5
C13—N1—C9	116.7 (7)	H50B—C50—H50C	109.5
C34—N3—Sb1	118.0 (5)	C28—C27—H27A	109.5
C38—N3—Sb1	123.7 (5)	C28—C27—H27B	109.5
C38—N3—C34	118.3 (6)	C28—C27—H27C	109.5
C15—C14—N2	119.5 (7)	H27A—C27—H27B	109.5
C22—C14—C15	120.9 (7)	H27A—C27—H27C	109.5
C22—C14—N2	119.5 (7)	H27B—C27—H27C	109.5
C39—N4—Sb2	119.6 (5)	C28—C26—H26A	109.5
C38—N4—Sb2	122.4 (5)	C28—C26—H26B	109.5
C38—N4—C39	118.0 (7)	C28—C26—H26C	109.5
C8—C9—N1	119.7 (7)	H26A—C26—H26B	109.5
C4—C9—N1	119.1 (7)	H26A—C26—H26C	109.5
C4—C9—C8	121.2 (7)	H26B—C26—H26C	109.5
C33—C34—N3	118.6 (7)	O1—C54—C53	106.3 (9)

C33—C34—C29	122.2 (7)	O1—C54—H54A	110.5
C29—C34—N3	119.2 (7)	O1—C54—H54B	110.5
C47—C39—N4	120.3 (7)	C53—C54—H54A	110.5
C47—C39—C40	121.0 (7)	C53—C54—H54B	110.5
C40—C39—N4	118.7 (7)	H54A—C54—H54B	108.7
C34—C33—C32	117.4 (8)	C51—C52—H52A	111.5
C34—C33—C35	123.2 (8)	C51—C52—H52B	111.5
C32—C33—C35	119.3 (8)	C53—C52—C51	101.5 (8)
C14—C15—C16	122.3 (7)	C53—C52—H52A	111.5
C19—C15—C14	118.0 (7)	C53—C52—H52B	111.5
C19—C15—C16	119.7 (8)	H52A—C52—H52B	109.3
C14—C22—C23	122.6 (7)	C62—O3—C59	108.5 (8)
C21—C22—C14	118.6 (8)	O3—C59—H59A	110.4
C21—C22—C23	118.8 (7)	O3—C59—H59B	110.4
C34—C29—C28	122.4 (7)	O3—C59—C60	106.6 (8)
C30—C29—C34	117.7 (8)	H59A—C59—H59B	108.6
C30—C29—C28	119.9 (8)	C60—C59—H59A	110.4
C22—C21—H21	119.5	C60—C59—H59B	110.4
C20—C21—C22	121.0 (8)	C59—C60—H60A	111.3
C20—C21—H21	119.5	C59—C60—H60B	111.3
C44—C45—H45	120.0	C59—C60—C61	102.1 (9)
C44—C45—C46	120.0 (8)	H60A—C60—H60B	109.2
C46—C45—H45	120.0	C61—C60—H60A	111.3
N1—C13—H13	119.2	C61—C60—H60B	111.3
N1—C13—N2	121.7 (7)	O3—C62—H62A	110.1
N2—C13—H13	119.2	O3—C62—H62B	110.1
C15—C19—H19	118.9	O3—C62—C61	108.2 (9)
C20—C19—C15	122.2 (8)	H62A—C62—H62B	108.4
C20—C19—H19	118.9	C61—C62—H62A	110.1
C40—C41—H41	107.7	C61—C62—H62B	110.1
C40—C41—C43	110.6 (7)	C60—C61—H61A	110.9

C40—C41—C42	112.7 (7)	C60—C61—H61B	110.9
C43—C41—H41	107.7	C62—C61—C60	104.4 (9)
C42—C41—H41	107.7	C62—C61—H61A	110.9
C42—C41—C43	110.3 (7)	C62—C61—H61B	110.9
C9—C8—C10	122.2 (7)	H61A—C61—H61B	108.9
C7—C8—C9	118.1 (7)	C58—O2—C55	108.6 (8)
C7—C8—C10	119.7 (7)	O2—C55—H55A	110.9
C22—C23—H23	108.1	O2—C55—H55B	110.9
C25—C23—C22	111.9 (7)	O2—C55—C56	104.3 (8)
C25—C23—H23	108.1	H55A—C55—H55B	108.9
C24—C23—C22	109.9 (8)	C56—C55—H55A	110.9
C24—C23—H23	108.1	C56—C55—H55B	110.9
C24—C23—C25	110.7 (8)	H57A—C57—H57B	109.4
C39—C47—C48	122.2 (7)	C58—C57—H57A	111.6
C46—C47—C39	119.4 (8)	C58—C57—H57B	111.6
C46—C47—C48	118.5 (7)	C58—C57—C56	100.8 (9)
C8—C7—H7	119.2	C56—C57—H57A	111.6
C6—C7—C8	121.6 (8)	C56—C57—H57B	111.6
C6—C7—H7	119.2	O2—C58—C57	108.1 (9)
C21—C20—H20	120.4	O2—C58—H58A	110.1
C19—C20—C21	119.3 (8)	O2—C58—H58B	110.1
C19—C20—H20	120.4	C57—C58—H58A	110.1
C39—C40—C41	121.2 (7)	C57—C58—H58B	110.1
C44—C40—C39	117.9 (7)	H58A—C58—H58B	108.4
C44—C40—C41	120.9 (7)	C55—C56—C57	102.3 (8)
C8—C10—H10	107.5	C55—C56—H56A	111.3
C8—C10—C12	112.5 (8)	C55—C56—H56B	111.3
C8—C10—C11	110.7 (8)	C57—C56—H56A	111.3
C12—C10—H10	107.5	C57—C56—H56B	111.3
C12—C10—C11	111.1 (8)	H56A—C56—H56B	109.2
C11—C10—H10	107.5	C66—O4—C63	104.5 (8)

C9—C4—C3	121.8 (7)	O4—C63—H63A	110.9
C5—C4—C9	117.8 (7)	O4—C63—H63B	110.9
C5—C4—C3	120.3 (8)	O4—C63—C64	104.2 (8)
C33—C32—H32	119.1	H63A—C63—H63B	108.9
C31—C32—C33	121.9 (9)	C64—C63—H63A	110.9
C31—C32—H32	119.1	C64—C63—H63B	110.9
C51—O1—C54	108.6 (8)	O4—C66—H66A	110.5
C33—C35—H35	108.0	O4—C66—H66B	110.5
C33—C35—C36	111.8 (8)	O4—C66—C65	106.2 (8)
C36—C35—H35	108.0	H66A—C66—H66B	108.7
C37—C35—C33	111.3 (8)	C65—C66—H66A	110.5
C37—C35—H35	108.0	C65—C66—H66B	110.5
C37—C35—C36	109.6 (8)	C63—C64—H64A	110.8
C15—C16—H16	108.0	C63—C64—H64B	110.8
C15—C16—C17	109.8 (7)	C63—C64—C65	104.9 (8)
C17—C16—H16	108.0	H64A—C64—H64B	108.8
C18—C16—C15	112.3 (8)	C65—C64—H64A	110.8
C18—C16—H16	108.0	C65—C64—H64B	110.8
C18—C16—C17	110.6 (8)	C66—C65—H65A	110.9
C45—C44—C40	121.7 (8)	C66—C65—H65B	110.9
C45—C44—H44	119.2	C64—C65—C66	104.2 (8)
C40—C44—H44	119.2	C64—C65—H65A	110.9
C32—C31—H31	120.4	C64—C65—H65B	110.9
C32—C31—C30	119.3 (8)	H65A—C65—H65B	108.9
C30—C31—H31	120.4	C70—O5—C67	104.2 (9)
C45—C46—C47	120.0 (8)	O5—C67—H67A	110.7
C45—C46—H46	120.0	O5—C67—H67B	110.7
C47—C46—H46	120.0	O5—C67—C68	105.1 (9)
C29—C28—H28	107.8	H67A—C67—H67B	108.8
C29—C28—C27	111.5 (8)	C68—C67—H67A	110.7
C29—C28—C26	110.6 (8)	C68—C67—H67B	110.7

C27—C28—H28	107.8	C67—C68—H68A	110.7
C26—C28—H28	107.8	C67—C68—H68B	110.7
C26—C28—C27	111.1 (8)	H68A—C68—H68B	108.8
C47—C48—H48	107.9	C69—C68—C67	105.2 (10)
C47—C48—C49	110.8 (8)	C69—C68—H68A	110.7
C47—C48—C50	110.9 (8)	C69—C68—H68B	110.7
C49—C48—H48	107.9	C68—C69—H69A	111.3
C50—C48—H48	107.9	C68—C69—H69B	111.3
C50—C48—C49	111.3 (8)	C68—C69—C70	102.5 (10)
C10—C12—H12A	109.5	H69A—C69—H69B	109.2
C10—C12—H12B	109.5	C70—C69—H69A	111.3
C10—C12—H12C	109.5	C70—C69—H69B	111.3
H12A—C12—H12B	109.5	O5—C70—C69	106.6 (11)
H12A—C12—H12C	109.5	O5—C70—H70A	110.4
H12B—C12—H12C	109.5	O5—C70—H70B	110.4
C4—C5—H5	119.1	C69—C70—H70A	110.4
C6—C5—C4	121.8 (8)	C69—C70—H70B	110.4
C6—C5—H5	119.1	H70A—C70—H70B	108.6
C16—C17—H17A	109.5	C14—N2—Sb2	118.9 (5)
C16—C17—H17B	109.5	C13—N2—Sb2	123.8 (5)
C16—C17—H17C	109.5	C13—N2—C14	117.3 (6)
H17A—C17—H17B	109.5	N3—C38—H38	118.5
H17A—C17—H17C	109.5	N4—C38—N3	123.0 (7)
H17B—C17—H17C	109.5	N4—C38—H38	118.5
C41—C43—H43A	109.5	C3—C2—H2A	109.5
C41—C43—H43B	109.5	C3—C2—H2B	109.5
C41—C43—H43C	109.5	C3—C2—H2C	109.5
H43A—C43—H43B	109.5	H2A—C2—H2B	109.5
H43A—C43—H43C	109.5	H2A—C2—H2C	109.5
H43B—C43—H43C	109.5	H2B—C2—H2C	109.5
C7—C6—C5	119.4 (8)	C71—O6—C74	107.5 (10)

C7—C6—H6	120.3	O6—C74—H74A	109.9
C5—C6—H6	120.3	O6—C74—H74B	109.9
C35—C36—H36A	109.5	O6—C74—C73	108.7 (12)
C35—C36—H36B	109.5	H74A—C74—H74B	108.3
C35—C36—H36C	109.5	C73—C74—H74A	109.9
H36A—C36—H36B	109.5	C73—C74—H74B	109.9
H36A—C36—H36C	109.5	C74—C73—H73A	111.5
H36B—C36—H36C	109.5	C74—C73—H73B	111.5
C4—C3—H3	108.0	C74—C73—C72	101.5 (13)
C4—C3—C1	111.4 (9)	H73A—C73—H73B	109.3
C4—C3—C2	111.7 (8)	C72—C73—H73A	111.5
C1—C3—H3	108.0	C72—C73—H73B	111.5
C1—C3—C2	109.5 (9)	O6—C71—H71A	110.5
C2—C3—H3	108.0	O6—C71—H71B	110.5
C23—C25—H25A	109.5	O6—C71—C72	106.1 (10)
C23—C25—H25B	109.5	H71A—C71—H71B	108.7
C23—C25—H25C	109.5	C72—C71—H71A	110.5
H25A—C25—H25B	109.5	C72—C71—H71B	110.5
H25A—C25—H25C	109.5	C73—C72—H72A	111.2
H25B—C25—H25C	109.5	C73—C72—H72B	111.2
C10—C11—H11A	109.5	C71—C72—C73	102.7 (13)
C10—C11—H11B	109.5	C71—C72—H72A	111.2
C10—C11—H11C	109.5	C71—C72—H72B	111.2
H11A—C11—H11B	109.5	H72A—C72—H72B	109.1
H11A—C11—H11C	109.5	C78—O7—C75	107.2 (13)
H11B—C11—H11C	109.5	O7—C75—H75A	110.8
C29—C30—H30	119.3	O7—C75—H75B	110.8
C31—C30—C29	121.5 (8)	O7—C75—C76	104.7 (13)
C31—C30—H30	119.3	H75A—C75—H75B	108.9
C3—C1—H1A	109.5	C76—C75—H75A	110.8
C3—C1—H1B	109.5	C76—C75—H75B	110.8

C3—C1—H1C	109.5	C75—C76—H76A	111.5
H1A—C1—H1B	109.5	C75—C76—H76B	111.5
H1A—C1—H1C	109.5	C75—C76—C77	101.6 (11)
H1B—C1—H1C	109.5	H76A—C76—H76B	109.3
C41—C42—H42A	109.5	C77—C76—H76A	111.5
C41—C42—H42B	109.5	C77—C76—H76B	111.5
C41—C42—H42C	109.5	C76—C77—H77A	111.1
H42A—C42—H42B	109.5	C76—C77—H77B	111.1
H42A—C42—H42C	109.5	H77A—C77—H77B	109.1
H42B—C42—H42C	109.5	C78—C77—C76	103.1 (11)
C35—C37—H37A	109.5	C78—C77—H77A	111.1
C35—C37—H37B	109.5	C78—C77—H77B	111.1
C35—C37—H37C	109.5	O7—C78—C77	107.1 (11)
H37A—C37—H37B	109.5	O7—C78—H78A	110.3
H37A—C37—H37C	109.5	O7—C78—H78B	110.3
H37B—C37—H37C	109.5	C77—C78—H78A	110.3
C48—C49—H49A	109.5	C77—C78—H78B	110.3
C48—C49—H49B	109.5	H78A—C78—H78B	108.5
C48—C49—H49C	109.5	C82—O8—C79	111.6 (16)
H49A—C49—H49B	109.5	O8—C79—H79A	111.3
H49A—C49—H49C	109.5	O8—C79—H79B	111.3
H49B—C49—H49C	109.5	O8—C79—C80	102.2 (15)
O1—C51—H51A	110.2	H79A—C79—H79B	109.2
O1—C51—H51B	110.2	C80—C79—H79A	111.3
O1—C51—C52	107.7 (8)	C80—C79—H79B	111.3
H51A—C51—H51B	108.5	C79—C80—H80A	112.1
C52—C51—H51A	110.2	C79—C80—H80B	112.1
C52—C51—H51B	110.2	C79—C80—C81	98.5 (15)
C16—C18—H18A	109.5	H80A—C80—H80B	109.7
C16—C18—H18B	109.5	C81—C80—H80A	112.1
C16—C18—H18C	109.5	C81—C80—H80B	112.1

H18A—C18—H18B	109.5	C80—C81—H81A	112.0
H18A—C18—H18C	109.5	C80—C81—H81B	112.0
H18B—C18—H18C	109.5	H81A—C81—H81B	109.7
C23—C24—H24A	109.5	C82—C81—C80	98.7 (15)
C23—C24—H24B	109.5	C82—C81—H81A	112.0
C23—C24—H24C	109.5	C82—C81—H81B	112.0
H24A—C24—H24B	109.5	O8—C82—C81	101.9 (15)
H24A—C24—H24C	109.5	O8—C82—H82A	111.4
H24B—C24—H24C	109.5	O8—C82—H82B	111.4
H53A—C53—H53B	109.3	C81—C82—H82A	111.4
C54—C53—H53A	111.5	C81—C82—H82B	111.4
C54—C53—H53B	111.5	H82A—C82—H82B	109.3
Sb1—N1—C9—C8	84.8 (8)	C7—C8—C10—C12	49.7 (11)
Sb1—N1—C9—C4	−93.6 (8)	C7—C8—C10—C11	−75.2 (10)
Sb1—N1—C13—N2	2.2 (11)	C40—C39—C47—C46	2.1 (13)
Sb1—N3—C34—C33	88.8 (8)	C40—C39—C47—C48	−176.1 (8)
Sb1—N3—C34—C29	−89.3 (8)	C10—C8—C7—C6	178.9 (9)
Sb1—N3—C38—N4	2.9 (11)	C4—C9—C8—C7	−1.3 (12)
Sb2—N4—C39—C47	−91.2 (8)	C4—C9—C8—C10	179.9 (8)
Sb2—N4—C39—C40	87.8 (8)	C4—C5—C6—C7	−0.4 (14)
Sb2—N4—C38—N3	−1.4 (11)	C32—C33—C35—C36	−61.6 (11)
N1—C9—C8—C7	−179.7 (7)	C32—C33—C35—C37	61.3 (12)
N1—C9—C8—C10	1.5 (12)	C32—C31—C30—C29	−1.5 (15)
N1—C9—C4—C5	−180.0 (8)	O1—C51—C52—C53	24.0 (13)
N1—C9—C4—C3	0.2 (12)	C35—C33—C32—C31	179.2 (9)
N1—C13—N2—Sb2	−1.3 (10)	C16—C15—C19—C20	−179.5 (9)
N1—C13—N2—C14	−179.9 (7)	C44—C45—C46—C47	−1.1 (15)
N3—C34—C33—C32	−178.8 (7)	C46—C45—C44—C40	1.1 (15)
N3—C34—C33—C35	3.3 (12)	C46—C47—C48—C49	−62.2 (11)
N3—C34—C29—C28	−0.6 (12)	C46—C47—C48—C50	61.9 (11)
N3—C34—C29—C30	177.2 (8)	C28—C29—C30—C31	179.9 (9)

C14—C15—C19—C20	0.9 (13)	C48—C47—C46—C45	177.8 (9)
C14—C15—C16—C17	106.7 (9)	C5—C4—C3—C1	65.3 (12)
C14—C15—C16—C18	−129.8 (9)	C5—C4—C3—C2	−57.5 (13)
C14—C22—C21—C20	1.8 (13)	C43—C41—C40—C39	97.7 (9)
C14—C22—C23—C25	119.4 (9)	C43—C41—C40—C44	−80.4 (10)
C14—C22—C23—C24	−117.1 (9)	C3—C4—C5—C6	179.1 (9)
N4—C39—C47—C46	−178.9 (8)	C30—C29—C28—C27	54.0 (11)
N4—C39—C47—C48	2.8 (13)	C30—C29—C28—C26	−70.2 (12)
N4—C39—C40—C41	0.7 (12)	C42—C41—C40—C39	−138.4 (9)
N4—C39—C40—C44	178.9 (8)	C42—C41—C40—C44	43.5 (11)
C9—N1—C13—N2	−178.0 (7)	C51—O1—C54—C53	−22.1 (13)
C9—C8—C7—C6	0.1 (13)	C54—O1—C51—C52	−1.6 (13)
C9—C8—C10—C12	−131.5 (9)	C54—C53—C52—C51	−35.5 (12)
C9—C8—C10—C11	103.6 (9)	C52—C53—C54—O1	36.5 (13)
C9—C4—C5—C6	−0.7 (14)	O3—C59—C60—C61	31.0 (12)
C9—C4—C3—C1	−114.8 (10)	O3—C62—C61—C60	18.2 (15)
C9—C4—C3—C2	122.4 (10)	C59—O3—C62—C61	1.4 (14)
C34—N3—C38—N4	−178.7 (7)	C59—C60—C61—C62	−29.4 (13)
C34—C33—C32—C31	1.3 (14)	C62—O3—C59—C60	−20.8 (12)
C34—C33—C35—C36	116.2 (10)	O2—C55—C56—C57	36.7 (11)
C34—C33—C35—C37	−120.9 (10)	C55—O2—C58—C57	−5.2 (13)
C34—C29—C28—C27	−128.2 (9)	C58—O2—C55—C56	−19.9 (12)
C34—C29—C28—C26	107.6 (10)	C58—C57—C56—C55	−38.5 (11)
C34—C29—C30—C31	2.0 (14)	C56—C57—C58—O2	27.7 (13)
C39—N4—C38—N3	−179.5 (7)	O4—C63—C64—C65	−31.0 (12)
C39—C47—C46—C45	−0.5 (14)	O4—C66—C65—C64	14.8 (13)
C39—C47—C48—C49	116.1 (10)	C63—O4—C66—C65	−34.6 (12)
C39—C47—C48—C50	−119.8 (10)	C63—C64—C65—C66	10.0 (13)
C39—C40—C44—C45	0.5 (13)	C66—O4—C63—C64	41.1 (11)
C33—C34—C29—C28	−178.7 (8)	O5—C67—C68—C69	−24.8 (13)
C33—C34—C29—C30	−0.8 (12)	C67—O5—C70—C69	−39.3 (15)

C33—C32—C31—C30	−0.2 (15)	C67—C68—C69—C70	1.6 (15)
C15—C14—C22—C21	−1.8 (12)	C68—C69—C70—O5	22.9 (16)
C15—C14—C22—C23	178.0 (8)	C70—O5—C67—C68	40.0 (12)
C15—C14—N2—Sb2	−95.5 (7)	N2—C14—C15—C19	178.6 (7)
C15—C14—N2—C13	83.1 (9)	N2—C14—C15—C16	−0.9 (11)
C15—C19—C20—C21	−0.9 (14)	N2—C14—C22—C21	−179.9 (7)
C22—C14—C15—C19	0.4 (12)	N2—C14—C22—C23	−0.1 (12)
C22—C14—C15—C16	−179.1 (8)	C38—N3—C34—C33	−89.7 (9)
C22—C14—N2—Sb2	82.6 (8)	C38—N3—C34—C29	92.2 (9)
C22—C14—N2—C13	−98.7 (9)	C38—N4—C39—C47	87.0 (10)
C22—C21—C20—C19	−0.5 (14)	C38—N4—C39—C40	−94.0 (9)
C29—C34—C33—C32	−0.8 (12)	O6—C74—C73—C72	27 (2)
C29—C34—C33—C35	−178.6 (8)	O6—C71—C72—C73	32.9 (17)
C21—C22—C23—C25	−60.8 (11)	C74—O6—C71—C72	−16.7 (17)
C21—C22—C23—C24	62.7 (11)	C74—C73—C72—C71	−36 (2)
C13—N1—C9—C8	−95.0 (9)	C71—O6—C74—C73	−7 (2)
C13—N1—C9—C4	86.6 (9)	O7—C75—C76—C77	−40 (2)
C19—C15—C16—C17	−72.8 (11)	C75—O7—C78—C77	−4 (4)
C19—C15—C16—C18	50.7 (11)	C75—C76—C77—C78	36 (2)
C41—C40—C44—C45	178.7 (9)	C76—C77—C78—O7	−20 (4)
C8—C9—C4—C5	1.6 (12)	C78—O7—C75—C76	28 (4)
C8—C9—C4—C3	−178.2 (8)	O8—C79—C80—C81	41 (3)
C8—C7—C6—C5	0.7 (14)	C79—O8—C82—C81	−17 (3)
C23—C22—C21—C20	−178.0 (8)	C79—C80—C81—C82	−51 (3)
C47—C39—C40—C41	179.7 (8)	C80—C81—C82—O8	42 (3)
C47—C39—C40—C44	−2.1 (12)	C82—O8—C79—C80	−16 (4)

2.

Crystal data

$C_{50}H_{70}ClN_4Sb$ $F(000) = 1864$

$M_r = 884.30$ $D_x = 1.225$ Mg m^{-3}

Monoclinic, $P2_1/c$	Synchrotron, λ = 0.71073 Å
a = 18.443 (4) Å	Cell parameters from 7706 reflections
b = 20.455 (4) Å	θ = 2–25°
c = 12.817 (3) Å	μ = 0.67 mm^{-1}
β = 97.46 (3)°	T = 100 K
V = 4794.3 (17) $Å^3$	Block, colourless
Z = 4	0.11 × 0.05 × 0.03
Data collection	
ADSC Quantum 210r Diffractometer	7706 observed [$I > 2\sigma(I)$] reflections
Radiation source: MX1 Beamline Australian Synchrotron	R_{int} = 0.039
Scan method: Phi scans	θ_{max} = 25°, θ_{min} = 1.1°
Absorption correction: Multi-scan, XDS (Kabsch, 1993)	h = −21→21
58107 measured reflections	k = −24→24
8002 independent reflections	l = −15→15
Refinement	
Refinement on F^2	0 restraints
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.029	$w = 1/[\sigma^2(F_o^2) + (0.034P)^2 + 4.7594P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.073	
S = 1.08	$(\Delta/\sigma)_{max}$ = 0.002
8002 reflections	$\Delta\rho_{max}$ = 1.01 e $Å^{-3}$
522 parameters	$\Delta\rho_{min}$ = −0.82 e $Å^{-3}$

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	y	z	U_{iso}^*/U_{eq}
Sb1	0.73700(2)	0.43057(2)	0.79144(2)	0.01702(7)
Cl1	0.76260(3)	0.31630(3)	0.77636(5)	0.03449(15)
N4	0.85421(10)	0.44312(8)	0.81255(13)	0.0180(3)
N2	0.70381(10)	0.44375(8)	0.62880(13)	0.0180(3)
N3	0.80322(9)	0.54279(8)	0.78694(12)	0.0149(3)
N1	0.61499(10)	0.38883(8)	0.69696(13)	0.0205(4)
C38	0.85976(11)	0.50854(9)	0.82272(14)	0.0160(4)
H38	0.903482	0.528608	0.854905	0.019
C34	0.80631(11)	0.61234(9)	0.79643(15)	0.0157(4)
C29	0.77287(11)	0.64296(10)	0.87598(16)	0.0196(4)
C13	0.63694(12)	0.41448(9)	0.61589(16)	0.0192(4)
H13	0.607769	0.413197	0.54914	0.023
C9	0.54793(12)	0.35438(10)	0.69358(16)	0.0226(4)
C14	0.72031(12)	0.48681(10)	0.54620(15)	0.0211(4)

C4	0.49409(13)	0.38230(11)	0.74805(17)	0.0261(5)
C22	0.68709(13)	0.54880(11)	0.53487(16)	0.0252(5)
C35	0.87175(12)	0.61622(10)	0.63245(15)	0.0218(4)
H35	0.844452	0.57454	0.615267	0.026
C33	0.83881(11)	0.64905(10)	0.72206(15)	0.0187(4)
C30	0.77304(13)	0.71103(10)	0.88019(17)	0.0254(5)
H30	0.750487	0.732463	0.933311	0.03
C39	0.90743(11)	0.40353(9)	0.87686(16)	0.0196(4)
C31	0.80535(13)	0.74797(10)	0.80866(18)	0.0282(5)
H31	0.805206	0.79434	0.812943	0.034
C32	0.83801(12)	0.71694(10)	0.73054(17)	0.0253(5)
H32	0.86033	0.742567	0.68173	0.03
C28	0.73653(12)	0.60415(10)	0.95587(16)	0.0228(4)
H28	0.752716	0.557654	0.951979	0.027
C8	0.53746(13)	0.29339(11)	0.64312(18)	0.0291(5)
C23	0.63825(14)	0.57568(10)	0.61163(18)	0.0273(5)
H23	0.652315	0.553908	0.681172	0.033
C5	0.42986(14)	0.34739(12)	0.7522(2)	0.0350(6)
H5	0.393031	0.364956	0.789454	0.042
C15	0.76419(13)	0.46304(12)	0.47305(17)	0.0279(5)
C3	0.50808(13)	0.44735(11)	0.80412(18)	0.0279(5)
H3	0.544975	0.471481	0.768205	0.033
C48	0.85662(13)	0.44163(11)	1.04474(17)	0.0263(5)
H48	0.823891	0.467081	0.991104	0.032
C41	0.95176(14)	0.36018(12)	0.70987(19)	0.0349(6)
H41	0.905077	0.381262	0.678353	0.042
C47	0.91167(12)	0.40539(10)	0.98723(17)	0.0222(4)
C21	0.69816(16)	0.58575(13)	0.44686(19)	0.0384(6)
H21	0.675647	0.627441	0.436613	0.046
C40	0.95604(13)	0.36488(10)	0.82821(18)	0.0259(5)
C46	0.96744(13)	0.37060(11)	1.04690(18)	0.0286(5)
H46	0.971092	0.371806	1.121491	0.034
C37	0.95233(13)	0.59891(14)	0.66220(18)	0.0341(5)
H37A	0.980258	0.638785	0.681882	0.051
H37B	0.97101	0.578331	0.602002	0.051
H37C	0.95742	0.568519	0.721809	0.051
C45	1.01745(14)	0.33444(11)	0.9999(2)	0.0331(5)

H45	1.055974	0.312023	1.041599	0.04
C25	0.64529(15)	0.64971(11)	0.6282(2)	0.0371(6)
H25A	0.696994	0.661304	0.645744	0.056
H25B	0.618416	0.66282	0.685963	0.056
H25C	0.624956	0.672343	0.563605	0.056
C36	0.86387(14)	0.65816(12)	0.53266(17)	0.0309(5)
H36A	0.813502	0.674174	0.517884	0.046
H36B	0.875597	0.631764	0.473276	0.046
H36C	0.897477	0.695401	0.542948	0.046
C10	0.59494(15)	0.26136(11)	0.5851(2)	0.0354(6)
H10	0.639297	0.289945	0.594197	0.042
C24	0.55758(15)	0.56005(12)	0.5750(2)	0.0353(6)
H24A	0.527165	0.578921	0.624576	0.053
H24B	0.550731	0.512545	0.572078	0.053
H24C	0.543334	0.578704	0.504889	0.053
C27	0.75858(16)	0.62772(14)	1.06863(19)	0.0399(6)
H27A	0.812024	0.628559	1.084048	0.06
H27B	0.738625	0.597921	1.117575	0.06
H27C	0.739221	0.671802	1.076614	0.06
C19	0.77391(15)	0.50285(14)	0.38728(18)	0.0391(6)
H19	0.803745	0.487999	0.337001	0.047
C1	0.54193(15)	0.43559(12)	0.9178(2)	0.0350(6)
H1A	0.507666	0.410708	0.954748	0.052
H1B	0.552362	0.477679	0.953105	0.052
H1C	0.587482	0.410832	0.918464	0.052
C44	1.01084(14)	0.33123(11)	0.8916(2)	0.0337(5)
H44	1.044536	0.305407	0.859366	0.04
C7	0.47165(14)	0.26126(12)	0.6487(2)	0.0376(6)
H7	0.46303	0.220339	0.614237	0.045
C6	0.41882(15)	0.28716(13)	0.7027(2)	0.0411(7)
H6	0.374638	0.263863	0.70613	0.049
C26	0.65373(15)	0.60544(15)	0.9293(2)	0.0428(6)
H26A	0.636353	0.650665	0.930775	0.064
H26B	0.631598	0.579439	0.981099	0.064
H26C	0.639878	0.587044	0.85894	0.064
C16	0.79554(15)	0.39468(14)	0.48081(19)	0.0366(6)
H16	0.801793	0.38124	0.556466	0.044

C20	0.74113(18)	0.56290(14)	0.3745(2)	0.0446(7)
H20	0.748082	0.589008	0.315346	0.054
C11	0.56870(17)	0.25610(14)	0.4664(2)	0.0456(7)
H11A	0.52445	0.22914	0.455222	0.068
H11B	0.607098	0.235938	0.431079	0.068
H11C	0.557853	0.299871	0.43746	0.068
C49	0.89309(15)	0.48999(13)	1.1251(2)	0.0384(6)
H49A	0.923383	0.466199	1.18116	0.058
H49B	0.855516	0.514911	1.155411	0.058
H49C	0.923869	0.52003	1.090648	0.058
C2	0.43985(15)	0.49040(13)	0.7984(2)	0.0411(6)
H2A	0.418928	0.496095	0.724654	0.062
H2B	0.453166	0.533179	0.82955	0.062
H2C	0.403744	0.469487	0.837217	0.062
C42	1.01490(18)	0.3977(2)	0.6721(2)	0.0675(11)
H42A	1.010517	0.444201	0.688406	0.101
H42B	1.013386	0.392071	0.595927	0.101
H42C	1.061385	0.380838	0.707754	0.101
C43	0.9502(2)	0.28895(17)	0.6740(3)	0.0776(14)
H43A	0.995966	0.267468	0.702524	0.116
H43B	0.944521	0.287216	0.596942	0.116
H43C	0.90895	0.266446	0.699451	0.116
C17	0.74176(19)	0.34714(15)	0.4188(3)	0.0545(8)
H17A	0.695202	0.34781	0.447988	0.082
H17B	0.762144	0.302841	0.424207	0.082
H17C	0.7336	0.360415	0.344785	0.082
C50	0.80866(16)	0.39307(15)	1.0960(2)	0.0442(6)
H50A	0.784706	0.363337	1.042259	0.066
H50B	0.771441	0.417044	1.128577	0.066
H50C	0.839174	0.367802	1.14991	0.066
C12	0.61724(18)	0.19443(13)	0.6323(3)	0.0502(8)
H12A	0.636923	0.19964	0.706634	0.075
H12B	0.65468	0.17513	0.594117	0.075
H12C	0.574387	0.165692	0.62643	0.075
C18	0.87034(18)	0.3901(2)	0.4406(2)	0.0628(10)
H18A	0.864556	0.3992	0.364915	0.094
H18B	0.890326	0.346017	0.453602	0.094

H18C	0.903831	0.422129	0.477666	0.094

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sb1	0.01757(11)	0.01786(10)	0.01538(9)	0.00056(4)	0.00123(5)	-0.00189(5)
Cl1	0.0329(3)	0.0160(2)	0.0503(3)	0.0016(2)	-0.0109(3)	-0.0015(2)
N4	0.0196(10)	0.0151(8)	0.0187(8)	-0.0010(6)	0.0004(7)	0.0010(6)
N2	0.0182(10)	0.0199(8)	0.0151(8)	-0.0010(6)	-0.0010(6)	-0.0026(7)
N3	0.0150(9)	0.0157(8)	0.0141(8)	-0.0006(6)	0.0025(6)	-0.0012(6)
N1	0.0183(10)	0.0197(8)	0.0227(9)	-0.0012(7)	0.0001(7)	-0.0023(7)
C38	0.0174(11)	0.0187(9)	0.0125(9)	-0.0017(7)	0.0040(7)	-0.0008(7)
C34	0.0139(11)	0.0152(9)	0.0173(9)	-0.0003(7)	-0.0012(7)	0.0009(7)
C29	0.0172(11)	0.0208(10)	0.0207(10)	0.0000(8)	0.0019(8)	0.0007(8)
C13	0.0189(11)	0.0163(9)	0.0211(10)	-0.0030(8)	-0.0020(8)	-0.0004(8)
C9	0.0191(12)	0.0221(10)	0.0246(10)	0.0056(8)	-0.0042(8)	-0.0031(8)
C14	0.0215(12)	0.0254(11)	0.0153(9)	-0.0003(8)	-0.0026(8)	-0.0075(8)
C4	0.0216(12)	0.0287(11)	0.0270(11)	0.0102(9)	0.0002(8)	-0.0015(9)
C22	0.0266(13)	0.0271(11)	0.0192(10)	0.0021(9)	-0.0072(8)	-0.0061(9)
C35	0.0230(12)	0.0262(10)	0.0170(10)	0.0042(8)	0.0053(8)	-0.0016(8)
C33	0.0147(11)	0.0222(10)	0.0188(10)	0.0016(8)	0.0008(7)	-0.0013(7)
C30	0.0270(13)	0.0194(10)	0.0299(11)	-0.0044(8)	0.0042(9)	0.0041(8)
C39	0.0180(11)	0.0156(9)	0.0240(10)	-0.0008(8)	-0.0017(8)	0.0001(8)
C31	0.0314(14)	0.0149(10)	0.0372(12)	-0.0011(9)	0.0002(10)	-0.0010(8)
C32	0.0260(13)	0.0214(10)	0.0278(11)	0.0058(8)	0.0014(9)	-0.0058(8)
C28	0.0277(12)	0.0209(10)	0.0216(10)	-0.0017(8)	0.0097(8)	0.0033(8)
C8	0.0273(13)	0.0222(11)	0.0341(12)	0.0043(9)	-0.0099(9)	-0.0025(9)
C23	0.0305(14)	0.0245(11)	0.0241(11)	0.0008(8)	-0.0068(9)	0.0035(9)
C5	0.0243(14)	0.0394(14)	0.0412(14)	0.0167(11)	0.0038(10)	-0.0027(10)
C15	0.0231(13)	0.0412(13)	0.0189(10)	-0.0039(9)	0.0005(8)	-0.0072(10)
C3	0.0251(13)	0.0290(11)	0.0311(12)	0.0034(9)	0.0100(9)	0.0001(9)
C48	0.0269(13)	0.0329(12)	0.0185(10)	0.0035(9)	0.0013(9)	0.0041(9)
C41	0.0306(14)	0.0410(14)	0.0317(13)	-0.0162(10)	-0.0005(10)	0.0154(10)
C47	0.0221(12)	0.0192(10)	0.0247(11)	0.0020(8)	0.0009(8)	-0.0018(8)
C21	0.0545(18)	0.0312(12)	0.0255(12)	0.0073(10)	-0.0097(11)	-0.0083(11)
C40	0.0223(12)	0.0231(10)	0.0310(12)	-0.0057(9)	-0.0015(9)	0.0027(8)
C46	0.0314(14)	0.0250(11)	0.0276(11)	0.0053(9)	-0.0035(9)	-0.0016(9)

C37	0.0246(14)	0.0540(16)	0.0248(11)	0.0077(11)	0.0074(9)	0.0044(11)
C45	0.0288(14)	0.0259(11)	0.0414(14)	0.0042(10)	-0.0072(10)	0.0062(9)
C25	0.0366(15)	0.0261(12)	0.0437(14)	-0.0045(10)	-0.0137(11)	0.0050(10)
C36	0.0359(14)	0.0362(13)	0.0211(11)	0.0079(9)	0.0050(9)	-0.0031(10)
C10	0.0331(15)	0.0246(12)	0.0453(14)	-0.0087(10)	-0.0070(11)	-0.0020(10)
C24	0.0315(15)	0.0291(12)	0.0423(14)	0.0014(10)	-0.0061(11)	0.0012(10)
C27	0.0493(17)	0.0481(15)	0.0223(12)	-0.0006(10)	0.0053(11)	-0.0047(12)
C19	0.0427(16)	0.0574(17)	0.0177(11)	-0.0029(11)	0.0054(10)	-0.0167(13)
C1	0.0341(15)	0.0402(14)	0.0315(13)	0.0007(10)	0.0076(11)	-0.0009(10)
C44	0.0296(14)	0.0279(12)	0.0420(14)	-0.0058(10)	-0.0010(10)	0.0104(10)
C7	0.0316(15)	0.0240(12)	0.0527(16)	0.0077(11)	-0.0118(11)	-0.0080(10)
C6	0.0272(15)	0.0353(13)	0.0572(17)	0.0198(12)	-0.0086(11)	-0.0146(11)
C26	0.0280(15)	0.0631(18)	0.0384(14)	0.0093(13)	0.0085(11)	-0.0112(12)
C16	0.0332(15)	0.0515(16)	0.0266(12)	-0.0049(11)	0.0091(10)	0.0081(11)
C20	0.062(2)	0.0505(17)	0.0198(12)	0.0092(11)	0.0004(12)	-0.0190(13)
C11	0.0507(18)	0.0381(14)	0.0449(15)	-0.0114(12)	-0.0054(12)	-0.0007(12)
C49	0.0405(16)	0.0414(14)	0.0321(13)	-0.0091(11)	0.0006(11)	0.0073(11)
C2	0.0388(16)	0.0411(14)	0.0447(15)	0.0047(12)	0.0102(12)	0.0096(11)
C42	0.041(2)	0.136(3)	0.0275(14)	-0.0136(18)	0.0118(13)	-0.0006(19)
C43	0.102(3)	0.059(2)	0.060(2)	-0.0387(17)	-0.035(2)	0.047(2)
C17	0.067(2)	0.0428(16)	0.0550(18)	-0.0237(14)	0.0129(15)	0.0020(14)
C50	0.0417(17)	0.0536(17)	0.0404(15)	0.0057(12)	0.0171(12)	-0.0045(13)
C12	0.055(2)	0.0302(14)	0.0605(19)	-0.0063(12)	-0.0107(14)	0.0098(12)
C18	0.046(2)	0.108(3)	0.0383(16)	0.0047(17)	0.0212(14)	0.0248(18)

Geometric parameters (Å, º)

Sb1—Cl1	2.3972 (7)	C46—H46	0.9500
Sb1—N4	2.1587 (19)	C46—C45	1.381 (4)
Sb1—N2	2.1121 (17)	C37—H37A	0.9800
Sb1—N3	2.6044 (17)	C37—H37B	0.9800
Sb1—N1	2.5593 (19)	C37—H37C	0.9800
N4—C38	1.347 (3)	C45—H45	0.9500
N4—C39	1.445 (3)	C45—C44	1.378 (4)
N2—C13	1.361 (3)	C25—H25A	0.9800
N2—C14	1.440 (3)	C25—H25B	0.9800

N3—C38	1.290 (3)	C25—H25C	0.9800
N3—C34	1.428 (3)	C36—H36A	0.9800
N1—C13	1.276 (3)	C36—H36B	0.9800
N1—C9	1.419 (3)	C36—H36C	0.9800
C38—H38	0.9500	C10—H10	1.0000
C34—C29	1.406 (3)	C10—C11	1.539 (4)
C34—C33	1.407 (3)	C10—C12	1.531 (4)
C29—C30	1.393 (3)	C24—H24A	0.9800
C29—C28	1.519 (3)	C24—H24B	0.9800
C13—H13	0.9500	C24—H24C	0.9800
C9—C4	1.407 (3)	C27—H27A	0.9800
C9—C8	1.407 (3)	C27—H27B	0.9800
C14—C22	1.408 (3)	C27—H27C	0.9800
C14—C15	1.403 (3)	C19—H19	0.9500
C4—C5	1.390 (3)	C19—C20	1.369 (4)
C4—C3	1.518 (3)	C1—H1A	0.9800
C22—C23	1.520 (3)	C1—H1B	0.9800
C22—C21	1.395 (3)	C1—H1C	0.9800
C35—H35	1.0000	C44—H44	0.9500
C35—C33	1.523 (3)	C7—H7	0.9500
C35—C37	1.527 (3)	C7—C6	1.373 (4)
C35—C36	1.531 (3)	C6—H6	0.9500
C33—C32	1.393 (3)	C26—H26A	0.9800
C30—H30	0.9500	C26—H26B	0.9800
C30—C31	1.381 (3)	C26—H26C	0.9800
C39—C47	1.407 (3)	C16—H16	1.0000
C39—C40	1.401 (3)	C16—C17	1.535 (4)
C31—H31	0.9500	C16—C18	1.537 (4)
C31—C32	1.387 (3)	C20—H20	0.9500
C32—H32	0.9500	C11—H11A	0.9800
C28—H28	1.0000	C11—H11B	0.9800

C28—C27	1.528 (3)	C11—H11C	0.9800
C28—C26	1.521 (4)	C49—H49A	0.9800
C8—C10	1.520 (4)	C49—H49B	0.9800
C8—C7	1.390 (3)	C49—H49C	0.9800
C23—H23	1.0000	C2—H2A	0.9800
C23—C25	1.532 (3)	C2—H2B	0.9800
C23—C24	1.535 (4)	C2—H2C	0.9800
C5—H5	0.9500	C42—H42A	0.9800
C5—C6	1.389 (4)	C42—H42B	0.9800
C15—C19	1.398 (3)	C42—H42C	0.9800
C15—C16	1.512 (4)	C43—H43A	0.9800
C3—H3	1.0000	C43—H43B	0.9800
C3—C1	1.528 (3)	C43—H43C	0.9800
C3—C2	1.530 (3)	C17—H17A	0.9800
C48—H48	1.0000	C17—H17B	0.9800
C48—C47	1.523 (3)	C17—H17C	0.9800
C48—C49	1.521 (3)	C50—H50A	0.9800
C48—C50	1.533 (3)	C50—H50B	0.9800
C41—H41	1.0000	C50—H50C	0.9800
C41—C40	1.512 (3)	C12—H12A	0.9800
C41—C42	1.525 (4)	C12—H12B	0.9800
C41—C43	1.527 (4)	C12—H12C	0.9800
C47—C46	1.395 (3)	C18—H18A	0.9800
C21—H21	0.9500	C18—H18B	0.9800
C21—C20	1.377 (4)	C18—H18C	0.9800
C40—C44	1.394 (3)		
Cl1—Sb1—N3	139.44 (4)	H37A—C37—H37C	109.5
Cl1—Sb1—N1	78.87 (4)	H37B—C37—H37C	109.5
N4—Sb1—Cl1	85.50 (5)	C46—C45—H45	120.4
N4—Sb1—N3	55.47 (6)	C44—C45—C46	119.2 (2)
N4—Sb1—N1	154.62 (6)	C44—C45—H45	120.4

N2—Sb1—Cl1	94.57 (5)	C23—C25—H25A	109.5
N2—Sb1—N4	105.41 (7)	C23—C25—H25B	109.5
N2—Sb1—N3	86.69 (6)	C23—C25—H25C	109.5
N2—Sb1—N1	56.73 (7)	H25A—C25—H25B	109.5
N1—Sb1—N3	132.03 (5)	H25A—C25—H25C	109.5
C38—N4—Sb1	101.10 (13)	H25B—C25—H25C	109.5
C38—N4—C39	117.64 (17)	C35—C36—H36A	109.5
C39—N4—Sb1	126.85 (13)	C35—C36—H36B	109.5
C13—N2—Sb1	101.86 (13)	C35—C36—H36C	109.5
C13—N2—C14	117.03 (17)	H36A—C36—H36B	109.5
C14—N2—Sb1	137.89 (13)	H36A—C36—H36C	109.5
C38—N3—Sb1	82.71 (11)	H36B—C36—H36C	109.5
C38—N3—C34	119.29 (16)	C8—C10—H10	107.6
C34—N3—Sb1	152.82 (12)	C8—C10—C11	111.3 (2)
C13—N1—Sb1	84.01 (13)	C8—C10—C12	111.1 (2)
C13—N1—C9	123.14 (18)	C11—C10—H10	107.6
C9—N1—Sb1	152.77 (13)	C12—C10—H10	107.6
N4—C38—H38	121.4	C12—C10—C11	111.2 (2)
N3—C38—N4	117.22 (18)	C23—C24—H24A	109.5
N3—C38—H38	121.4	C23—C24—H24B	109.5
C29—C34—N3	119.30 (17)	C23—C24—H24C	109.5
C29—C34—C33	121.28 (18)	H24A—C24—H24B	109.5
C33—C34—N3	119.31 (17)	H24A—C24—H24C	109.5
C34—C29—C28	121.99 (18)	H24B—C24—H24C	109.5
C30—C29—C34	118.32 (19)	C28—C27—H27A	109.5
C30—C29—C28	119.69 (18)	C28—C27—H27B	109.5
N2—C13—H13	121.3	C28—C27—H27C	109.5
N1—C13—N2	117.39 (18)	H27A—C27—H27B	109.5
N1—C13—H13	121.3	H27A—C27—H27C	109.5
C4—C9—N1	116.85 (19)	H27B—C27—H27C	109.5
C8—C9—N1	121.4 (2)	C15—C19—H19	119.5

C8—C9—C4	121.6 (2)	C20—C19—C15	121.1 (3)
C22—C14—N2	119.75 (19)	C20—C19—H19	119.5
C15—C14—N2	118.36 (19)	C3—C1—H1A	109.5
C15—C14—C22	121.6 (2)	C3—C1—H1B	109.5
C9—C4—C3	120.2 (2)	C3—C1—H1C	109.5
C5—C4—C9	118.1 (2)	H1A—C1—H1B	109.5
C5—C4—C3	121.7 (2)	H1A—C1—H1C	109.5
C14—C22—C23	123.06 (19)	H1B—C1—H1C	109.5
C21—C22—C14	117.7 (2)	C40—C44—H44	119.1
C21—C22—C23	119.2 (2)	C45—C44—C40	121.7 (2)
C33—C35—H35	107.7	C45—C44—H44	119.1
C33—C35—C37	112.61 (18)	C8—C7—H7	119.2
C33—C35—C36	112.26 (18)	C6—C7—C8	121.7 (2)
C37—C35—H35	107.7	C6—C7—H7	119.2
C37—C35—C36	108.79 (18)	C5—C6—H6	120.0
C36—C35—H35	107.7	C7—C6—C5	120.1 (2)
C34—C33—C35	121.47 (18)	C7—C6—H6	120.0
C32—C33—C34	117.99 (19)	C28—C26—H26A	109.5
C32—C33—C35	120.51 (18)	C28—C26—H26B	109.5
C29—C30—H30	119.3	C28—C26—H26C	109.5
C31—C30—C29	121.3 (2)	H26A—C26—H26B	109.5
C31—C30—H30	119.3	H26A—C26—H26C	109.5
C47—C39—N4	120.22 (18)	H26B—C26—H26C	109.5
C40—C39—N4	119.27 (18)	C15—C16—H16	108.2
C40—C39—C47	120.49 (19)	C15—C16—C17	109.6 (2)
C30—C31—H31	120.2	C15—C16—C18	112.8 (3)
C30—C31—C32	119.59 (19)	C17—C16—H16	108.2
C32—C31—H31	120.2	C17—C16—C18	109.6 (2)
C33—C32—H32	119.3	C18—C16—H16	108.2
C31—C32—C33	121.5 (2)	C21—C20—H20	119.7
C31—C32—H32	119.3	C19—C20—C21	120.5 (2)

C29—C28—H28	107.6	C19—C20—H20	119.7
C29—C28—C27	112.73 (19)	C10—C11—H11A	109.5
C29—C28—C26	110.99 (19)	C10—C11—H11B	109.5
C27—C28—H28	107.6	C10—C11—H11C	109.5
C26—C28—H28	107.6	H11A—C11—H11B	109.5
C26—C28—C27	110.0 (2)	H11A—C11—H11C	109.5
C9—C8—C10	123.0 (2)	H11B—C11—H11C	109.5
C7—C8—C9	117.7 (2)	C48—C49—H49A	109.5
C7—C8—C10	119.4 (2)	C48—C49—H49B	109.5
C22—C23—H23	108.0	C48—C49—H49C	109.5
C22—C23—C25	113.6 (2)	H49A—C49—H49B	109.5
C22—C23—C24	111.03 (19)	H49A—C49—H49C	109.5
C25—C23—H23	108.0	H49B—C49—H49C	109.5
C25—C23—C24	108.04 (19)	C3—C2—H2A	109.5
C24—C23—H23	108.0	C3—C2—H2B	109.5
C4—C5—H5	119.6	C3—C2—H2C	109.5
C6—C5—C4	120.9 (2)	H2A—C2—H2B	109.5
C6—C5—H5	119.6	H2A—C2—H2C	109.5
C14—C15—C16	121.7 (2)	H2B—C2—H2C	109.5
C19—C15—C14	117.9 (2)	C41—C42—H42A	109.5
C19—C15—C16	120.2 (2)	C41—C42—H42B	109.5
C4—C3—H3	107.4	C41—C42—H42C	109.5
C4—C3—C1	109.67 (19)	H42A—C42—H42B	109.5
C4—C3—C2	113.2 (2)	H42A—C42—H42C	109.5
C1—C3—H3	107.4	H42B—C42—H42C	109.5
C1—C3—C2	111.6 (2)	C41—C43—H43A	109.5
C2—C3—H3	107.4	C41—C43—H43B	109.5
C47—C48—H48	107.5	C41—C43—H43C	109.5
C47—C48—C50	110.5 (2)	H43A—C43—H43B	109.5
C49—C48—H48	107.5	H43A—C43—H43C	109.5
C49—C48—C47	112.4 (2)	H43B—C43—H43C	109.5

C49—C48—C50	111.1 (2)	C16—C17—H17A	109.5
C50—C48—H48	107.5	C16—C17—H17B	109.5
C40—C41—H41	107.9	C16—C17—H17C	109.5
C40—C41—C42	110.1 (2)	H17A—C17—H17B	109.5
C40—C41—C43	111.1 (2)	H17A—C17—H17C	109.5
C42—C41—H41	107.9	H17B—C17—H17C	109.5
C42—C41—C43	111.7 (3)	C48—C50—H50A	109.5
C43—C41—H41	107.9	C48—C50—H50B	109.5
C39—C47—C48	123.12 (19)	C48—C50—H50C	109.5
C46—C47—C39	118.6 (2)	H50A—C50—H50B	109.5
C46—C47—C48	118.27 (19)	H50A—C50—H50C	109.5
C22—C21—H21	119.4	H50B—C50—H50C	109.5
C20—C21—C22	121.2 (3)	C10—C12—H12A	109.5
C20—C21—H21	119.4	C10—C12—H12B	109.5
C39—C40—C41	122.0 (2)	C10—C12—H12C	109.5
C44—C40—C39	118.5 (2)	H12A—C12—H12B	109.5
C44—C40—C41	119.5 (2)	H12A—C12—H12C	109.5
C47—C46—H46	119.3	H12B—C12—H12C	109.5
C45—C46—C47	121.4 (2)	C16—C18—H18A	109.5
C45—C46—H46	119.3	C16—C18—H18B	109.5
C35—C37—H37A	109.5	C16—C18—H18C	109.5
C35—C37—H37B	109.5	H18A—C18—H18B	109.5
C35—C37—H37C	109.5	H18A—C18—H18C	109.5
H37A—C37—H37B	109.5	H18B—C18—H18C	109.5
Sb1—N4—C38—N3	−20.39 (19)	C14—C15—C16—C17	89.9 (3)
Sb1—N4—C39—C47	−68.9 (2)	C14—C15—C16—C18	−147.7 (2)
Sb1—N4—C39—C40	112.9 (2)	C4—C9—C8—C10	−179.0 (2)
Sb1—N2—C13—N1	−0.8 (2)	C4—C9—C8—C7	0.1 (3)
Sb1—N2—C14—C22	−81.6 (3)	C4—C5—C6—C7	0.0 (4)
Sb1—N2—C14—C15	104.2 (2)	C22—C14—C15—C19	−0.3 (3)
Sb1—N3—C38—N4	16.60 (15)	C22—C14—C15—C16	−175.6 (2)

Sb1—N3—C34—C29	39.0 (3)	C22—C21—C20—C19	0.3 (4)
Sb1—N3—C34—C33	−137.2 (2)	C35—C33—C32—C31	177.0 (2)
Sb1—N1—C13—N2	0.66 (17)	C33—C34—C29—C30	−0.5 (3)
Sb1—N1—C9—C4	70.2 (4)	C33—C34—C29—C28	179.06 (19)
Sb1—N1—C9—C8	−106.3 (3)	C30—C29—C28—C27	−47.4 (3)
N4—C39—C47—C48	7.3 (3)	C30—C29—C28—C26	76.5 (3)
N4—C39—C47—C46	−174.95 (19)	C30—C31—C32—C33	0.3 (4)
N4—C39—C40—C41	−3.6 (3)	C39—N4—C38—N3	−162.82 (17)
N4—C39—C40—C44	174.8 (2)	C39—C47—C46—C45	−0.5 (3)
N2—C14—C22—C23	5.0 (3)	C39—C40—C44—C45	0.9 (4)
N2—C14—C22—C21	−172.86 (19)	C28—C29—C30—C31	−179.8 (2)
N2—C14—C15—C19	173.76 (19)	C8—C9—C4—C5	0.9 (3)
N2—C14—C15—C16	−1.5 (3)	C8—C9—C4—C3	178.3 (2)
N3—C34—C29—C30	−176.51 (18)	C8—C7—C6—C5	1.0 (4)
N3—C34—C29—C28	3.0 (3)	C23—C22—C21—C20	−179.1 (2)
N3—C34—C33—C35	−0.9 (3)	C5—C4—C3—C1	86.5 (3)
N3—C34—C33—C32	177.10 (17)	C5—C4—C3—C2	−38.9 (3)
N1—C9—C4—C5	−175.60 (19)	C15—C14—C22—C23	179.0 (2)
N1—C9—C4—C3	1.8 (3)	C15—C14—C22—C21	1.1 (3)
N1—C9—C8—C10	−2.6 (3)	C15—C19—C20—C21	0.6 (4)
N1—C9—C8—C7	176.4 (2)	C3—C4—C5—C6	−178.3 (2)
C38—N4—C39—C47	62.7 (3)	C48—C47—C46—C45	177.3 (2)
C38—N4—C39—C40	−115.4 (2)	C41—C40—C44—C45	179.4 (2)
C38—N3—C34—C29	−101.8 (2)	C47—C39—C40—C41	178.2 (2)
C38—N3—C34—C33	82.1 (2)	C47—C39—C40—C44	−3.3 (3)
C34—N3—C38—N4	179.65 (16)	C47—C46—C45—C44	−1.8 (4)
C34—C29—C30—C31	−0.3 (3)	C21—C22—C23—C25	−37.1 (3)
C34—C29—C28—C27	133.1 (2)	C21—C22—C23—C24	84.9 (3)
C34—C29—C28—C26	−103.0 (2)	C40—C39—C47—C48	−174.6 (2)
C34—C33—C32—C31	−0.9 (3)	C40—C39—C47—C46	3.1 (3)
C29—C34—C33—C35	−176.91 (19)	C46—C45—C44—C40	1.6 (4)

C29—C34—C33—C32	1.0 (3)	C37—C35—C33—C34	−89.5 (2)
C29—C30—C31—C32	0.4 (4)	C37—C35—C33—C32	92.6 (2)
C13—N2—C14—C22	73.7 (2)	C36—C35—C33—C34	147.3 (2)
C13—N2—C14—C15	−100.5 (2)	C36—C35—C33—C32	−30.6 (3)
C13—N1—C9—C4	−114.5 (2)	C10—C8—C7—C6	178.1 (2)
C13—N1—C9—C8	69.0 (3)	C19—C15—C16—C17	−85.3 (3)
C9—N1—C13—N2	−177.18 (18)	C19—C15—C16—C18	37.1 (3)
C9—C4—C5—C6	−1.0 (3)	C7—C8—C10—C11	66.4 (3)
C9—C4—C3—C1	−90.9 (2)	C7—C8—C10—C12	−58.2 (3)
C9—C4—C3—C2	143.8 (2)	C16—C15—C19—C20	174.8 (2)
C9—C8—C10—C11	−114.6 (2)	C49—C48—C47—C39	−125.8 (2)
C9—C8—C10—C12	120.8 (2)	C49—C48—C47—C46	56.5 (3)
C9—C8—C7—C6	−1.0 (3)	C42—C41—C40—C39	107.1 (3)
C14—N2—C13—N1	−164.19 (18)	C42—C41—C40—C44	−71.3 (3)
C14—C22—C23—C25	145.1 (2)	C43—C41—C40—C39	−128.6 (3)
C14—C22—C23—C24	−92.9 (2)	C43—C41—C40—C44	53.0 (3)
C14—C22—C21—C20	−1.1 (4)	C50—C48—C47—C39	109.5 (2)
C14—C15—C19—C20	−0.6 (4)	C50—C48—C47—C46	−68.2 (3)

3.

Crystal data	
$C_{50}H_{70}BrN_4Sb$	$F(000) = 1936$
$M_r = 928.76$	$D_x = 1.244$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$, $\lambda = 0.71073$ Å
$a = 18.7239$ (14) Å	Cell parameters from 8130 reflections
$b = 20.5497$ (17) Å	$\theta = 2.2$–$22.4°$
$c = 12.9785$ (10) Å	$\mu = 1.40$ mm^{-1}
$\beta = 96.886$ (4)°	$T = 123$ K
$V = 4957.7$ (7) Å^3	Block, yellow
$Z = 4$	0.5 × 0.35 × 0.07
Data collection	
Bruker *APEX*-II CCD Diffractometer	5851 observed [$I > 2\sigma(I)$] reflections
Radiation source: fine-focus sealed tube Graphite monochromator	$R_{int} = 0.109$
Scan method: φ and ω scans	$\theta_{max} = 25°$, $\theta_{min} = 1.5°$

Absorption correction: Multi-scan, *SADABS2012*/1 (Bruker,2012). T_{min} = 0.444, T_{max} =0.746	h = −22→22
63607 measured reflections	k = −23→24
8731 independent reflections	l = −15→15
Refinement	
Refinement on F^2	0 restraints
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.040	$w = 1/[\sigma^2(F_o^2) + (0.0409P)^2 + 1.9059P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.102	
S = 1.01	$(\Delta/\sigma)_{max}$ = 0.001
8731 reflections	$\Delta\rho_{max}$ = 0.62 e Å^{-3}
522 parameters	$\Delta\rho_{min}$ = −0.74 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}^*/U_{eq}
Sb1	0.73919(2)	0.56976(2)	0.78439(2)	0.04091(10)
Br1	0.76869(3)	0.69031(2)	0.76428(5)	0.08041(18)
N2	0.80244(15)	0.45545(14)	0.7867(2)	0.0362(7)
N3	0.70405(15)	0.55409(14)	0.6256(2)	0.0395(7)
N1	0.85411(15)	0.55473(14)	0.8053(2)	0.0386(7)
N4	0.61794(16)	0.61100(15)	0.6928(2)	0.0436(8)
C13	0.85842(18)	0.48990(17)	0.8182(3)	0.0370(9)
H13	0.901434	0.470028	0.849573	0.044
C14	0.80496(18)	0.38667(17)	0.7979(3)	0.0368(9)
C15	0.83916(19)	0.34890(18)	0.7281(3)	0.0442(9)
C39	0.5506(2)	0.64398(19)	0.6915(3)	0.0470(10)
C38	0.6380(2)	0.58312(17)	0.6145(3)	0.0426(9)
H38	0.608127	0.582386	0.549958	0.051
C34	0.71985(19)	0.51111(19)	0.5428(3)	0.0437(9)
C9	0.9084(2)	0.59421(18)	0.8656(3)	0.0478(10)
C16	0.8759(2)	0.3792(2)	0.6420(3)	0.0532(11)
H16	0.854863	0.423517	0.627842	0.064
C22	0.7699(2)	0.35719(18)	0.8753(3)	0.0470(10)
C29	0.6879(2)	0.4501(2)	0.5324(3)	0.0532(11)
C4	0.9100(2)	0.5976(2)	0.9738(3)	0.0553(11)
C19	0.8374(2)	0.2816(2)	0.7388(4)	0.0625(12)
H19	0.860829	0.255136	0.693036	0.075
C28	0.6391(2)	0.4225(2)	0.6072(3)	0.0584(11)

H28	0.650928	0.445179	0.675287	0.07
C23	0.7325(2)	0.3968(2)	0.9517(3)	0.0629(12)
H23	0.746581	0.443347	0.944177	0.075
C40	0.4989(2)	0.6148(2)	0.7469(3)	0.0544(11)
C8	0.9584(2)	0.6274(2)	0.8137(4)	0.0602(12)
C33	0.7630(2)	0.5348(2)	0.4705(3)	0.0612(12)
C21	0.7694(2)	0.2899(2)	0.8806(4)	0.0630(12)
H21	0.745202	0.269287	0.932059	0.076
C47	0.5388(2)	0.7043(2)	0.6428(4)	0.0630(12)
C10	0.9569(3)	0.6257(2)	0.6974(4)	0.0723(14)
H10	0.908785	0.608805	0.667528	0.087
C3	0.8553(2)	0.5656(2)	1.0334(3)	0.0671(13)
H3	0.822379	0.539643	0.982685	0.08
C41	0.5139(2)	0.5513(2)	0.8020(3)	0.0642(12)
H41	0.551284	0.528578	0.76634	0.077
C20	0.8026(3)	0.2526(2)	0.8140(4)	0.0725(14)
H20	0.801643	0.206478	0.81951	0.087
C44	0.4357(2)	0.6489(3)	0.7539(4)	0.0760(15)
H44	0.400474	0.631049	0.792675	0.091
C5	0.9656(3)	0.6334(2)	1.0286(4)	0.0740(14)
H5	0.967998	0.636234	1.101992	0.089
C18	0.8644(3)	0.3404(3)	0.5410(3)	0.0806(15)
H18A	0.892833	0.300282	0.548748	0.121
H18B	0.879793	0.366547	0.484467	0.121
H18C	0.813352	0.329546	0.525095	0.121
C7	1.0128(3)	0.6615(3)	0.8740(5)	0.0866(16)
H7	1.048259	0.683473	0.840656	0.104
C26	0.6480(3)	0.3495(2)	0.6265(4)	0.0838(16)
H26A	0.625451	0.325553	0.565794	0.126
H26B	0.624825	0.337326	0.687572	0.126
H26C	0.699259	0.338699	0.638527	0.126
C6	1.0163(3)	0.6641(3)	0.9799(5)	0.0913(17)
H6	1.054088	0.687436	1.019108	0.11
C30	0.6986(3)	0.4130(2)	0.4444(4)	0.0820(16)
H30	0.676566	0.371445	0.434547	0.098
C27	0.5596(3)	0.4360(2)	0.5691(4)	0.0866(16)
H27A	0.551774	0.483074	0.563221	0.13

H27B	0.529398	0.417861	0.618642	0.13
H27C	0.546979	0.415667	0.501025	0.13
C17	0.9564(2)	0.3872(3)	0.6738(4)	0.0896(17)
H17A	0.964397	0.414632	0.735903	0.134
H17B	0.978345	0.407791	0.617122	0.134
H17C	0.978294	0.344426	0.688796	0.134
C43	0.5467(3)	0.5621(3)	0.9144(4)	0.0937(17)
H43A	0.591171	0.587352	0.915361	0.141
H43B	0.557361	0.519996	0.948058	0.141
H43C	0.512473	0.586057	0.9517	0.141
C46	0.4732(3)	0.7350(3)	0.6511(4)	0.0866(16)
H46	0.463372	0.775788	0.617905	0.104
C35	0.7929(3)	0.6030(3)	0.4755(4)	0.0860(16)
H35	0.801057	0.615708	0.550363	0.103
C48	0.5935(3)	0.7378(2)	0.5841(4)	0.0796(15)
H48	0.63794	0.710392	0.591442	0.096
C32	0.7717(3)	0.4951(3)	0.3854(4)	0.0861(16)
H32	0.800626	0.510057	0.334883	0.103
C45	0.4230(3)	0.7080(3)	0.7058(5)	0.0898(18)
H45	0.378974	0.730123	0.710643	0.108
C31	0.7402(4)	0.4361(3)	0.3733(4)	0.100(2)
H31	0.74716	0.410401	0.314507	0.12
C49	0.5661(3)	0.7421(3)	0.4679(4)	0.111(2)
H49A	0.557667	0.69812	0.439716	0.166
H49B	0.602208	0.763988	0.431373	0.166
H49C	0.521095	0.766825	0.458418	0.166
C42	0.4485(3)	0.5058(3)	0.7948(5)	0.1040(19)
H42A	0.411374	0.525043	0.832461	0.156
H42B	0.463095	0.463601	0.82552	0.156
H42C	0.429348	0.499805	0.721794	0.156
C24	0.7552(4)	0.3772(3)	1.0636(4)	0.119(2)
H24A	0.737589	0.40949	1.110141	0.179
H24B	0.807787	0.374996	1.07632	0.179
H24C	0.734824	0.334486	1.07672	0.179
C25	0.6516(3)	0.3928(3)	0.9274(5)	0.113(2)
H25A	0.636553	0.347122	0.926448	0.169
H25B	0.636808	0.412435	0.859338	0.169

H25C	0.628924	0.416326	0.980608	0.169
C11	1.0137(3)	0.5786(3)	0.6672(5)	0.124(2)
H11A	1.061661	0.594514	0.694445	0.186
H11B	1.010138	0.575586	0.591402	0.186
H11C	1.005965	0.535576	0.696299	0.186
C2	0.8896(3)	0.5188(3)	1.1150(4)	0.104(2)
H2A	0.91781	0.486333	1.082145	0.156
H2B	0.851935	0.496937	1.148341	0.156
H2C	0.921216	0.542959	1.167243	0.156
C12	0.9665(3)	0.6932(3)	0.6512(5)	0.121(2)
H12A	0.93071	0.723043	0.673769	0.181
H12B	0.960117	0.690256	0.575243	0.181
H12C	1.014945	0.709406	0.674829	0.181
C1	0.8093(3)	0.6164(3)	1.0816(5)	0.125(2)
H1A	0.839951	0.64203	1.133104	0.187
H1B	0.772017	0.594338	1.115457	0.187
H1C	0.786705	0.645281	1.027137	0.187
C50	0.6140(3)	0.8046(3)	0.6291(5)	0.121(2)
H50A	0.571393	0.832693	0.622668	0.181
H50B	0.650849	0.823961	0.591	0.181
H50C	0.632923	0.800135	0.702451	0.181
C36	0.8653(3)	0.6101(4)	0.4311(5)	0.152(3)
H36A	0.900549	0.580059	0.467229	0.228
H36B	0.882769	0.654854	0.441118	0.228
H36C	0.858699	0.599791	0.356862	0.228
C37	0.7376(4)	0.6508(3)	0.4207(6)	0.139(3)
H37A	0.73057	0.641323	0.346135	0.208
H37B	0.755389	0.695438	0.431663	0.208
H37C	0.691779	0.646163	0.449239	0.208

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sb1	0.04499(16)	0.04314(17)	0.03471(15)	-0.00164(12)	0.00522(11)	0.00390(12)
Br1	0.0799(3)	0.0379(3)	0.1157(4)	-0.0061(3)	-0.0201(3)	0.0033(2)
N2	0.0412(17)	0.0336(17)	0.0344(17)	-0.0002(13)	0.0064(14)	0.0012(14)
N3	0.0414(17)	0.0382(18)	0.0389(18)	0.0046(14)	0.0044(14)	0.0058(14)

N1	0.0428(17)	0.0326(18)	0.0395(18)	0.0013(14)	0.0014(14)	-0.0029(14)
N4	0.0427(18)	0.0435(19)	0.044(2)	0.0047(16)	0.0034(16)	0.0069(15)
C13	0.037(2)	0.041(2)	0.034(2)	0.0014(17)	0.0057(17)	0.0045(18)
C14	0.033(2)	0.032(2)	0.044(2)	-0.0012(17)	-0.0008(17)	0.0010(16)
C15	0.039(2)	0.039(2)	0.053(3)	-0.0001(19)	0.0007(19)	0.0048(18)
C39	0.042(2)	0.045(2)	0.052(3)	-0.010(2)	-0.004(2)	0.0088(19)
C38	0.048(2)	0.038(2)	0.041(2)	0.0031(18)	-0.0001(19)	0.0009(18)
C34	0.045(2)	0.048(3)	0.037(2)	-0.0017(19)	0.0010(18)	0.0100(19)
C9	0.048(2)	0.037(2)	0.057(3)	-0.001(2)	-0.001(2)	-0.0013(19)
C16	0.061(3)	0.052(3)	0.050(3)	-0.009(2)	0.018(2)	0.005(2)
C22	0.049(2)	0.039(2)	0.053(3)	0.0039(19)	0.007(2)	-0.0045(19)
C29	0.063(3)	0.054(3)	0.038(2)	-0.006(2)	-0.012(2)	0.013(2)
C4	0.056(3)	0.053(3)	0.054(3)	-0.005(2)	-0.003(2)	-0.001(2)
C19	0.063(3)	0.046(3)	0.079(3)	-0.008(2)	0.009(3)	0.013(2)
C28	0.065(3)	0.048(3)	0.058(3)	-0.005(2)	-0.010(2)	-0.002(2)
C23	0.076(3)	0.056(3)	0.062(3)	0.007(2)	0.030(3)	-0.009(2)
C40	0.049(3)	0.060(3)	0.053(3)	-0.015(2)	0.004(2)	0.008(2)
C8	0.057(3)	0.050(3)	0.071(3)	0.008(2)	-0.001(2)	-0.014(2)
C33	0.064(3)	0.076(3)	0.043(3)	0.000(2)	0.007(2)	0.010(3)
C21	0.069(3)	0.051(3)	0.070(3)	0.013(2)	0.012(2)	-0.009(2)
C47	0.056(3)	0.048(3)	0.080(3)	-0.008(2)	-0.014(2)	0.013(2)
C10	0.068(3)	0.080(4)	0.070(3)	0.023(3)	0.008(3)	-0.022(3)
C3	0.072(3)	0.087(4)	0.042(2)	-0.003(3)	0.005(2)	-0.006(3)
C41	0.064(3)	0.069(3)	0.065(3)	-0.005(2)	0.026(2)	-0.004(2)
C20	0.080(3)	0.042(3)	0.095(4)	0.006(3)	0.009(3)	0.002(3)
C44	0.055(3)	0.084(4)	0.090(4)	-0.029(3)	0.014(3)	0.009(3)
C5	0.084(4)	0.070(3)	0.064(3)	-0.010(3)	-0.010(3)	-0.014(3)
C18	0.088(4)	0.095(4)	0.059(3)	-0.020(3)	0.012(3)	0.007(3)
C7	0.083(4)	0.081(4)	0.093(4)	0.011(3)	-0.002(3)	-0.039(3)
C26	0.081(3)	0.056(3)	0.106(4)	0.011(3)	-0.023(3)	-0.006(3)
C6	0.090(4)	0.075(4)	0.101(5)	-0.006(3)	-0.021(4)	-0.032(3)
C30	0.118(4)	0.065(3)	0.058(3)	-0.018(3)	-0.010(3)	0.009(3)
C27	0.070(3)	0.074(4)	0.111(4)	0.000(3)	-0.008(3)	-0.006(3)
C17	0.059(3)	0.136(5)	0.077(4)	-0.019(3)	0.021(3)	-0.017(3)
C43	0.110(4)	0.102(4)	0.072(4)	0.006(3)	0.022(3)	0.006(3)
C46	0.081(4)	0.056(3)	0.115(5)	-0.007(3)	-0.020(3)	0.022(3)
C35	0.090(4)	0.114(5)	0.059(3)	0.001(3)	0.032(3)	-0.023(4)

C48	0.079(3)	0.056(3)	0.098(4)	0.025(3)	-0.015(3)	0.000(3)
C32	0.102(4)	0.116(5)	0.044(3)	-0.001(3)	0.024(3)	0.024(4)
C45	0.065(3)	0.085(4)	0.116(5)	-0.037(4)	-0.005(3)	0.028(3)
C31	0.145(6)	0.101(5)	0.054(3)	-0.021(3)	0.012(4)	0.033(4)
C49	0.122(5)	0.106(5)	0.099(5)	0.031(4)	-0.011(4)	0.003(4)
C42	0.102(4)	0.089(4)	0.125(5)	-0.001(4)	0.031(4)	-0.023(4)
C24	0.138(6)	0.162(7)	0.058(4)	-0.008(4)	0.012(4)	0.018(5)
C25	0.077(4)	0.157(6)	0.109(5)	-0.024(4)	0.028(4)	0.025(4)
C11	0.132(6)	0.162(7)	0.086(4)	0.025(4)	0.045(4)	0.028(5)
C2	0.109(4)	0.126(5)	0.073(4)	0.030(4)	-0.006(3)	-0.024(4)
C12	0.135(5)	0.106(5)	0.114(5)	0.053(4)	-0.012(4)	-0.046(4)
C1	0.126(5)	0.156(7)	0.100(5)	-0.018(4)	0.043(4)	0.025(5)
C50	0.130(5)	0.062(4)	0.161(6)	0.017(4)	-0.021(5)	-0.024(4)
C36	0.120(5)	0.252(9)	0.096(5)	-0.026(5)	0.059(4)	-0.079(6)
C37	0.179(7)	0.093(5)	0.149(6)	0.054(5)	0.040(6)	-0.009(5)

Geometric parameters (Å, º)

Sb1—Br1	2.5581 (6)	C18—H18A	0.9800
Sb1—N2	2.629 (3)	C18—H18B	0.9800
Sb1—N3	2.111 (3)	C18—H18C	0.9800
Sb1—N1	2.158 (3)	C7—H7	0.9500
Sb1—N4	2.576 (3)	C7—C6	1.369 (7)
N2—C13	1.290 (4)	C26—H26A	0.9800
N2—C14	1.421 (4)	C26—H26B	0.9800
N3—C38	1.365 (4)	C26—H26C	0.9800
N3—C34	1.449 (4)	C6—H6	0.9500
N1—C13	1.344 (4)	C30—H30	0.9500
N1—C9	1.453 (5)	C30—C31	1.364 (8)
N4—C39	1.429 (4)	C27—H27A	0.9800
N4—C38	1.263 (4)	C27—H27B	0.9800
C13—H13	0.9500	C27—H27C	0.9800
C14—C15	1.405 (5)	C17—H17A	0.9800
C14—C22	1.402 (5)	C17—H17B	0.9800

C15—C16	1.515 (5)	C17—H17C	0.9800
C15—C19	1.391 (5)	C43—H43A	0.9800
C39—C40	1.407 (5)	C43—H43B	0.9800
C39—C47	1.397 (6)	C43—H43C	0.9800
C38—H38	0.9500	C46—H46	0.9500
C34—C29	1.388 (5)	C46—C45	1.362 (7)
C34—C33	1.397 (5)	C35—H35	1.0000
C9—C4	1.402 (5)	C35—C36	1.543 (7)
C9—C8	1.396 (5)	C35—C37	1.538 (8)
C16—H16	1.0000	C48—H48	1.0000
C16—C18	1.527 (6)	C48—C49	1.536 (7)
C16—C17	1.524 (6)	C48—C50	1.523 (7)
C22—C23	1.518 (5)	C32—H32	0.9500
C22—C21	1.385 (5)	C32—C31	1.349 (8)
C29—C28	1.520 (6)	C45—H45	0.9500
C29—C30	1.407 (6)	C31—H31	0.9500
C4—C3	1.507 (6)	C49—H49A	0.9800
C4—C5	1.397 (6)	C49—H49B	0.9800
C19—H19	0.9500	C49—H49C	0.9800
C19—C20	1.374 (6)	C42—H42A	0.9800
C28—H28	1.0000	C42—H42B	0.9800
C28—C26	1.528 (6)	C42—H42C	0.9800
C28—C27	1.536 (6)	C24—H24A	0.9800
C23—H23	1.0000	C24—H24B	0.9800
C23—C24	1.518 (7)	C24—H24C	0.9800
C23—C25	1.512 (7)	C25—H25A	0.9800
C40—C41	1.499 (6)	C25—H25B	0.9800
C40—C44	1.389 (6)	C25—H25C	0.9800
C8—C10	1.506 (6)	C11—H11A	0.9800
C8—C7	1.395 (6)	C11—H11B	0.9800
C33—C35	1.507 (7)	C11—H11C	0.9800

C33—C32	1.398 (6)	C2—H2A	0.9800
C21—H21	0.9500	C2—H2B	0.9800
C21—C20	1.361 (6)	C2—H2C	0.9800
C47—C46	1.397 (6)	C12—H12A	0.9800
C47—C48	1.513 (6)	C12—H12B	0.9800
C10—H10	1.0000	C12—H12C	0.9800
C10—C11	1.523 (7)	C1—H1A	0.9800
C10—C12	1.530 (6)	C1—H1B	0.9800
C3—H3	1.0000	C1—H1C	0.9800
C3—C2	1.514 (6)	C50—H50A	0.9800
C3—C1	1.534 (7)	C50—H50B	0.9800
C41—H41	1.0000	C50—H50C	0.9800
C41—C43	1.529 (6)	C36—H36A	0.9800
C41—C42	1.533 (6)	C36—H36B	0.9800
C20—H20	0.9500	C36—H36C	0.9800
C44—H44	0.9500	C37—H37A	0.9800
C44—C45	1.372 (7)	C37—H37B	0.9800
C5—H5	0.9500	C37—H37C	0.9800
C5—C6	1.359 (7)		
Br1—Sb1—N2	139.81 (6)	C6—C7—C8	121.9 (5)
Br1—Sb1—N4	79.84 (7)	C6—C7—H7	119.1
N3—Sb1—Br1	95.39 (8)	C28—C26—H26A	109.5
N3—Sb1—N2	87.84 (10)	C28—C26—H26B	109.5
N3—Sb1—N1	106.86 (11)	C28—C26—H26C	109.5
N3—Sb1—N4	56.34 (10)	H26A—C26—H26B	109.5
N1—Sb1—Br1	85.82 (8)	H26A—C26—H26C	109.5
N1—Sb1—N2	55.24 (10)	H26B—C26—H26C	109.5
N1—Sb1—N4	156.22 (10)	C5—C6—C7	119.7 (5)
N4—Sb1—N2	132.07 (9)	C5—C6—H6	120.1
C13—N2—Sb1	82.0 (2)	C7—C6—H6	120.1
C13—N2—C14	119.9 (3)	C29—C30—H30	119.7

C14—N2—Sb1	154.1 (2)	C31—C30—C29	120.6 (5)
C38—N3—Sb1	102.1 (2)	C31—C30—H30	119.7
C38—N3—C34	116.8 (3)	C28—C27—H27A	109.5
C34—N3—Sb1	138.6 (2)	C28—C27—H27B	109.5
C13—N1—Sb1	101.6 (2)	C28—C27—H27C	109.5
C13—N1—C9	117.3 (3)	H27A—C27—H27B	109.5
C9—N1—Sb1	127.6 (2)	H27A—C27—H27C	109.5
C39—N4—Sb1	152.7 (2)	H27B—C27—H27C	109.5
C38—N4—Sb1	83.8 (2)	C16—C17—H17A	109.5
C38—N4—C39	123.5 (3)	C16—C17—H17B	109.5
N2—C13—N1	118.0 (3)	C16—C17—H17C	109.5
N2—C13—H13	121.0	H17A—C17—H17B	109.5
N1—C13—H13	121.0	H17A—C17—H17C	109.5
C15—C14—N2	119.7 (3)	H17B—C17—H17C	109.5
C22—C14—N2	119.4 (3)	C41—C43—H43A	109.5
C22—C14—C15	120.8 (3)	C41—C43—H43B	109.5
C14—C15—C16	122.1 (3)	C41—C43—H43C	109.5
C19—C15—C14	117.9 (4)	H43A—C43—H43B	109.5
C19—C15—C16	120.0 (4)	H43A—C43—H43C	109.5
C40—C39—N4	116.8 (3)	H43B—C43—H43C	109.5
C47—C39—N4	121.2 (4)	C47—C46—H46	119.2
C47—C39—C40	121.9 (4)	C45—C46—C47	121.6 (5)
N3—C38—H38	121.1	C45—C46—H46	119.2
N4—C38—N3	117.8 (3)	C33—C35—H35	107.4
N4—C38—H38	121.1	C33—C35—C36	114.2 (5)
C29—C34—N3	119.9 (3)	C33—C35—C37	110.4 (5)
C29—C34—C33	121.8 (4)	C36—C35—H35	107.4
C33—C34—N3	118.1 (4)	C37—C35—H35	107.4
C4—C9—N1	119.8 (3)	C37—C35—C36	109.8 (5)
C8—C9—N1	118.6 (4)	C47—C48—H48	107.6
C8—C9—C4	121.6 (4)	C47—C48—C49	110.8 (4)

C15—C16—H16	107.8	C47—C48—C50	111.8 (5)
C15—C16—C18	112.9 (4)	C49—C48—H48	107.6
C15—C16—C17	111.5 (4)	C50—C48—H48	107.6
C18—C16—H16	107.8	C50—C48—C49	111.3 (4)
C17—C16—H16	107.8	C33—C32—H32	119.2
C17—C16—C18	108.8 (3)	C31—C32—C33	121.7 (5)
C14—C22—C23	121.9 (3)	C31—C32—H32	119.2
C21—C22—C14	118.3 (4)	C44—C45—H45	119.8
C21—C22—C23	119.8 (4)	C46—C45—C44	120.3 (5)
C34—C29—C28	124.1 (4)	C46—C45—H45	119.8
C34—C29—C30	117.8 (4)	C30—C31—H31	119.6
C30—C29—C28	118.0 (4)	C32—C31—C30	120.8 (5)
C9—C4—C3	123.9 (4)	C32—C31—H31	119.6
C5—C4—C9	117.5 (4)	C48—C49—H49A	109.5
C5—C4—C3	118.6 (4)	C48—C49—H49B	109.5
C15—C19—H19	119.3	C48—C49—H49C	109.5
C20—C19—C15	121.4 (4)	H49A—C49—H49B	109.5
C20—C19—H19	119.3	H49A—C49—H49C	109.5
C29—C28—H28	107.7	H49B—C49—H49C	109.5
C29—C28—C26	114.2 (4)	C41—C42—H42A	109.5
C29—C28—C27	111.1 (4)	C41—C42—H42B	109.5
C26—C28—H28	107.7	C41—C42—H42C	109.5
C26—C28—C27	108.2 (4)	H42A—C42—H42B	109.5
C27—C28—H28	107.7	H42A—C42—H42C	109.5
C22—C23—H23	107.5	H42B—C42—H42C	109.5
C24—C23—C22	112.6 (4)	C23—C24—H24A	109.5
C24—C23—H23	107.5	C23—C24—H24B	109.5
C25—C23—C22	111.3 (4)	C23—C24—H24C	109.5
C25—C23—H23	107.5	H24A—C24—H24B	109.5
C25—C23—C24	110.1 (4)	H24A—C24—H24C	109.5
C39—C40—C41	121.0 (4)	H24B—C24—H24C	109.5

C44—C40—C39	117.5 (4)	C23—C25—H25A	109.5
C44—C40—C41	121.4 (4)	C23—C25—H25B	109.5
C9—C8—C10	122.6 (4)	C23—C25—H25C	109.5
C7—C8—C9	117.4 (4)	H25A—C25—H25B	109.5
C7—C8—C10	119.9 (4)	H25A—C25—H25C	109.5
C34—C33—C35	122.5 (4)	H25B—C25—H25C	109.5
C32—C33—C34	117.3 (5)	C10—C11—H11A	109.5
C32—C33—C35	119.9 (4)	C10—C11—H11B	109.5
C22—C21—H21	119.2	C10—C11—H11C	109.5
C20—C21—C22	121.7 (4)	H11A—C11—H11B	109.5
C20—C21—H21	119.2	H11A—C11—H11C	109.5
C39—C47—C46	117.3 (5)	H11B—C11—H11C	109.5
C39—C47—C48	123.5 (4)	C3—C2—H2A	109.5
C46—C47—C48	119.2 (5)	C3—C2—H2B	109.5
C8—C10—H10	107.7	C3—C2—H2C	109.5
C8—C10—C11	110.1 (4)	H2A—C2—H2B	109.5
C8—C10—C12	112.5 (5)	H2A—C2—H2C	109.5
C11—C10—H10	107.7	H2B—C2—H2C	109.5
C11—C10—C12	110.8 (5)	C10—C12—H12A	109.5
C12—C10—H10	107.7	C10—C12—H12B	109.5
C4—C3—H3	107.4	C10—C12—H12C	109.5
C4—C3—C2	112.3 (4)	H12A—C12—H12B	109.5
C4—C3—C1	111.2 (4)	H12A—C12—H12C	109.5
C2—C3—H3	107.4	H12B—C12—H12C	109.5
C2—C3—C1	111.0 (4)	C3—C1—H1A	109.5
C1—C3—H3	107.4	C3—C1—H1B	109.5
C40—C41—H41	106.6	C3—C1—H1C	109.5
C40—C41—C43	111.0 (4)	H1A—C1—H1B	109.5
C40—C41—C42	113.5 (4)	H1A—C1—H1C	109.5
C43—C41—H41	106.6	H1B—C1—H1C	109.5
C43—C41—C42	111.9 (4)	C48—C50—H50A	109.5

C42—C41—H41	106.6	C48—C50—H50B	109.5
C19—C20—H20	120.0	C48—C50—H50C	109.5
C21—C20—C19	119.9 (4)	H50A—C50—H50B	109.5
C21—C20—H20	120.0	H50A—C50—H50C	109.5
C40—C44—H44	119.3	H50B—C50—H50C	109.5
C45—C44—C40	121.3 (5)	C35—C36—H36A	109.5
C45—C44—H44	119.3	C35—C36—H36B	109.5
C4—C5—H5	119.1	C35—C36—H36C	109.5
C6—C5—C4	121.8 (5)	H36A—C36—H36B	109.5
C6—C5—H5	119.1	H36A—C36—H36C	109.5
C16—C18—H18A	109.5	H36B—C36—H36C	109.5
C16—C18—H18B	109.5	C35—C37—H37A	109.5
C16—C18—H18C	109.5	C35—C37—H37B	109.5
H18A—C18—H18B	109.5	C35—C37—H37C	109.5
H18A—C18—H18C	109.5	H37A—C37—H37B	109.5
H18B—C18—H18C	109.5	H37A—C37—H37C	109.5
C8—C7—H7	119.1	H37B—C37—H37C	109.5
Sb1—N2—C13—N1	−15.5 (3)	C34—C29—C30—C31	1.2 (7)
Sb1—N2—C14—C15	137.4 (4)	C34—C33—C35—C36	150.3 (5)
Sb1—N2—C14—C22	−39.2 (7)	C34—C33—C35—C37	−85.3 (6)
Sb1—N3—C38—N4	2.2 (4)	C34—C33—C32—C31	−0.3 (8)
Sb1—N3—C34—C29	83.9 (4)	C9—N1—C13—N2	163.0 (3)
Sb1—N3—C34—C33	−101.0 (4)	C9—C4—C3—C2	122.6 (5)
Sb1—N1—C13—N2	19.3 (3)	C9—C4—C3—C1	−112.4 (5)
Sb1—N1—C9—C4	65.8 (4)	C9—C4—C5—C6	0.2 (7)
Sb1—N1—C9—C8	−115.0 (4)	C9—C8—C10—C11	−101.6 (5)
Sb1—N4—C39—C40	−67.8 (6)	C9—C8—C10—C12	134.2 (5)
Sb1—N4—C39—C47	108.3 (6)	C9—C8—C7—C6	−1.7 (8)
Sb1—N4—C38—N3	−1.8 (3)	C16—C15—C19—C20	−177.9 (4)
N2—C14—C15—C16	1.9 (5)	C22—C14—C15—C16	178.5 (3)
N2—C14—C15—C19	−177.0 (3)	C22—C14—C15—C19	−0.4 (5)

N2—C14—C22—C23	−3.3 (5)	C22—C21—C20—C19	−0.4 (7)
N2—C14—C22—C21	176.1 (3)	C29—C34—C33—C35	174.6 (4)
N3—C34—C29—C28	−3.6 (6)	C29—C34—C33—C32	1.2 (6)
N3—C34—C29—C30	173.2 (4)	C29—C30—C31—C32	−0.3 (9)
N3—C34—C33—C35	−0.4 (6)	C4—C9—C8—C10	−178.7 (4)
N3—C34—C33—C32	−173.8 (4)	C4—C9—C8—C7	3.2 (6)
N1—C9—C4—C3	−4.0 (6)	C4—C5—C6—C7	1.3 (8)
N1—C9—C4—C5	176.6 (4)	C19—C15—C16—C18	37.7 (5)
N1—C9—C8—C10	2.1 (6)	C19—C15—C16—C17	−85.1 (5)
N1—C9—C8—C7	−175.9 (4)	C28—C29—C30—C31	178.2 (5)
N4—C39—C40—C41	−1.5 (5)	C23—C22—C21—C20	−179.6 (4)
N4—C39—C40—C44	174.6 (4)	C40—C39—C47—C46	0.1 (6)
N4—C39—C47—C46	−175.8 (4)	C40—C39—C47—C48	179.0 (4)
N4—C39—C47—C48	3.0 (6)	C40—C44—C45—C46	−1.1 (8)
C13—N2—C14—C15	−78.1 (4)	C8—C9—C4—C3	176.9 (4)
C13—N2—C14—C22	105.3 (4)	C8—C9—C4—C5	−2.5 (6)
C13—N1—C9—C4	−67.3 (5)	C8—C7—C6—C5	−0.5 (9)
C13—N1—C9—C8	111.9 (4)	C33—C34—C29—C28	−178.5 (4)
C14—N2—C13—N1	179.3 (3)	C33—C34—C29—C30	−1.7 (6)
C14—C15—C16—C18	−141.1 (4)	C33—C32—C31—C30	−0.2 (9)
C14—C15—C16—C17	96.1 (4)	C21—C22—C23—C24	51.3 (6)
C14—C15—C19—C20	1.0 (6)	C21—C22—C23—C25	−72.9 (6)
C14—C22—C23—C24	−129.2 (5)	C47—C39—C40—C41	−177.6 (4)
C14—C22—C23—C25	106.5 (5)	C47—C39—C40—C44	−1.5 (6)
C14—C22—C21—C20	0.9 (6)	C47—C46—C45—C44	−0.5 (8)
C15—C14—C22—C23	−180.0 (4)	C10—C8—C7—C6	−179.8 (5)
C15—C14—C22—C21	−0.5 (6)	C3—C4—C5—C6	−179.2 (5)
C15—C19—C20—C21	−0.6 (7)	C41—C40—C44—C45	178.1 (4)
C39—N4—C38—N3	179.1 (3)	C44—C40—C41—C43	−84.6 (5)
C39—C40—C41—C43	91.3 (5)	C44—C40—C41—C42	42.5 (6)
C39—C40—C41—C42	−141.6 (4)	C5—C4—C3—C2	−58.0 (6)

C39—C40—C44—C45	2.0 (7)	C5—C4—C3—C1	67.0 (6)
C39—C47—C46—C45	1.0 (7)	C7—C8—C10—C11	76.3 (6)
C39—C47—C48—C49	113.9 (5)	C7—C8—C10—C12	−47.8 (6)
C39—C47—C48—C50	−121.3 (5)	C30—C29—C28—C26	40.1 (5)
C38—N3—C34—C29	−73.9 (4)	C30—C29—C28—C27	−82.6 (5)
C38—N3—C34—C33	101.2 (4)	C46—C47—C48—C49	−67.3 (6)
C38—N4—C39—C40	110.3 (4)	C46—C47—C48—C50	57.5 (6)
C38—N4—C39—C47	−73.6 (5)	C35—C33—C32—C31	−173.8 (5)
C34—N3—C38—N4	167.4 (3)	C48—C47—C46—C45	−178.0 (5)
C34—C29—C28—C26	−143.1 (4)	C32—C33—C35—C36	−36.5 (7)
C34—C29—C28—C27	94.2 (5)	C32—C33—C35—C37	87.9 (6)

4.

Crystal data	
$C_{50}H_{70}IN_4Sb$	$F(000) = 2008$
$M_r = 975.75$	$D_x = 1.303$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$, $\lambda = 0.71073$ Å
$a = 18.616$ (2) Å	Cell parameters from 8087 reflections
$b = 20.713$ (2) Å	$\theta = 2.2$–$20.3°$
$c = 12.9942$ (13) Å	$\mu = 1.21$mm^{-1}
$\beta = 96.750$ (5)°	$T = 123$ K
$V = 4975.8$ (9) Å^3	Block, yellow
$Z = 4$	0.45 × 0.3 × 0.08
Data collection	
Bruker *APEX*-II CCD Diffractometer	5504 observed [$I > 2\sigma(I)$] reflections
Radiation source: fine-focus sealed tube Graphite monochromator	$R_{int} = 0.089$
Scan method: φ and ω scans	$\theta_{max} = 25°$, $\theta_{min} = 1.5°$
Absorption correction: Multi-scan, *SADABS2012*/1 (Bruker,2012). $T_{min} = 0.437$, $T_{max} = 0.746$	$h = -22 \rightarrow 22$
63063 measured reflections	$k = -24 \rightarrow 24$
8728 independent reflections	$l = -15 \rightarrow 14$
Refinement	
Refinement on F^2	0 restraints
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.045$	$w = 1/[\sigma^2(F_o^2) + (0.0537P)^2 + 1.427P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.118$	
$S = 1.01$	$(\Delta/\sigma)_{max} = 0.002$
8728 reflections	$\Delta\rho_{max} = 0.85$ e Å^{-3}
521 parameters	$\Delta\rho_{min} = -1.17$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}^{*}/U_{eq}
Sb1	0.74069(2)	0.56947(2)	0.78243(2)	0.04235(12)
I1	0.77416(2)	0.69870(2)	0.75958(4)	0.07893(17)
N2	0.8024(2)	0.45491(17)	0.7883(3)	0.0377(9)
N3	0.7031(2)	0.55199(16)	0.6251(3)	0.0400(9)
N4	0.6181(2)	0.61129(18)	0.6909(3)	0.0439(10)
N1	0.8561(2)	0.55241(16)	0.8008(3)	0.0407(9)
C14	0.8040(2)	0.3863(2)	0.8012(4)	0.0389(11)
C13	0.8594(3)	0.4881(2)	0.8165(3)	0.0413(11)
H13	0.902582	0.468047	0.847403	0.05
C38	0.6380(3)	0.5816(2)	0.6137(4)	0.0435(12)
H38	0.607909	0.580309	0.549442	0.052
C15	0.8385(2)	0.3479(2)	0.7321(4)	0.0456(12)
C39	0.5511(3)	0.6435(2)	0.6899(4)	0.0495(13)
C22	0.7685(3)	0.3584(2)	0.8789(4)	0.0509(13)
C34	0.7190(3)	0.5085(2)	0.5433(4)	0.0446(12)
C40	0.4994(3)	0.6150(2)	0.7470(4)	0.0561(14)
C9	0.9115(3)	0.5914(2)	0.8592(4)	0.0460(12)
C16	0.8764(3)	0.3763(2)	0.6459(4)	0.0578(15)
H16	0.857397	0.421021	0.632533	0.069
C29	0.6863(3)	0.4475(2)	0.5347(4)	0.0524(14)
C4	0.9125(3)	0.5975(2)	0.9674(4)	0.0546(14)
C27	0.6376(3)	0.4220(2)	0.6105(4)	0.0578(14)
H27	0.650271	0.445	0.677894	0.069
C33	0.7617(3)	0.5307(3)	0.4687(4)	0.0600(15)
C41	0.5149(3)	0.5517(3)	0.8024(4)	0.0638(15)
H41	0.552983	0.529327	0.767503	0.077
C21	0.7672(3)	0.2918(3)	0.8846(5)	0.0660(16)
H21	0.741947	0.272045	0.935757	0.079
C23	0.7308(3)	0.3988(3)	0.9538(4)	0.0659(16)
H23	0.744663	0.444878	0.943849	0.079
C47	0.5380(3)	0.7027(2)	0.6399(5)	0.0628(16)
C8	0.9620(3)	0.6228(2)	0.8064(5)	0.0593(15)
C3	0.8578(3)	0.5670(3)	1.0286(4)	0.0669(16)

H3	0.823614	0.541784	0.978907	0.08
C19	0.8363(3)	0.2809(2)	0.7450(5)	0.0660(16)
H19	0.85998	0.253709	0.700786	0.079
C17	0.9568(3)	0.3812(3)	0.6770(5)	0.090(2)
H17A	0.966117	0.407459	0.739817	0.134
H17B	0.979641	0.40138	0.620836	0.134
H17C	0.976967	0.337869	0.690415	0.134
C10	0.9605(3)	0.6190(3)	0.6903(5)	0.0720(17)
H10	0.910921	0.604669	0.661359	0.086
C44	0.4356(3)	0.6480(3)	0.7543(5)	0.0804(19)
H44	0.400525	0.630183	0.793626	0.096
C5	0.9681(4)	0.6334(3)	1.0205(5)	0.0768(18)
H5	0.970324	0.637522	1.093585	0.092
C20	0.8002(3)	0.2539(3)	0.8208(5)	0.0729(18)
H20	0.798695	0.208256	0.828072	0.087
C18	0.8626(3)	0.3386(3)	0.5443(5)	0.0846(19)
H18A	0.888357	0.297282	0.551407	0.127
H18B	0.880027	0.363733	0.488301	0.127
H18C	0.810623	0.330653	0.527967	0.127
C26	0.6454(3)	0.3496(2)	0.6312(5)	0.083(2)
H26A	0.625401	0.325666	0.569383	0.125
H26B	0.61919	0.337899	0.68962	0.125
H26C	0.696731	0.338822	0.647948	0.125
C28	0.5583(3)	0.4359(3)	0.5735(5)	0.0846(19)
H28A	0.550141	0.482694	0.572444	0.127
H28B	0.52767	0.415619	0.620753	0.127
H28C	0.546022	0.418457	0.50357	0.127
C42	0.5464(4)	0.5636(3)	0.9138(5)	0.096(2)
H42A	0.510239	0.584903	0.951099	0.144
H42B	0.589212	0.591301	0.915003	0.144
H42C	0.560249	0.522312	0.947224	0.144
C7	1.0168(3)	0.6580(3)	0.8644(6)	0.086(2)
H7	1.052703	0.678921	0.830145	0.103
C32	0.7712(4)	0.4913(4)	0.3853(5)	0.0831(19)
H32	0.80086	0.505394	0.335009	0.1
C45	0.4223(4)	0.7064(4)	0.7053(6)	0.094(2)
H45	0.377866	0.728112	0.710328	0.113

C30	0.6968(4)	0.4106(3)	0.4468(5)	0.0802(19)
H30	0.674273	0.369577	0.437076	0.096
C46	0.4722(4)	0.7335(3)	0.6495(6)	0.092(2)
H46	0.46217	0.773988	0.616554	0.11
C31	0.7390(5)	0.4332(4)	0.3748(5)	0.098(2)
H31	0.745527	0.407237	0.316333	0.118
C12	0.9744(4)	0.6845(3)	0.6410(5)	0.102(2)
H12A	0.941418	0.716854	0.664063	0.152
H12B	0.966242	0.680668	0.565319	0.152
H12C	1.024537	0.697767	0.662004	0.152
C48	0.5907(3)	0.7360(3)	0.5786(5)	0.0811(19)
H48	0.635903	0.709403	0.586231	0.097
C6	1.0193(4)	0.6627(3)	0.9706(6)	0.096(2)
H6	1.0569	0.686613	1.009036	0.115
C35	0.7907(4)	0.5985(3)	0.4726(5)	0.083(2)
H35	0.799446	0.612035	0.546941	0.099
C43	0.4499(4)	0.5069(3)	0.7955(6)	0.105(2)
H43A	0.463699	0.466282	0.831238	0.157
H43B	0.433029	0.498004	0.722599	0.157
H43C	0.410939	0.52742	0.828339	0.157
C25	0.7539(4)	0.3820(4)	1.0660(5)	0.124(3)
H25A	0.735201	0.414523	1.110789	0.185
H25B	0.806802	0.381036	1.078786	0.185
H25C	0.734547	0.339495	1.081295	0.185
C2	0.8920(4)	0.5199(3)	1.1107(5)	0.097(2)
H2A	0.926068	0.543201	1.160765	0.146
H2B	0.917868	0.486093	1.077256	0.146
H2C	0.854084	0.500306	1.146636	0.146
C11	1.0141(4)	0.5686(3)	0.6596(6)	0.114(3)
H11A	1.063526	0.582566	0.683331	0.172
H11B	1.008325	0.563789	0.584013	0.172
H11C	1.004641	0.527102	0.691653	0.172
C50	0.6117(4)	0.8036(3)	0.6221(6)	0.123(3)
H50A	0.648496	0.822382	0.582973	0.185
H50B	0.631122	0.799914	0.69526	0.185
H50C	0.568824	0.831391	0.615527	0.185
C37	0.7349(5)	0.6445(3)	0.4165(7)	0.134(3)

H37A	0.732139	0.637435	0.341554	0.202
H37B	0.749342	0.68926	0.432452	0.202
H37C	0.687407	0.636401	0.439449	0.202
C49	0.5635(4)	0.7382(3)	0.4618(5)	0.108(2)
H49A	0.517794	0.762159	0.451227	0.162
H49B	0.55577	0.694135	0.435462	0.162
H49C	0.599544	0.759809	0.424666	0.162
C24	0.6496(4)	0.3946(4)	0.9311(6)	0.115(3)
H24A	0.634048	0.350106	0.941436	0.172
H24B	0.634821	0.407531	0.859181	0.172
H24C	0.627163	0.423412	0.977926	0.172
C1	0.8133(4)	0.6183(4)	1.0781(6)	0.116(3)
H1A	0.773976	0.597321	1.109414	0.175
H1B	0.792898	0.648821	1.024829	0.175
H1C	0.844534	0.641603	1.131699	0.175
C36	0.8618(4)	0.6058(4)	0.4250(6)	0.143(3)
H36A	0.896943	0.574144	0.456334	0.215
H36B	0.880937	0.649454	0.43821	0.215
H36C	0.852962	0.598363	0.350125	0.215

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sb1	0.0473(2)	0.0430(2)	0.0366(2)	-0.00226(15)	0.00460(15)	0.00321(15)
I1	0.0801(3)	0.0376(2)	0.1122(4)	-0.0090(2)	-0.0176(2)	0.00338(18)
N2	0.043(2)	0.033(2)	0.038(2)	0.0004(17)	0.0082(19)	0.0017(18)
N3	0.047(2)	0.038(2)	0.034(2)	0.0020(17)	-0.0005(19)	0.0059(18)
N4	0.043(2)	0.041(2)	0.048(3)	0.002(2)	0.007(2)	0.0037(19)
N1	0.052(3)	0.031(2)	0.039(2)	0.0026(17)	0.0026(19)	-0.0025(18)
C14	0.038(3)	0.036(3)	0.042(3)	0.001(2)	-0.001(2)	0.002(2)
C13	0.045(3)	0.042(3)	0.037(3)	0.006(2)	0.008(2)	0.005(2)
C38	0.047(3)	0.035(3)	0.046(3)	0.007(2)	-0.006(3)	0.003(2)
C15	0.041(3)	0.044(3)	0.051(3)	-0.001(3)	0.002(3)	0.001(2)
C39	0.046(3)	0.046(3)	0.055(4)	-0.010(3)	-0.004(3)	0.009(2)
C22	0.051(3)	0.041(3)	0.061(4)	0.005(3)	0.009(3)	-0.003(2)
C34	0.050(3)	0.047(3)	0.034(3)	-0.006(2)	-0.004(2)	0.011(2)
C40	0.049(3)	0.061(3)	0.059(4)	-0.021(3)	0.008(3)	0.005(3)

C9	0.050(3)	0.036(3)	0.052(4)	0.002(2)	0.002(3)	-0.002(2)
C16	0.067(4)	0.054(3)	0.055(4)	-0.010(3)	0.012(3)	0.011(3)
C29	0.064(4)	0.049(3)	0.042(3)	-0.006(3)	-0.006(3)	0.010(3)
C4	0.059(4)	0.047(3)	0.057(4)	-0.005(3)	0.001(3)	-0.006(3)
C27	0.069(4)	0.048(3)	0.053(4)	-0.003(3)	-0.009(3)	-0.008(3)
C33	0.059(4)	0.076(4)	0.045(4)	-0.001(3)	0.005(3)	0.011(3)
C41	0.065(4)	0.061(4)	0.069(4)	0.000(3)	0.023(3)	-0.002(3)
C21	0.072(4)	0.052(4)	0.077(4)	0.015(3)	0.019(3)	-0.010(3)
C23	0.078(4)	0.060(4)	0.065(4)	0.005(3)	0.032(3)	-0.008(3)
C47	0.061(4)	0.045(3)	0.078(4)	-0.003(3)	-0.013(3)	0.011(3)
C8	0.064(4)	0.048(3)	0.065(4)	0.011(3)	0.005(3)	-0.013(3)
C3	0.071(4)	0.089(4)	0.038(3)	-0.011(3)	-0.002(3)	-0.005(3)
C19	0.064(4)	0.043(3)	0.090(5)	-0.004(3)	0.008(3)	0.014(3)
C17	0.077(5)	0.124(6)	0.071(5)	-0.021(4)	0.022(4)	-0.030(4)
C10	0.074(4)	0.068(4)	0.076(5)	0.020(3)	0.018(4)	-0.009(3)
C44	0.054(4)	0.088(5)	0.099(5)	-0.031(4)	0.008(4)	0.015(4)
C5	0.093(5)	0.069(4)	0.064(4)	-0.009(3)	-0.009(4)	-0.012(4)
C20	0.084(5)	0.040(3)	0.094(5)	0.014(3)	0.008(4)	-0.002(3)
C18	0.087(5)	0.097(5)	0.071(5)	-0.023(4)	0.014(4)	0.010(4)
C26	0.092(5)	0.052(4)	0.096(5)	0.015(3)	-0.026(4)	-0.015(3)
C28	0.072(4)	0.076(4)	0.102(5)	0.000(4)	-0.005(4)	-0.008(3)
C42	0.108(6)	0.105(5)	0.076(5)	0.013(4)	0.018(4)	0.007(4)
C7	0.081(5)	0.080(4)	0.094(6)	0.006(4)	0.006(4)	-0.041(4)
C32	0.104(5)	0.093(5)	0.057(4)	0.003(4)	0.029(4)	0.022(4)
C45	0.062(5)	0.085(5)	0.128(7)	-0.043(5)	-0.017(5)	0.023(4)
C30	0.124(6)	0.054(4)	0.058(4)	-0.010(3)	-0.008(4)	0.003(4)
C46	0.081(5)	0.056(4)	0.130(7)	-0.012(4)	-0.025(5)	0.020(4)
C31	0.158(8)	0.089(5)	0.048(4)	-0.015(4)	0.018(5)	0.035(5)
C12	0.120(6)	0.088(5)	0.095(5)	0.041(4)	0.004(4)	-0.029(4)
C48	0.081(5)	0.052(4)	0.104(5)	0.025(3)	-0.017(4)	-0.001(3)
C6	0.098(6)	0.082(5)	0.100(6)	-0.002(4)	-0.020(5)	-0.039(4)
C35	0.096(5)	0.102(5)	0.054(4)	0.002(4)	0.026(4)	-0.032(4)
C43	0.099(5)	0.093(5)	0.128(6)	0.005(4)	0.039(5)	-0.024(4)
C25	0.135(7)	0.171(8)	0.065(5)	-0.007(5)	0.012(5)	0.026(6)
C2	0.105(5)	0.115(6)	0.069(5)	0.023(4)	-0.004(4)	-0.017(4)
C11	0.136(7)	0.125(6)	0.089(6)	0.022(5)	0.042(5)	0.026(5)
C50	0.133(7)	0.058(4)	0.166(8)	0.019(4)	-0.037(6)	-0.010(4)

C37	0.174(9)	0.082(5)	0.152(8)	0.052(5)	0.038(7)	0.000(5)
C49	0.113(6)	0.102(5)	0.101(6)	0.037(4)	-0.016(5)	-0.009(4)
C24	0.078(5)	0.169(7)	0.100(6)	-0.024(5)	0.023(4)	0.034(5)
C1	0.118(6)	0.154(7)	0.085(6)	-0.019(5)	0.040(5)	0.019(5)
C36	0.136(8)	0.211(9)	0.093(6)	-0.016(6)	0.057(6)	-0.076(7)

Geometric parameters (Å, º)

Sb1—I1	2.7722 (5)	C5—H5	0.9500
Sb1—N2	2.634 (3)	C5—C6	1.357 (8)
Sb1—N3	2.113 (4)	C20—H20	0.9500
Sb1—N4	2.595 (4)	C18—H18A	0.9800
Sb1—N1	2.163 (4)	C18—H18B	0.9800
N2—C14	1.431 (5)	C18—H18C	0.9800
N2—C13	1.281 (5)	C26—H26A	0.9800
N3—C38	1.350 (5)	C26—H26B	0.9800
N3—C34	1.450 (5)	C26—H26C	0.9800
N4—C38	1.268 (5)	C28—H28A	0.9800
N4—C39	1.413 (6)	C28—H28B	0.9800
N1—C13	1.348 (5)	C28—H28C	0.9800
N1—C9	1.451 (6)	C42—H42A	0.9800
C14—C15	1.410 (6)	C42—H42B	0.9800
C14—C22	1.395 (6)	C42—H42C	0.9800
C13—H13	0.9500	C7—H7	0.9500
C38—H38	0.9500	C7—C6	1.380 (9)
C15—C16	1.511 (7)	C32—H32	0.9500
C15—C19	1.398 (6)	C32—C31	1.344 (9)
C39—C40	1.412 (7)	C45—H45	0.9500
C39—C47	1.395 (7)	C45—C46	1.365 (9)
C22—C21	1.383 (6)	C30—H30	0.9500
C22—C23	1.516 (7)	C30—C31	1.372 (9)
C34—C29	1.401 (6)	C46—H46	0.9500
C34—C33	1.401 (7)	C31—H31	0.9500

C40—C41	1.506 (7)	C12—H12A	0.9800
C40—C44	1.385 (7)	C12—H12B	0.9800
C9—C4	1.410 (7)	C12—H12C	0.9800
C9—C8	1.390 (7)	C48—H48	1.0000
C16—H16	1.0000	C48—C50	1.543 (8)
C16—C17	1.508 (7)	C48—C49	1.543 (8)
C16—C18	1.529 (7)	C6—H6	0.9500
C29—C27	1.511 (7)	C35—H35	1.0000
C29—C30	1.407 (7)	C35—C37	1.530 (9)
C4—C3	1.502 (7)	C35—C36	1.533 (8)
C4—C5	1.390 (7)	C43—H43A	0.9800
C27—H27	1.0000	C43—H43B	0.9800
C27—C26	1.527 (7)	C43—H43C	0.9800
C27—C28	1.526 (7)	C25—H25A	0.9800
C33—C32	1.385 (8)	C25—H25B	0.9800
C33—C35	1.503 (8)	C25—H25C	0.9800
C41—H41	1.0000	C2—H2A	0.9800
C41—C42	1.517 (8)	C2—H2B	0.9800
C41—C43	1.520 (7)	C2—H2C	0.9800
C21—H21	0.9500	C11—H11A	0.9800
C21—C20	1.343 (7)	C11—H11B	0.9800
C23—H23	1.0000	C11—H11C	0.9800
C23—C25	1.511 (8)	C50—H50A	0.9800
C23—C24	1.509 (8)	C50—H50B	0.9800
C47—C46	1.399 (8)	C50—H50C	0.9800
C47—C48	1.503 (8)	C37—H37A	0.9800
C8—C10	1.507 (8)	C37—H37B	0.9800
C8—C7	1.399 (8)	C37—H37C	0.9800
C3—H3	1.0000	C49—H49A	0.9800
C3—C2	1.528 (7)	C49—H49B	0.9800
C3—C1	1.535 (8)	C49—H49C	0.9800

C19—H19	0.9500	C24—H24A	0.9800
C19—C20	1.374 (7)	C24—H24B	0.9800
C17—H17A	0.9800	C24—H24C	0.9800
C17—H17B	0.9800	C1—H1A	0.9800
C17—H17C	0.9800	C1—H1B	0.9800
C10—H10	1.0000	C1—H1C	0.9800
C10—C12	1.535 (7)	C36—H36A	0.9800
C10—C11	1.529 (8)	C36—H36B	0.9800
C44—H44	0.9500	C36—H36C	0.9800
C44—C45	1.375 (9)		
N2—Sb1—I1	140.37 (8)	C16—C18—H18B	109.5
N3—Sb1—I1	96.60 (9)	C16—C18—H18C	109.5
N3—Sb1—N2	88.15 (12)	H18A—C18—H18B	109.5
N3—Sb1—N4	55.96 (13)	H18A—C18—H18C	109.5
N3—Sb1—N1	106.91 (14)	H18B—C18—H18C	109.5
N4—Sb1—I1	79.93 (8)	C27—C26—H26A	109.5
N4—Sb1—N2	132.17 (12)	C27—C26—H26B	109.5
N1—Sb1—I1	86.37 (9)	C27—C26—H26C	109.5
N1—Sb1—N2	54.91 (12)	H26A—C26—H26B	109.5
N1—Sb1—N4	156.04 (13)	H26A—C26—H26C	109.5
C14—N2—Sb1	154.3 (3)	H26B—C26—H26C	109.5
C13—N2—Sb1	82.5 (3)	C27—C28—H28A	109.5
C13—N2—C14	119.6 (4)	C27—C28—H28B	109.5
C38—N3—Sb1	102.7 (3)	C27—C28—H28C	109.5
C38—N3—C34	117.4 (4)	H28A—C28—H28B	109.5
C34—N3—Sb1	137.9 (3)	H28A—C28—H28C	109.5
C38—N4—Sb1	83.0 (3)	H28B—C28—H28C	109.5
C38—N4—C39	124.1 (4)	C41—C42—H42A	109.5
C39—N4—Sb1	152.8 (3)	C41—C42—H42B	109.5
C13—N1—Sb1	101.9 (3)	C41—C42—H42C	109.5
C13—N1—C9	116.9 (4)	H42A—C42—H42B	109.5

C9—N1—Sb1	127.0 (3)	H42A—C42—H42C	109.5
C15—C14—N2	119.4 (4)	H42B—C42—H42C	109.5
C22—C14—N2	119.4 (4)	C8—C7—H7	119.6
C22—C14—C15	121.2 (4)	C6—C7—C8	120.8 (6)
N2—C13—N1	117.7 (4)	C6—C7—H7	119.6
N2—C13—H13	121.2	C33—C32—H32	119.6
N1—C13—H13	121.2	C31—C32—C33	120.8 (6)
N3—C38—H38	120.8	C31—C32—H32	119.6
N4—C38—N3	118.4 (4)	C44—C45—H45	119.7
N4—C38—H38	120.8	C46—C45—C44	120.7 (6)
C14—C15—C16	122.7 (4)	C46—C45—H45	119.7
C19—C15—C14	117.4 (5)	C29—C30—H30	119.5
C19—C15—C16	119.9 (5)	C31—C30—C29	120.9 (6)
C40—C39—N4	116.9 (4)	C31—C30—H30	119.5
C47—C39—N4	121.7 (5)	C47—C46—H46	119.4
C47—C39—C40	121.3 (5)	C45—C46—C47	121.1 (6)
C14—C22—C23	122.0 (4)	C45—C46—H46	119.4
C21—C22—C14	117.7 (5)	C32—C31—C30	121.3 (6)
C21—C22—C23	120.3 (5)	C32—C31—H31	119.3
C29—C34—N3	119.6 (4)	C30—C31—H31	119.3
C29—C34—C33	121.2 (5)	C10—C12—H12A	109.5
C33—C34—N3	119.0 (4)	C10—C12—H12B	109.5
C39—C40—C41	120.8 (5)	C10—C12—H12C	109.5
C44—C40—C39	118.2 (5)	H12A—C12—H12B	109.5
C44—C40—C41	121.0 (6)	H12A—C12—H12C	109.5
C4—C9—N1	119.8 (4)	H12B—C12—H12C	109.5
C8—C9—N1	118.9 (5)	C47—C48—H48	106.8
C8—C9—C4	121.3 (5)	C47—C48—C50	112.1 (6)
C15—C16—H16	107.7	C47—C48—C49	112.0 (5)
C15—C16—C18	113.3 (5)	C50—C48—H48	106.8
C17—C16—C15	111.3 (5)	C50—C48—C49	111.8 (5)

C17—C16—H16	107.7	C49—C48—H48	106.8
C17—C16—C18	109.0 (4)	C5—C6—C7	120.2 (6)
C18—C16—H16	107.7	C5—C6—H6	119.9
C34—C29—C27	123.5 (4)	C7—C6—H6	119.9
C34—C29—C30	117.0 (5)	C33—C35—H35	108.1
C30—C29—C27	119.4 (5)	C33—C35—C37	110.2 (6)
C9—C4—C3	124.0 (5)	C33—C35—C36	113.6 (6)
C5—C4—C9	117.7 (5)	C37—C35—H35	108.1
C5—C4—C3	118.3 (5)	C37—C35—C36	108.5 (6)
C29—C27—H27	107.8	C36—C35—H35	108.1
C29—C27—C26	113.9 (5)	C41—C43—H43A	109.5
C29—C27—C28	111.2 (4)	C41—C43—H43B	109.5
C26—C27—H27	107.8	C41—C43—H43C	109.5
C28—C27—H27	107.8	H43A—C43—H43B	109.5
C28—C27—C26	108.1 (4)	H43A—C43—H43C	109.5
C34—C33—C35	120.9 (5)	H43B—C43—H43C	109.5
C32—C33—C34	118.8 (6)	C23—C25—H25A	109.5
C32—C33—C35	120.0 (6)	C23—C25—H25B	109.5
C40—C41—H41	107.0	C23—C25—H25C	109.5
C40—C41—C42	110.2 (5)	H25A—C25—H25B	109.5
C40—C41—C43	113.4 (5)	H25A—C25—H25C	109.5
C42—C41—H41	107.0	H25B—C25—H25C	109.5
C42—C41—C43	111.8 (5)	C3—C2—H2A	109.5
C43—C41—H41	107.0	C3—C2—H2B	109.5
C22—C21—H21	118.7	C3—C2—H2C	109.5
C20—C21—C22	122.6 (5)	H2A—C2—H2B	109.5
C20—C21—H21	118.7	H2A—C2—H2C	109.5
C22—C23—H23	107.3	H2B—C2—H2C	109.5
C25—C23—C22	113.1 (5)	C10—C11—H11A	109.5
C25—C23—H23	107.3	C10—C11—H11B	109.5
C24—C23—C22	111.7 (5)	C10—C11—H11C	109.5

C24—C23—H23	107.3	H11A—C11—H11B	109.5
C24—C23—C25	109.9 (5)	H11A—C11—H11C	109.5
C39—C47—C46	117.8 (6)	H11B—C11—H11C	109.5
C39—C47—C48	124.1 (5)	C48—C50—H50A	109.5
C46—C47—C48	118.1 (6)	C48—C50—H50B	109.5
C9—C8—C10	122.4 (5)	C48—C50—H50C	109.5
C9—C8—C7	118.1 (6)	H50A—C50—H50B	109.5
C7—C8—C10	119.5 (5)	H50A—C50—H50C	109.5
C4—C3—H3	107.3	H50B—C50—H50C	109.5
C4—C3—C2	112.6 (5)	C35—C37—H37A	109.5
C4—C3—C1	111.4 (5)	C35—C37—H37B	109.5
C2—C3—H3	107.3	C35—C37—H37C	109.5
C2—C3—C1	110.5 (5)	H37A—C37—H37B	109.5
C1—C3—H3	107.3	H37A—C37—H37C	109.5
C15—C19—H19	119.5	H37B—C37—H37C	109.5
C20—C19—C15	121.0 (5)	C48—C49—H49A	109.5
C20—C19—H19	119.5	C48—C49—H49B	109.5
C16—C17—H17A	109.5	C48—C49—H49C	109.5
C16—C17—H17B	109.5	H49A—C49—H49B	109.5
C16—C17—H17C	109.5	H49A—C49—H49C	109.5
H17A—C17—H17B	109.5	H49B—C49—H49C	109.5
H17A—C17—H17C	109.5	C23—C24—H24A	109.5
H17B—C17—H17C	109.5	C23—C24—H24B	109.5
C8—C10—H10	107.4	C23—C24—H24C	109.5
C8—C10—C12	112.8 (5)	H24A—C24—H24B	109.5
C8—C10—C11	111.1 (5)	H24A—C24—H24C	109.5
C12—C10—H10	107.4	H24B—C24—H24C	109.5
C11—C10—H10	107.4	C3—C1—H1A	109.5
C11—C10—C12	110.3 (5)	C3—C1—H1B	109.5
C40—C44—H44	119.6	C3—C1—H1C	109.5
C45—C44—C40	120.8 (7)	H1A—C1—H1B	109.5

C45—C44—H44	119.6	H1A—C1—H1C	109.5
C4—C5—H5	119.1	H1B—C1—H1C	109.5
C6—C5—C4	121.8 (6)	C35—C36—H36A	109.5
C6—C5—H5	119.1	C35—C36—H36B	109.5
C21—C20—C19	120.1 (5)	C35—C36—H36C	109.5
C21—C20—H20	119.9	H36A—C36—H36B	109.5
C19—C20—H20	119.9	H36A—C36—H36C	109.5
C16—C18—H18A	109.5	H36B—C36—H36C	109.5
Sb1—N2—C14—C15	137.3 (5)	C34—N3—C38—N4	168.7 (4)
Sb1—N2—C14—C22	−39.6 (9)	C34—C29—C27—C26	−143.9 (5)
Sb1—N2—C13—N1	−15.4 (4)	C34—C29—C27—C28	93.7 (6)
Sb1—N3—C38—N4	1.8 (5)	C34—C29—C30—C31	1.9 (8)
Sb1—N3—C34—C29	85.7 (6)	C34—C33—C32—C31	1.3 (9)
Sb1—N3—C34—C33	−100.0 (5)	C34—C33—C35—C37	−86.3 (7)
Sb1—N4—C38—N3	−1.5 (4)	C34—C33—C35—C36	151.7 (6)
Sb1—N4—C39—C40	−66.0 (8)	C40—C39—C47—C46	1.1 (8)
Sb1—N4—C39—C47	110.5 (7)	C40—C39—C47—C48	179.5 (5)
Sb1—N1—C13—N2	19.2 (5)	C40—C44—C45—C46	−0.9 (10)
Sb1—N1—C9—C4	63.7 (5)	C9—N1—C13—N2	162.0 (4)
Sb1—N1—C9—C8	−115.4 (4)	C9—C4—C3—C2	119.7 (6)
N2—C14—C15—C16	2.0 (7)	C9—C4—C3—C1	−115.4 (6)
N2—C14—C15—C19	−177.5 (4)	C9—C4—C5—C6	1.1 (8)
N2—C14—C22—C21	175.9 (5)	C9—C8—C10—C12	137.0 (6)
N2—C14—C22—C23	−2.9 (7)	C9—C8—C10—C11	−98.5 (7)
N3—C34—C29—C27	−3.6 (7)	C9—C8—C7—C6	−1.7 (9)
N3—C34—C29—C30	172.4 (4)	C16—C15—C19—C20	−178.0 (5)
N3—C34—C33—C32	−174.0 (5)	C29—C34—C33—C32	0.2 (7)
N3—C34—C33—C35	−0.2 (7)	C29—C34—C33—C35	174.0 (5)
N4—C39—C40—C41	−2.3 (7)	C29—C30—C31—C32	−0.5 (10)
N4—C39—C40—C44	174.9 (5)	C4—C9—C8—C10	−177.7 (5)
N4—C39—C47—C46	−175.2 (5)	C4—C9—C8—C7	3.5 (8)

N4—C39—C47—C48	3.2 (8)	C4—C5—C6—C7	0.7 (10)
N1—C9—C4—C3	−1.6 (7)	C27—C29—C30—C31	178.1 (6)
N1—C9—C4—C5	177.8 (4)	C33—C34—C29—C27	−177.7 (5)
N1—C9—C8—C10	1.3 (7)	C33—C34—C29—C30	−1.7 (7)
N1—C9—C8—C7	−177.4 (5)	C33—C32—C31—C30	−1.1 (11)
C14—N2—C13—N1	178.5 (4)	C41—C40—C44—C45	178.7 (6)
C14—C15—C16—C17	97.9 (5)	C21—C22—C23—C25	53.2 (8)
C14—C15—C16—C18	−138.8 (5)	C21—C22—C23—C24	−71.3 (7)
C14—C15—C19—C20	1.5 (8)	C23—C22—C21—C20	−179.3 (6)
C14—C22—C21—C20	1.9 (8)	C47—C39—C40—C41	−178.8 (5)
C14—C22—C23—C25	−128.0 (6)	C47—C39—C40—C44	−1.6 (8)
C14—C22—C23—C24	107.4 (6)	C8—C9—C4—C3	177.5 (5)
C13—N2—C14—C15	−76.1 (5)	C8—C9—C4—C5	−3.2 (7)
C13—N2—C14—C22	106.9 (5)	C8—C7—C6—C5	−0.3 (11)
C13—N1—C9—C4	−68.6 (6)	C3—C4—C5—C6	−179.5 (6)
C13—N1—C9—C8	112.3 (5)	C19—C15—C16—C17	−82.7 (6)
C38—N3—C34—C29	−74.9 (5)	C19—C15—C16—C18	40.6 (7)
C38—N3—C34—C33	99.4 (5)	C10—C8—C7—C6	179.5 (6)
C38—N4—C39—C40	108.9 (5)	C44—C40—C41—C42	−84.0 (6)
C38—N4—C39—C47	−74.6 (6)	C44—C40—C41—C43	42.3 (7)
C15—C14—C22—C21	−1.0 (7)	C44—C45—C46—C47	0.4 (11)
C15—C14—C22—C23	−179.8 (5)	C5—C4—C3—C2	−59.6 (7)
C15—C19—C20—C21	−0.8 (9)	C5—C4—C3—C1	65.2 (7)
C39—N4—C38—N3	−179.1 (4)	C7—C8—C10—C12	−44.2 (8)
C39—C40—C41—C42	93.1 (6)	C7—C8—C10—C11	80.3 (7)
C39—C40—C41—C43	−140.6 (5)	C32—C33—C35—C37	87.4 (7)
C39—C40—C44—C45	1.5 (8)	C32—C33—C35—C36	−34.5 (8)
C39—C47—C46—C45	−0.5 (9)	C30—C29—C27—C26	40.2 (7)
C39—C47—C48—C50	−120.8 (6)	C30—C29—C27—C28	−82.2 (6)
C39—C47—C48—C49	112.6 (6)	C46—C47—C48—C50	57.6 (7)
C22—C14—C15—C16	178.9 (5)	C46—C47—C48—C49	−69.0 (7)

C22—C14—C15—C19	−0.6 (7)	C48—C47—C46—C45	−179.0 (6)
C22—C21—C20—C19	−1.0 (9)	C35—C33—C32—C31	−172.6 (6)

5.

Crystal data	
$C_{25}H_{35}Br_2N_2Sb$	$Z = 2$
$M_r = 645.12$	$F(000) = 640$
Triclinic, *P*-1	$D_x = 1.642$ Mg m^{-3}
$a = 10.105$ (2) Å	Synchrotron, $\lambda = 0.71073$ Å
$b = 10.332$ (2) Å	Cell parameters from 6298 reflections
$c = 14.240$ (3) Å	$\theta = 2$–25°
$\alpha = 96.69$ (3) °	$\mu = 4.13$ mm^{-1}
$\beta = 103.93$ (3)°	$T = 100$ K
$\gamma = 111.72$ (3) °	Cube, yellow
$V = 4794.3$ (17) Å^3	0.1 × 0.04 × 0.02
Data collection	
ADSC Quantum 210r Diffractometer	6079 observed [$I > 2\sigma(I)$] reflections
Radiation source: MX1 Beamline Australian Synchrotron	$R_{int} = 0.032$
Scan method: Phi scans	$\theta_{max} = 31.9°$, $\theta_{min} = 2.4°$
Absorption correction: Multi-scan, XDS (Kabsch, 1993)	$h = -14 \rightarrow 14$
23524 measured reflections	$k = -14 \rightarrow 14$
6298 independent reflections	$l = -18 \rightarrow 18$
Refinement	
Refinement on F^2	0 restraints
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.028$	$w = 1/[\sigma^2(F_o^2) + (0.0394P)^2 + 1.7194P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.075$	
$S = 1.07$	$(\Delta/\sigma)_{max} = 0.003$
6298 reflections	$\Delta\rho_{max} = 0.50$ e Å^{-3}
279 parameters	$\Delta\rho_{min} = -1.25$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}^*/U_{eq}
Sb1	0.39366(2)	0.57235(2)	0.85010(2)	0.01444(5)
Br1	0.55529(3)	0.73608(2)	1.02516(2)	0.01988(6)
Br2	0.25079(3)	0.72234(3)	0.80529(2)	0.02796(7)
N1	0.57025(19)	0.66793(18)	0.79381(13)	0.0124(3)
N2	0.3676(2)	0.51144(19)	0.67425(14)	0.0151(3)
C10	0.7817(2)	0.5702(2)	0.90412(17)	0.0160(4)

H10	0.672943	0.534523	0.898438	0.019
C3	0.9817(2)	0.8099(2)	0.90879(17)	0.0157(4)
H3	1.054777	0.77803	0.939372	0.019
C1	0.7249(2)	0.7659(2)	0.83235(16)	0.0117(3)
C14	0.2830(2)	0.4227(2)	0.57749(16)	0.0144(4)
C6	0.7681(2)	0.9060(2)	0.81703(16)	0.0137(4)
C2	0.8299(2)	0.7182(2)	0.88170(16)	0.0134(4)
C13	0.5085(2)	0.5954(2)	0.69805(16)	0.0131(4)
H13	0.563553	0.604972	0.651889	0.016
C7	0.6539(3)	0.9632(2)	0.77384(18)	0.0170(4)
H7	0.556221	0.879527	0.739066	0.02
C23	0.2786(3)	0.6417(2)	0.51231(18)	0.0194(4)
H23	0.301999	0.681506	0.584718	0.023
C16	0.1567(3)	0.3892(3)	0.40455(17)	0.0209(4)
H16	0.127694	0.427244	0.349446	0.025
C5	0.9209(2)	0.9947(2)	0.84786(17)	0.0167(4)
H5	0.952902	1.089822	0.83865	0.02
C4	1.0272(2)	0.9468(2)	0.89171(17)	0.0167(4)
H4	1.130791	1.007699	0.909948	0.02
C21	0.2718(3)	0.2119(2)	0.65622(19)	0.0200(4)
H21	0.371161	0.281366	0.703045	0.024
C15	0.2388(2)	0.4820(2)	0.49811(17)	0.0162(4)
C8	0.6971(3)	1.0513(3)	0.6979(2)	0.0266(5)
H8A	0.787909	1.138679	0.731471	0.04
H8B	0.615296	1.076848	0.666978	0.04
H8C	0.715827	0.994652	0.646558	0.04
C19	0.2376(2)	0.2733(2)	0.56631(17)	0.0159(4)
C12	0.8666(3)	0.5757(3)	1.01055(18)	0.0212(4)
H12A	0.973585	0.608249	1.01797	0.032
H12B	0.828539	0.480051	1.024063	0.032
H12C	0.85196	0.642352	1.057592	0.032
C9	0.6320(3)	1.0516(3)	0.8581(2)	0.0251(5)
H9A	0.598977	0.99185	0.903764	0.038
H9B	0.556195	1.08614	0.830331	0.038
H9C	0.726961	1.133472	0.894285	0.038
C17	0.1168(3)	0.2429(3)	0.39064(18)	0.0227(5)
H17	0.063121	0.18196	0.326337	0.027

C11	0.7991(3)	0.4648(3)	0.82823(19)	0.0260(5)
H11A	0.738209	0.458346	0.761436	0.039
H11B	0.765667	0.37024	0.843817	0.039
H11C	0.904459	0.498365	0.830835	0.039
C24	0.1483(3)	0.6731(3)	0.4560(2)	0.0292(6)
H24A	0.126355	0.640131	0.38438	0.044
H24B	0.175771	0.776332	0.472152	0.044
H24C	0.059572	0.622939	0.475592	0.044
C20	0.1531(3)	0.1979(3)	0.7093(2)	0.0238(5)
H20A	0.146027	0.289893	0.72304	0.036
H20B	0.181695	0.170014	0.772007	0.036
H20C	0.055807	0.124802	0.666777	0.036
C18	0.1560(3)	0.1857(2)	0.47164(19)	0.0209(4)
H18	0.126627	0.085292	0.462109	0.025
C22	0.2798(3)	0.0667(3)	0.6325(2)	0.0305(6)
H22A	0.180534	-0.005746	0.592449	0.046
H22B	0.312636	0.039146	0.694553	0.046
H22C	0.351164	0.074027	0.59525	0.046
C25	0.4177(3)	0.7200(3)	0.4825(2)	0.0258(5)
H25A	0.503102	0.70731	0.523404	0.039
H25B	0.439554	0.822127	0.492653	0.039
H25C	0.39966	0.680628	0.412286	0.039

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sb1	0.01144(7)	0.01627(7)	0.01325(8)	0.00351(5)	0.00466(6)	0.00259(5)
Br1	0.01938(11)	0.02213(11)	0.01410(11)	0.00015(8)	0.00478(9)	0.00562(8)
Br2	0.02293(12)	0.04259(15)	0.02845(14)	0.01107(11)	0.01050(11)	0.02195(11)
N1	0.0106(7)	0.0134(7)	0.0114(8)	0.0026(6)	0.0039(7)	0.0029(6)
N2	0.0119(8)	0.0165(8)	0.0117(8)	0.0010(6)	0.0034(7)	0.0012(6)
C10	0.0151(9)	0.0161(9)	0.0191(10)	0.0071(8)	0.0054(8)	0.0081(7)
C3	0.0107(8)	0.0204(9)	0.0149(10)	0.0041(8)	0.0029(8)	0.0060(7)
C1	0.0105(8)	0.0110(8)	0.0116(9)	0.0015(7)	0.0040(7)	0.0025(6)
C14	0.0108(8)	0.0179(9)	0.0119(9)	0.0015(7)	0.0038(8)	0.0032(7)
C6	0.0157(9)	0.0123(8)	0.0125(9)	0.0024(7)	0.0044(8)	0.0051(7)
C2	0.0143(9)	0.0146(8)	0.0129(9)	0.0046(7)	0.0057(8)	0.0065(7)

C13	0.0137(9)	0.0127(8)	0.0132(9)	0.0040(7)	0.0041(8)	0.0056(7)
C7	0.0184(9)	0.0153(9)	0.0196(10)	0.0063(8)	0.0051(9)	0.0091(7)
C23	0.0229(10)	0.0194(10)	0.0155(10)	0.0066(8)	0.0069(9)	0.0069(8)
C16	0.0209(10)	0.0260(11)	0.0123(10)	0.0034(8)	0.0044(9)	0.0066(8)
C5	0.0167(9)	0.0125(8)	0.0173(10)	0.0028(7)	0.0054(8)	0.0022(7)
C4	0.0116(9)	0.0170(9)	0.0157(10)	0.0016(8)	0.0044(8)	0.0001(7)
C21	0.0158(9)	0.0161(9)	0.0223(11)	0.0042(8)	0.0007(9)	0.0036(8)
C15	0.0146(9)	0.0199(9)	0.0131(10)	0.0042(8)	0.0057(8)	0.0049(7)
C8	0.0325(13)	0.0291(12)	0.0268(13)	0.0168(10)	0.0113(11)	0.0176(10)
C19	0.0118(8)	0.0171(9)	0.0167(10)	0.0028(8)	0.0049(8)	0.0036(7)
C12	0.0240(11)	0.0258(11)	0.0194(11)	0.0116(9)	0.0093(10)	0.0128(9)
C9	0.0311(12)	0.0254(11)	0.0274(13)	0.0074(10)	0.0124(11)	0.0183(10)
C17	0.0203(10)	0.0257(11)	0.0138(10)	-0.0029(9)	0.0042(9)	0.0034(9)
C11	0.0411(14)	0.0166(10)	0.0215(12)	0.0056(9)	0.0090(11)	0.0132(10)
C24	0.0263(12)	0.0311(13)	0.0358(15)	0.0145(11)	0.0122(12)	0.0143(10)
C20	0.0216(11)	0.0221(11)	0.0197(12)	0.0058(9)	0.0054(10)	0.0006(8)
C18	0.0185(10)	0.0181(10)	0.0204(11)	-0.0020(8)	0.0051(9)	0.0040(8)
C22	0.0265(12)	0.0214(11)	0.0428(16)	0.0097(11)	0.0058(12)	0.0112(10)
C25	0.0201(11)	0.0255(11)	0.0254(13)	0.0110(10)	0.0048(10)	0.0023(9)

Geometric parameters (Å, º)

Sb1—Br1	2.5989 (14)	C4—H4	0.9500
Sb1—Br2	2.5172 (7)	C21—H21	1.0000
Sb1—N1	2.091 (2)	C21—C19	1.517 (3)
Sb1—N2	2.435 (2)	C21—C20	1.539 (4)
N1—C1	1.433 (3)	C21—C22	1.534 (3)
N1—C13	1.348 (3)	C8—H8A	0.9800
N2—C14	1.424 (3)	C8—H8B	0.9800
N2—C13	1.295 (3)	C8—H8C	0.9800
C10—H10	1.0000	C19—C18	1.394 (3)
C10—C2	1.521 (3)	C12—H12A	0.9800
C10—C12	1.534 (3)	C12—H12B	0.9800
C10—C11	1.531 (3)	C12—H12C	0.9800
C3—H3	0.9500	C9—H9A	0.9800

C3—C2	1.397 (3)	C9—H9B	0.9800
C3—C4	1.387 (3)	C9—H9C	0.9800
C1—C6	1.409 (3)	C17—H17	0.9500
C1—C2	1.405 (3)	C17—C18	1.396 (4)
C14—C15	1.405 (3)	C11—H11A	0.9800
C14—C19	1.414 (3)	C11—H11B	0.9800
C6—C7	1.519 (3)	C11—H11C	0.9800
C6—C5	1.396 (3)	C24—H24A	0.9800
C13—H13	0.9500	C24—H24B	0.9800
C7—H7	1.0000	C24—H24C	0.9800
C7—C8	1.534 (4)	C20—H20A	0.9800
C7—C9	1.531 (3)	C20—H20B	0.9800
C23—H23	1.0000	C20—H20C	0.9800
C23—C15	1.522 (3)	C18—H18	0.9500
C23—C24	1.533 (3)	C22—H22A	0.9800
C23—C25	1.529 (4)	C22—H22B	0.9800
C16—H16	0.9500	C22—H22C	0.9800
C16—C15	1.401 (3)	C25—H25A	0.9800
C16—C17	1.389 (3)	C25—H25B	0.9800
C5—H5	0.9500	C25—H25C	0.9800
C5—C4	1.390 (3)		
Br2—Sb1—Br1	94.98 (3)	C22—C21—C20	109.4 (2)
N1—Sb1—Br1	90.13 (6)	C14—C15—C23	121.5 (2)
N1—Sb1—Br2	98.93 (5)	C16—C15—C14	117.8 (2)
N1—Sb1—N2	58.20 (7)	C16—C15—C23	120.6 (2)
N2—Sb1—Br1	148.10 (5)	C7—C8—H8A	109.5
N2—Sb1—Br2	87.08 (5)	C7—C8—H8B	109.5
C1—N1—Sb1	137.39 (14)	C7—C8—H8C	109.5
C13—N1—Sb1	100.51 (14)	H8A—C8—H8B	109.5
C13—N1—C1	121.57 (19)	H8A—C8—H8C	109.5
C14—N2—Sb1	149.66 (15)	H8B—C8—H8C	109.5

C13—N2—Sb1	86.44 (14)	C14—C19—C21	120.2 (2)
C13—N2—C14	123.0 (2)	C18—C19—C14	118.0 (2)
C2—C10—H10	107.6	C18—C19—C21	121.7 (2)
C2—C10—C12	111.47 (19)	C10—C12—H12A	109.5
C2—C10—C11	111.3 (2)	C10—C12—H12B	109.5
C12—C10—H10	107.6	C10—C12—H12C	109.5
C11—C10—H10	107.6	H12A—C12—H12B	109.5
C11—C10—C12	111.17 (18)	H12A—C12—H12C	109.5
C2—C3—H3	119.5	H12B—C12—H12C	109.5
C4—C3—H3	119.5	C7—C9—H9A	109.5
C4—C3—C2	120.99 (19)	C7—C9—H9B	109.5
C6—C1—N1	119.20 (18)	C7—C9—H9C	109.5
C2—C1—N1	119.01 (18)	H9A—C9—H9B	109.5
C2—C1—C6	121.76 (19)	H9A—C9—H9C	109.5
C15—C14—N2	120.54 (19)	H9B—C9—H9C	109.5
C15—C14—C19	121.7 (2)	C16—C17—H17	120.2
C19—C14—N2	117.6 (2)	C16—C17—C18	119.7 (2)
C1—C6—C7	121.91 (19)	C18—C17—H17	120.2
C5—C6—C1	117.69 (19)	C10—C11—H11A	109.5
C5—C6—C7	120.32 (19)	C10—C11—H11B	109.5
C3—C2—C10	120.33 (18)	C10—C11—H11C	109.5
C3—C2—C1	118.14 (19)	H11A—C11—H11B	109.5
C1—C2—C10	121.52 (18)	H11A—C11—H11C	109.5
N1—C13—H13	122.8	H11B—C11—H11C	109.5
N2—C13—N1	114.4 (2)	C23—C24—H24A	109.5
N2—C13—H13	122.8	C23—C24—H24B	109.5
C6—C7—H7	107.9	C23—C24—H24C	109.5
C6—C7—C8	112.6 (2)	H24A—C24—H24B	109.5
C6—C7—C9	109.54 (19)	H24A—C24—H24C	109.5
C8—C7—H7	107.9	H24B—C24—H24C	109.5
C9—C7—H7	107.9	C21—C20—H20A	109.5

C9—C7—C8	110.8 (2)	C21—C20—H20B	109.5
C15—C23—H23	107.5	C21—C20—H20C	109.5
C15—C23—C24	112.4 (2)	H20A—C20—H20B	109.5
C15—C23—C25	111.9 (2)	H20A—C20—H20C	109.5
C24—C23—H23	107.5	H20B—C20—H20C	109.5
C25—C23—H23	107.5	C19—C18—C17	121.2 (2)
C25—C23—C24	109.8 (2)	C19—C18—H18	119.4
C15—C16—H16	119.3	C17—C18—H18	119.4
C17—C16—H16	119.3	C21—C22—H22A	109.5
C17—C16—C15	121.4 (2)	C21—C22—H22B	109.5
C6—C5—H5	119.3	C21—C22—H22C	109.5
C4—C5—C6	121.39 (19)	H22A—C22—H22B	109.5
C4—C5—H5	119.3	H22A—C22—H22C	109.5
C3—C4—C5	119.84 (19)	H22B—C22—H22C	109.5
C3—C4—H4	120.1	C23—C25—H25A	109.5
C5—C4—H4	120.1	C23—C25—H25B	109.5
C19—C21—H21	107.9	C23—C25—H25C	109.5
C19—C21—C20	109.14 (19)	H25A—C25—H25B	109.5
C19—C21—C22	114.4 (2)	H25A—C25—H25C	109.5
C20—C21—H21	107.9	H25B—C25—H25C	109.5
C22—C21—H21	107.9		
Sb1—N1—C1—C6	−108.4 (2)	C13—N2—C14—C15	−74.5 (3)
Sb1—N1—C1—C2	73.6 (3)	C13—N2—C14—C19	109.5 (2)
Sb1—N1—C13—N2	7.3 (2)	C7—C6—C5—C4	177.1 (2)
Sb1—N2—C14—C15	121.3 (3)	C16—C17—C18—C19	−1.4 (4)
Sb1—N2—C14—C19	−54.6 (4)	C5—C6—C7—C8	45.0 (3)
Sb1—N2—C13—N1	−6.15 (17)	C5—C6—C7—C9	−78.8 (3)
N1—C1—C6—C7	8.8 (3)	C4—C3—C2—C10	−177.9 (2)
N1—C1—C6—C5	−174.5 (2)	C4—C3—C2—C1	3.0 (3)
N1—C1—C2—C10	−6.2 (3)	C21—C19—C18—C17	175.8 (2)
N1—C1—C2—C3	172.88 (19)	C15—C14—C19—C21	−172.7 (2)

N2—C14—C15—C23	−0.3 (3)	C15—C14—C19—C18	4.8 (3)
N2—C14—C15—C16	179.6 (2)	C15—C16—C17—C18	1.5 (4)
N2—C14—C19—C21	3.2 (3)	C19—C14—C15—C23	175.5 (2)
N2—C14—C19—C18	−179.3 (2)	C19—C14—C15—C16	−4.7 (3)
C1—N1—C13—N2	−179.69 (18)	C12—C10—C2—C3	45.4 (3)
C1—C6—C7—C8	−138.4 (2)	C12—C10—C2—C1	−135.5 (2)
C1—C6—C7—C9	97.8 (3)	C17—C16—C15—C14	1.5 (4)
C1—C6—C5—C4	0.3 (3)	C17—C16—C15—C23	−178.7 (2)
C14—N2—C13—N1	−178.20 (19)	C11—C10—C2—C3	−79.3 (3)
C14—C19—C18—C17	−1.7 (3)	C11—C10—C2—C1	99.8 (2)
C6—C1—C2—C10	175.9 (2)	C24—C23—C15—C14	−138.5 (2)
C6—C1—C2—C3	−5.1 (3)	C24—C23—C15—C16	41.6 (3)
C6—C5—C4—C3	−2.3 (4)	C20—C21—C19—C14	82.1 (2)
C2—C3—C4—C5	0.6 (4)	C20—C21—C19—C18	−95.3 (3)
C2—C1—C6—C7	−173.3 (2)	C22—C21—C19—C14	−155.0 (2)
C2—C1—C6—C5	3.4 (3)	C22—C21—C19—C18	27.6 (3)
C13—N1—C1—C6	81.8 (3)	C25—C23—C15—C14	97.3 (3)
C13—N1—C1—C2	−96.2 (2)	C25—C23—C15—C16	−82.5 (3)

6.

Crystal data	
$C_{25}H_{35}I_2N_2Sb$	$Z = 2$
$M_r = 739.10$	$F(000) = 712$
Triclinic, *P*-1	$D_x = 1.746$ Mg m^{-3}
$a = 10.4137$ (4) Å	Mo $K\alpha$, $\lambda = 0.71073$ Å
$b = 10.5559$ (4) Å	Cell parameters from 3979 reflections
$c = 14.6097$ (5) Å	$\theta = 2.2$–$26.2°$
$\alpha = 95.876$ (2)°	$\mu = 3.19$ mm^{-1}
$\beta = 104.946$ (2)°	$T = 123$ K
$\gamma = 111.754$ (2)°	Cube, orange
$V = 1405.64$ (9) Å^3	0.45 × 0.15 × 0.08
Data collection	
Bruker *APEX*-II CCD Diffractometer	4879 observed [$I > 2\sigma(I)$] reflections
Radiation source: fine-focus sealed tube Graphite monochromator	$R_{int} = 0.077$
Scan method: φ and ω scans	$\theta_{max} = 27.5°$, $\theta_{min} = 1.5°$

Absorption correction: Multi-scan, *SADABS2012*/1 (Bruker,2012). T_{min} = 0.345, T_{max} = 0.746	h = −13→13
35754 measured reflections	k = −13→13
6393 independent reflections	l = −18→18
Refinement	
Refinement on F^2	0 restraints
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.071	$w = 1/[\sigma^2(F_o^2) + (0.1654P)^2 + 0.3766P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.227	
S = 1.04	$(\Delta/\sigma)_{max} < 0.001$
6393 reflections	$\Delta\rho_{max}$ = 2.98 e Å^{-3}
279 parameters	$\Delta\rho_{min}$ = −2.24 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}^*/U_{eq}
Sb1	0.60489(4)	0.42674(5)	0.15250(3)	0.04374(19)
I2	0.43935(6)	0.24904(6)	-0.03233(4)	0.0624(2)
I1	0.76641(7)	0.27915(9)	0.20995(5)	0.0823(3)
N2	0.4324(5)	0.3345(5)	0.2076(4)	0.0370(11)
N1	0.6298(6)	0.4896(6)	0.3236(4)	0.0411(12)
C14	0.2806(7)	0.2394(6)	0.1704(4)	0.0371(13)
C15	0.2387(8)	0.1025(7)	0.1865(5)	0.0417(14)
C13	0.4943(6)	0.4053(6)	0.3000(4)	0.0361(12)
H13	0.441931	0.394105	0.345197	0.043
C1	0.7123(6)	0.5753(7)	0.4186(4)	0.0389(13)
C2	0.7477(7)	0.5161(8)	0.4975(5)	0.0461(15)
C22	0.1785(7)	0.2835(7)	0.1183(5)	0.0418(14)
C9	0.7619(7)	0.7209(8)	0.4288(5)	0.0472(15)
C21	0.0318(8)	0.1926(9)	0.0902(6)	0.0560(19)
H21	-0.039972	0.221749	0.056874	0.067
C23	0.2237(8)	0.4274(8)	0.0946(5)	0.0498(16)
H23	0.329022	0.461303	0.099278	0.06
C20	-0.0112(8)	0.0617(9)	0.1097(6)	0.060(2)
H20	-0.112025	0.00135	0.090916	0.073
C19	0.0907(8)	0.0184(7)	0.1560(6)	0.0545(18)
H19	0.059014	-0.073181	0.168005	0.065
C16	0.3477(9)	0.0478(8)	0.2335(6)	0.0576(19)
H16	0.444462	0.12972	0.261471	0.069

C7	0.8712(10)	0.7471(10)	0.6002(6)	0.066(2)
H7	0.924735	0.806089	0.662983	0.079
C8	0.8405(9)	0.8044(9)	0.5228(6)	0.063(2)
H8	0.872908	0.903043	0.532422	0.075
C11	0.7379(8)	0.7837(8)	0.3409(6)	0.060(2)
H11	0.643553	0.716765	0.291574	0.072
C3	0.7041(9)	0.3584(9)	0.4853(6)	0.059(2)
H3	0.664238	0.315931	0.414065	0.071
C6	0.8259(9)	0.6055(10)	0.5887(5)	0.0583(19)
H6	0.848091	0.567424	0.643865	0.07
C24	0.1386(11)	0.4212(12)	-0.0100(7)	0.074(3)
H24A	0.145039	0.349915	-0.054902	0.112
H24B	0.180486	0.512478	-0.025968	0.112
H24C	0.036109	0.397233	-0.015689	0.112
C10	0.8601(11)	0.8003(12)	0.2963(7)	0.078(3)
H10A	0.953393	0.868913	0.342155	0.117
H10B	0.839092	0.832626	0.235884	0.117
H10C	0.865764	0.710086	0.282398	0.117
C5	0.8329(13)	0.3251(14)	0.5274(11)	0.096(4)
H5A	0.902071	0.355608	0.491232	0.144
H5B	0.799369	0.224053	0.522465	0.144
H5C	0.881017	0.374023	0.595751	0.144
C4	0.5808(13)	0.2930(12)	0.5293(9)	0.087(3)
H4A	0.616133	0.333903	0.599113	0.131
H4B	0.551519	0.191744	0.518965	0.131
H4C	0.496813	0.312093	0.497687	0.131
C17	0.3612(16)	-0.0492(13)	0.1562(10)	0.098(4)
H17A	0.266206	-0.127744	0.123813	0.147
H17B	0.432664	-0.084686	0.186421	0.147
H17C	0.393524	0.002177	0.108292	0.147
C12	0.7290(12)	0.9242(11)	0.3616(10)	0.090(3)
H12A	0.669298	0.92051	0.404052	0.134
H12B	0.684683	0.944638	0.300325	0.134
H12C	0.827442	0.997775	0.393559	0.134
C25	0.2120(17)	0.5308(10)	0.1672(8)	0.091(4)
H25A	0.113878	0.492986	0.173056	0.137
H25B	0.230173	0.61878	0.145494	0.137

H25C	0.284356	0.547994	0.230528	0.137
C18	0.3170(15)	-0.0197(16)	0.3140(10)	0.104(4)
H18A	0.341442	0.052121	0.371433	0.156
H18B	0.375904	-0.07339	0.32938	0.156
H18C	0.213205	-0.082689	0.294515	0.156

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sb1	0.0356(3)	0.0474(3)	0.0424(3)	0.0125(2)	0.01266(18)	0.0100(2)
I2	0.0580(3)	0.0685(4)	0.0463(3)	-0.0012(2)	0.0135(2)	0.0164(3)
I1	0.0674(4)	0.1199(6)	0.0894(5)	0.0386(4)	0.0303(3)	0.0631(4)
N2	0.031(2)	0.041(3)	0.034(2)	0.008(2)	0.0095(19)	0.010(2)
N1	0.034(2)	0.043(3)	0.036(2)	0.006(2)	0.008(2)	0.006(2)
C14	0.035(3)	0.034(3)	0.036(3)	0.005(2)	0.012(2)	0.008(2)
C15	0.046(3)	0.035(3)	0.042(3)	0.004(3)	0.017(3)	0.015(3)
C13	0.037(3)	0.034(3)	0.037(3)	0.010(2)	0.011(2)	0.014(2)
C1	0.029(3)	0.041(3)	0.037(3)	0.004(2)	0.008(2)	0.007(2)
C2	0.040(3)	0.054(4)	0.038(3)	0.007(3)	0.009(3)	0.015(3)
C22	0.035(3)	0.045(3)	0.040(3)	0.011(3)	0.009(2)	0.012(3)
C9	0.038(3)	0.047(3)	0.048(4)	0.006(3)	0.011(3)	0.012(3)
C21	0.036(3)	0.070(5)	0.056(4)	0.012(4)	0.013(3)	0.018(3)
C23	0.048(4)	0.060(4)	0.053(4)	0.026(3)	0.019(3)	0.029(3)
C20	0.036(3)	0.060(4)	0.067(5)	0.003(4)	0.017(3)	0.002(3)
C19	0.052(4)	0.037(3)	0.070(5)	0.008(3)	0.028(4)	0.009(3)
C16	0.057(4)	0.042(3)	0.077(5)	0.017(4)	0.018(4)	0.024(3)
C7	0.059(5)	0.071(5)	0.043(4)	-0.005(4)	0.003(3)	0.014(4)
C8	0.051(4)	0.052(4)	0.059(4)	-0.008(4)	0.004(3)	0.008(4)
C11	0.043(4)	0.051(4)	0.063(5)	0.018(4)	0.000(3)	0.005(3)
C3	0.059(4)	0.062(4)	0.055(4)	0.024(4)	0.014(3)	0.022(4)
C6	0.057(4)	0.079(5)	0.035(3)	0.013(3)	0.007(3)	0.028(4)
C24	0.077(6)	0.100(7)	0.063(5)	0.042(5)	0.021(4)	0.049(6)
C10	0.067(5)	0.090(7)	0.056(5)	0.019(5)	0.017(4)	0.011(5)
C5	0.077(7)	0.092(8)	0.131(10)	0.040(7)	0.035(7)	0.042(6)
C4	0.082(7)	0.081(7)	0.091(7)	0.037(6)	0.030(6)	0.019(6)
C17	0.122(10)	0.087(7)	0.104(9)	0.017(7)	0.034(8)	0.065(8)
C12	0.075(6)	0.063(5)	0.119(9)	0.033(6)	0.007(6)	0.029(5)

C25	0.152(11)	0.057(5)	0.076(6)	0.017(5)	0.040(7)	0.052(7)
C18	0.100(9)	0.129(11)	0.104(9)	0.061(8)	0.030(7)	0.062(8)

Geometric parameters (Å, º)

Sb1—I2	2.8190 (6)	C7—C6	1.368 (13)
Sb1—I1	2.7282 (8)	C8—H8	0.9500
Sb1—N2	2.105 (5)	C11—H11	1.0000
Sb1—N1	2.441 (5)	C11—C10	1.536 (14)
N2—C14	1.439 (7)	C11—C12	1.525 (14)
N2—C13	1.336 (8)	C3—H3	1.0000
N1—C13	1.287 (8)	C3—C5	1.506 (15)
N1—C1	1.426 (8)	C3—C4	1.548 (14)
C14—C15	1.411 (9)	C6—H6	0.9500
C14—C22	1.396 (9)	C24—H24A	0.9800
C15—C19	1.383 (10)	C24—H24B	0.9800
C15—C16	1.502 (11)	C24—H24C	0.9800
C13—H13	0.9500	C10—H10A	0.9800
C1—C2	1.398 (9)	C10—H10B	0.9800
C1—C9	1.406 (9)	C10—H10C	0.9800
C2—C3	1.532 (11)	C5—H5A	0.9800
C2—C6	1.394 (10)	C5—H5B	0.9800
C22—C21	1.390 (9)	C5—H5C	0.9800
C22—C23	1.520 (10)	C4—H4A	0.9800
C9—C8	1.404 (10)	C4—H4B	0.9800
C9—C11	1.510 (11)	C4—H4C	0.9800
C21—H21	0.9500	C17—H17A	0.9800
C21—C20	1.372 (13)	C17—H17B	0.9800
C23—H23	1.0000	C17—H17C	0.9800
C23—C24	1.536 (11)	C12—H12A	0.9800
C23—C25	1.504 (13)	C12—H12B	0.9800
C20—H20	0.9500	C12—H12C	0.9800
C20—C19	1.358 (12)	C25—H25A	0.9800

C19—H19	0.9500	C25—H25B	0.9800
C16—H16	1.0000	C25—H25C	0.9800
C16—C17	1.515 (15)	C18—H18A	0.9800
C16—C18	1.480 (15)	C18—H18B	0.9800
C7—H7	0.9500	C18—H18C	0.9800
C7—C8	1.358 (13)		
I1—Sb1—I2	95.93 (3)	C9—C11—C12	114.2 (8)
N2—Sb1—I2	91.24 (13)	C10—C11—H11	107.9
N2—Sb1—I1	100.11 (15)	C12—C11—H11	107.9
N2—Sb1—N1	57.86 (17)	C12—C11—C10	109.1 (9)
N1—Sb1—I2	148.77 (12)	C2—C3—H3	107.5
N1—Sb1—I1	86.23 (14)	C2—C3—C4	110.3 (8)
C14—N2—Sb1	137.9 (4)	C5—C3—C2	112.0 (8)
C13—N2—Sb1	100.1 (4)	C5—C3—H3	107.5
C13—N2—C14	121.5 (5)	C5—C3—C4	111.7 (8)
C13—N1—Sb1	86.3 (4)	C4—C3—H3	107.5
C13—N1—C1	123.0 (6)	C2—C6—H6	119.5
C1—N1—Sb1	150.2 (4)	C7—C6—C2	121.1 (7)
C15—C14—N2	118.9 (6)	C7—C6—H6	119.5
C22—C14—N2	119.6 (5)	C23—C24—H24A	109.5
C22—C14—C15	121.5 (6)	C23—C24—H24B	109.5
C14—C15—C16	122.5 (6)	C23—C24—H24C	109.5
C19—C15—C14	116.8 (7)	H24A—C24—H24B	109.5
C19—C15—C16	120.7 (6)	H24A—C24—H24C	109.5
N2—C13—H13	122.3	H24B—C24—H24C	109.5
N1—C13—N2	115.5 (6)	C11—C10—H10A	109.5
N1—C13—H13	122.3	C11—C10—H10B	109.5
C2—C1—N1	120.8 (6)	C11—C10—H10C	109.5
C2—C1—C9	121.6 (6)	H10A—C10—H10B	109.5
C9—C1—N1	117.5 (6)	H10A—C10—H10C	109.5
C1—C2—C3	121.8 (6)	H10B—C10—H10C	109.5

C6—C2—C1	117.9 (7)	C3—C5—H5A	109.5
C6—C2—C3	120.3 (7)	C3—C5—H5B	109.5
C14—C22—C23	121.8 (6)	C3—C5—H5C	109.5
C21—C22—C14	117.9 (6)	H5A—C5—H5B	109.5
C21—C22—C23	120.2 (7)	H5A—C5—H5C	109.5
C1—C9—C11	120.8 (6)	H5B—C5—H5C	109.5
C8—C9—C1	117.2 (7)	C3—C4—H4A	109.5
C8—C9—C11	121.9 (7)	C3—C4—H4B	109.5
C22—C21—H21	119.4	C3—C4—H4C	109.5
C20—C21—C22	121.1 (8)	H4A—C4—H4B	109.5
C20—C21—H21	119.4	H4A—C4—H4C	109.5
C22—C23—H23	107.1	H4B—C4—H4C	109.5
C22—C23—C24	111.7 (7)	C16—C17—H17A	109.5
C24—C23—H23	107.1	C16—C17—H17B	109.5
C25—C23—C22	111.7 (7)	C16—C17—H17C	109.5
C25—C23—H23	107.1	H17A—C17—H17B	109.5
C25—C23—C24	111.8 (8)	H17A—C17—H17C	109.5
C21—C20—H20	120.1	H17B—C17—H17C	109.5
C19—C20—C21	119.8 (7)	C11—C12—H12A	109.5
C19—C20—H20	120.1	C11—C12—H12B	109.5
C15—C19—H19	118.7	C11—C12—H12C	109.5
C20—C19—C15	122.6 (7)	H12A—C12—H12B	109.5
C20—C19—H19	118.7	H12A—C12—H12C	109.5
C15—C16—H16	107.1	H12B—C12—H12C	109.5
C15—C16—C17	109.1 (8)	C23—C25—H25A	109.5
C17—C16—H16	107.1	C23—C25—H25B	109.5
C18—C16—C15	114.4 (8)	C23—C25—H25C	109.5
C18—C16—H16	107.1	H25A—C25—H25B	109.5
C18—C16—C17	111.5 (9)	H25A—C25—H25C	109.5
C8—C7—H7	119.6	H25B—C25—H25C	109.5
C8—C7—C6	120.8 (7)	C16—C18—H18A	109.5

C6—C7—H7	119.6	C16—C18—H18B	109.5
C9—C8—H8	119.3	C16—C18—H18C	109.5
C7—C8—C9	121.3 (8)	H18A—C18—H18B	109.5
C7—C8—H8	119.3	H18A—C18—H18C	109.5
C9—C11—H11	107.9	H18B—C18—H18C	109.5
C9—C11—C10	109.8 (7)		
Sb1—N2—C14—C15	107.9 (7)	C1—C2—C3—C5	126.6 (9)
Sb1—N2—C14—C22	−71.2 (9)	C1—C2—C3—C4	−108.3 (9)
Sb1—N2—C13—N1	−5.1 (6)	C1—C2—C6—C7	−2.4 (12)
Sb1—N1—C13—N2	4.4 (5)	C1—C9—C8—C7	2.0 (12)
Sb1—N1—C1—C2	−122.5 (8)	C1—C9—C11—C10	−84.6 (9)
Sb1—N1—C1—C9	54.6 (12)	C1—C9—C11—C12	152.4 (8)
N2—C14—C15—C19	175.2 (6)	C2—C1—C9—C8	−4.2 (11)
N2—C14—C15—C16	−5.4 (10)	C2—C1—C9—C11	172.6 (7)
N2—C14—C22—C21	−175.0 (6)	C22—C14—C15—C19	−5.8 (10)
N2—C14—C22—C23	3.3 (10)	C22—C14—C15—C16	173.7 (7)
N1—C1—C2—C3	1.9 (11)	C22—C21—C20—C19	−1.0 (13)
N1—C1—C2—C6	−178.6 (7)	C9—C1—C2—C3	−175.1 (7)
N1—C1—C9—C8	178.7 (7)	C9—C1—C2—C6	4.4 (11)
N1—C1—C9—C11	−4.4 (10)	C21—C22—C23—C24	−43.7 (10)
C14—N2—C13—N1	−178.3 (6)	C21—C22—C23—C25	82.3 (10)
C14—C15—C19—C20	2.2 (11)	C21—C20—C19—C15	1.1 (13)
C14—C15—C16—C17	−103.9 (9)	C23—C22—C21—C20	179.1 (7)
C14—C15—C16—C18	130.4 (9)	C19—C15—C16—C17	75.6 (10)
C14—C22—C21—C20	−2.5 (11)	C19—C15—C16—C18	−50.2 (11)
C14—C22—C23—C24	138.0 (7)	C16—C15—C19—C20	−177.3 (8)
C14—C22—C23—C25	−96.0 (10)	C8—C9—C11—C10	92.0 (10)
C15—C14—C22—C21	5.9 (10)	C8—C9—C11—C12	−30.9 (11)
C15—C14—C22—C23	−175.7 (7)	C8—C7—C6—C2	0.3 (15)
C13—N2—C14—C15	−82.1 (8)	C11—C9—C8—C7	−174.8 (9)
C13—N2—C14—C22	98.8 (7)	C3—C2—C6—C7	177.1 (8)

C13—N1—C1—C2	68.7 (9)	C6—C2—C3—C5	−52.9 (11)
C13—N1—C1—C9	−114.2 (7)	C6—C2—C3—C4	72.2 (10)
C1—N1—C13—N2	178.8 (6)	C6—C7—C8—C9	−0.1 (15)