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Unexpected reactions of NHC*—Cu^{I} and —Ag^{I} bromides with potassium thio- or selenocyanate

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The reactions of N-heterocyclic carbene Cu^{I} and Ag^{I} halides with potassium thio- or selenocyanate gave unexpected products. The attempted substitution reaction of bromido(1,3-dibenzyl-4,5-diphenylimidazol-2-ylidene)silver (NHC*—Ag—Br) with KSCN yielded bis[bis(1,3-dibenzyl-4,5-diphenylimidazol-2-ylidene)silver(I)] tris(thiocyanato)argentate(I) diethyl ether disolvate, $[Ag(C_{29}H_{24}N_2)_2][Ag(NCS)_3]\cdot 2C_4H_{10}O$ or $[NHC^*_2Ag]_2[Ag(SCN)_3]\cdot 2Et_2O$, (**1**), while reaction with KSeCN led to bis(μ-1,3-dibenzyl-4,5-diphenyl-2-selenoimidazole-κ^2Se:Se)bis[bromido(1,3-dibenzyl-4,5-diphenyl-2-selenoimidazole-κSe)silver(I)] dichloromethane hexasolvate, $[Ag_2Br_2(C_{29}H_{24}N_2Se)_4]\cdot 6CH_2Cl_2$ or $(NHC^*Se)_4Ag_2Br_2\cdot 6CH_2Cl_2$, (**2**), *via* oxidation of the NHC* fragment to 2-selenoimidazole. This oxidation was observed again in the reaction of NHC*—Cu—Br with KSeCN, yielding *catena*-poly[[[(1,3-dibenzyl-4,5-diphenyl-2-selenoimidazole-κSe)copper(I)]-μ-cyanido-κ^2C:N] acetonitrile monosolvate], $\{[Cu(CN)(C_{29}H_{24}N_2Se)]\cdot C_2H_3N\}_n$ or NHC*Se—CuCN·CH_3CN, (**3**). Compound (**1**) represents an organic/inorganic salt with Ag^{I} in a linear coordination in each of the two cations and in a trigonal coordination in the anion, accompanied by diethyl ether solvent molecules. The tri-blade boomerang-shaped complex anion $[Ag(SCN)_3]^{2-}$ present in (**1**) is characterized by X-ray diffraction for the first time. Compound (**2**) comprises an isolated centrosymmetric molecule with Ag^{I} in a distorted tetrahedral $BrSe_3$ coordination, together with dichloromethane solvent molecules. Compound (**3**) exhibits a linear polymeric $^1_\infty[Cu—C{\equiv}N—Cu—]$ chain structure with a selenoimidazole moiety additionally coordinating to each Cu^{I} atom, and completed by acetonitrile solvent molecules. Electron densities associated with an additional ether solvent molecule in (**1**) and two additional dichloromethane solvent molecules in (**2**) were removed with the SQUEEZE procedure [Spek (2015). *Acta Cryst.* C**71**, 9–18] in *PLATON*.

1. Chemical context

Copper and silver and their compounds exhibit fungicidal properties. For example, a copper dihydroxide suspension in water – *The Bordeaux Mixture* – is a well-known early fungicide used in vineyards, while metallic silver has been used as an antimicrobial agent to purify drinking water for a long time. Alexander the Great stored drinking water in silver vessels during his military campaigns (White, 2002). Later, silver nitrate was used to treat wounds and infectious diseases even before the discovery of bacteria (Klasen, 2000). Silver sulfadiazine, discovered in the 1960s, was found to be more effective and safer than silver nitrate in treating burn wounds and is currently the most widely used remedy in burn centres (Fox, 1968). Silver is considered nontoxic to mammalian cells within the determined exposure limits of 0.01–0.1 mg m^{-3} (Drake & Hazelwood, 2005). Nevertheless, silver compounds may cause skin discoloration, known as Argyria (Kim *et al.*, 2009). The active species, the Ag^{I} cation, inhibits the respiratory path of

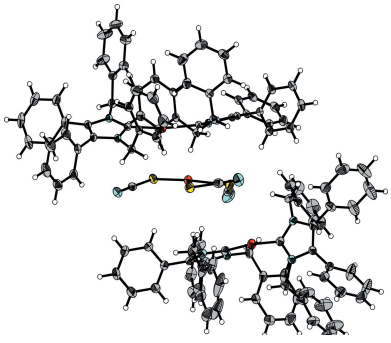
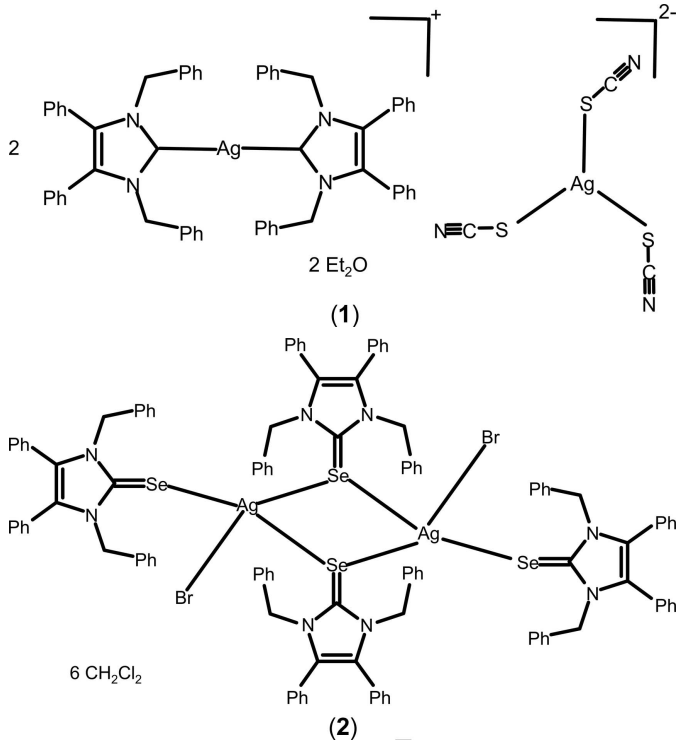


Table 1
Selected internuclear distances and bond angles (Å, °) for (**1**), (**2**) and (**3**).

Atoms	Distance	Atoms	Angle
(**1**)			
Ag1—C8	2.091 (2)	S1—Ag3—S2	127.68 (2)
Ag1—C37	2.085 (2)	S2—Ag3—S3	103.96 (2)
Ag2—C66	2.097 (2)	S3—Ag3—S1	126.94 (2)
Ag2—C95	2.102 (2)	Sum	358.58
Ag3—S1	2.4657 (5)	C8—Ag1—C37	173.06 (8)
Ag3—S2	2.5377 (6)	C66—Ag2—C95	172.01 (7)
Ag3—S3	2.4940 (6)	Ag3—S —C117	100.90 (7)
		Ag3—S2—C118	93.45 (8)
Ag3···N3	4.161 (2)	Ag3—S3—C119	105.56 (9)
Ag3···C66	3.069 (2)	S1—C117—N9	177.8 (2)
		S2—C118—N10	179.4 (3)
		S3—C119—N11	177.1 (2)
(**2**)			
Ag—Se1	2.6899 (4)	Br—Ag—Se1	102.274 (13)
Ag—Se2	2.7677 (4)	Br—Ag—Se2	109.628 (12)
Ag—Se2#1	2.7187 (4)	Br—Ag—Se2#1	126.883 (14)
Ag—Br	2.6631 (4)	Se1—Ag—Se2	110.623 (12)
		Se1—Ag—Se2#1	100.026 (11)
		Se2—Ag—Se2#1	106.352 (11)
		Ag—Se1—C8	94.72 (8)
		Ag—Se2—C37	100.72 (8)
		Ag#1—Se2—C37	108.43 (8)
		Ag—Se2—Ag#1	73.649 (11)
(**3**)			
Cu1—Se1	2.3900 (6)	Se1—Cu1—C59	125.06 (12)
Cu1—C59	1.898 (4)	Se1—Cu1—N6#2	110.25 (9)
Cu1—N6#2	1.939 (3)	C59—Cu1—N6#2	124.68 (14)
		Sum	359.99
Cu2—Se2	2.3861 (6)	Se2—Cu2—C60	126.88 (11)
Cu2—C60	1.895 (4)	Se2—Cu2—N5	110.28 (10)
Cu2—N5	1.937 (3)	C60—Cu2—N5	122.84 (15)
		Sum	360.00
		Cu1—Se1—C8	95.96 (10)
		Cu2—Se2—C37	93.84 (11)

Symmetry codes: (#1) $-x+1, -y+1, -z+2$; (#2) $-x+2, y+\frac{1}{2}, -z+\frac{3}{2}$.

sensitive strain organisms, destroys the cell wall, impairs essential enzymes, obstructs metabolic activity and/or causes RNA and DNA alteration (Silver, 2003; Starodub & Trevors, 1989). This topic saw renewed interest when Youngs and co-workers published the clean synthesis of N-heterocyclic (NHC) silver acetate derivatives from easily accessible imidazolium halides (Liang *et al.*, 2018); NHC–silver acetates exhibit good chemical stability through covalently bonded silver, which results in significant antibiotic activity. Particularly well suited are complexes with benzyl-substituted ligands like 1,3-dibenzyl-4,5-diphenylimidazol-2-ylidene (NHC*; Fig. 1), *e.g.* NHC*–Ag–OAc (SBC3) (Patil *et al.*, 2011; Streciwilk *et al.*, 2014; Hackenberg & Tacke, 2014), which combine synthesis from a commercially available precursor (4,5-diphenylimidazole) with high antimicrobial activity *in vitro* (Sharkey *et al.*, 2012) and *in vivo* (Browne *et al.* 2014). In the homologue gold series, the introduction of pseudohalide anions led to stable and bioactive compounds (Dada *et al.*, 2017). In this context, the attempted syntheses of the analogous NHC*—Ag^{I} and —Cu^{I} thio- and selenocyanates as potential antimicrobial species led to unexpected results with the formation of bis[bis(1,3-dibenzyl-4,5-diphenylimidazol-2-ylidene)silver(I)] tris(thiocyanato)argentate(I) diethyl ether disolvate, (**1**), bis(μ-1,3-dibenzyl-4,5-diphenyl-2-selenoimidazole-κ^2*Se*:*Se*)bis[bromido(1,3-dibenzyl-4,5-diphenyl-2-selenoimidazole-κ*Se*)silver(I)] dichloromethane hexasolvate, (**2**), and *catena*-poly[[[(1,3-dibenzyl-4,5-diphenyl-2-selenoimidazole-κ*Se*)-copper(I)]-μ-cyanido-κ^2*C*:*N*] acetonitrile monosolvate], {[Cu(CN)($C_{29}H_{24}N_2$Se)]·C_2H_3N}$_n$ or NHC*Se—CuCN·CH_3CN, (**3**), the crystal structures of which are reported in this communication.



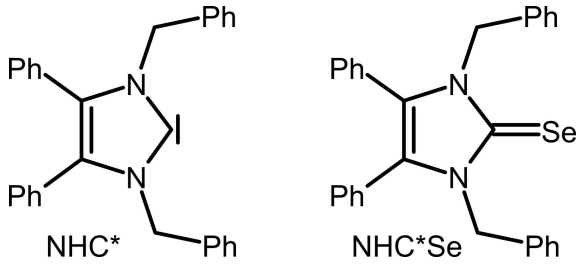


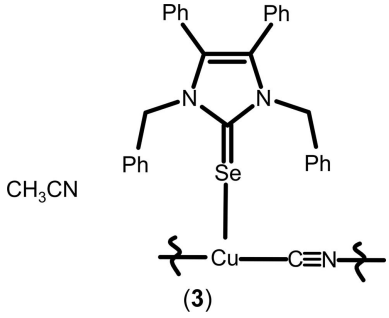
Figure 1
Lewis structures of the ligands NHC* and NHC*Se.

2. Structural commentary

2.1. [NHC*$_2$Ag]$_2$[Ag(SCN)$_3$]·2Et$_2$O, (1)

Both of the crystallographically distinct [NHC*$_2$Ag]$^+$ cations (Ag1 and Ag2) in the organic/inorganic salt show a nearly linear C—Ag—C angle and two almost identical Ag—C bond lengths (Table 1). In between these two bulky cations is located one [Ag(SCN)$_3$]$^{2-}$ anion with a rare coordination number of three for monovalent silver(I) (Ag3). The corresponding Ag—S bond lengths cover the range 2.4657 (5)–2.5377 (6) Å. The flexibility of the [Ag(SCN)$_3$]$^{2-}$ anion also shows itself in the bond angles, with Ag—S—C angles ranging from 93.45 (8) to 105.56 (9)°, and S—Ag—S

angles ranging from 104.96 (2) to 127.68 (2)° (Table 1). As expected, all three SCN^- ligands are virtually linear. The sum of the S—Ag—S bond angles (Table 1) indicates that the anion is almost planar [the deviation of the Ag3 from the least-squares plane of the three S atoms is 0.1270 (5) Å]. The $[Ag(SCN)_3]^{2-}$ anion is situated between the two crystallographically independent cations, but not in the middle (Fig. 2): cation 1 (Ag1) has a shortest distance of 4.161 (2) Å from N3 to Ag3 (line 2 in Fig. 2), whereas cation 2 (Ag2) has a shortest distance of 3.069 (2) Å from C66 to Ag3 (line 1 in Fig. 2). As a consequence of this close association, the benzyl groups in cation 2 are all aligned away from the anion. Due to its greater distance from the anion, the benzyl groups of cation 1 have greater flexibility, allowing it to take a shape suitable to fill gaps in the packing caused by the constraint on cation 2 (Fig. 3). The remaining gaps are filled by two noncoordinating diethyl ether molecules, one of which is highly disordered and could not be refined in terms of atomic sites. The SQUEEZE option (Spek, 2015) in *PLATON* was used to compensate for the ill-defined electron density.



(**3**)

2.2. $(NHC^*Se)_4Ag_2Br_2·6CH_2Cl_2$, (2)

Compound (**2**) is characterized by a molecular structure complemented by dichloromethane solvent molecules. Two Ag^I cations and two bridging NHC*Se ligands build up a centrosymmetric four-membered Ag_2Se_2 ring. Each silver cation carries a further terminal NHC*Se ligand and a terminal bromide ligand, in each case leading to a coordination number of 4 in the shape of a distorted tetrahedron (Table 1 and Fig. 4). One of the bridging Ag—Se distances is 2.7677 (4) Å, significantly longer than the other [2.7187 (4) Å]

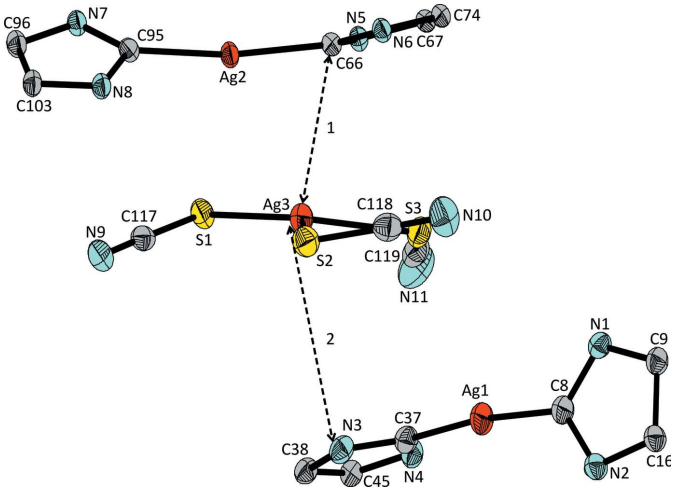


Figure 2
The $[Ag(SCN)_3]^{2-}$ anion in (**1**) with the two closest $[Ag(NHC^*)_2]^+$ cations. Substituents on the imidazole moiety have been omitted for clarity and displacement ellipsoids are drawn at the 50% probability level.

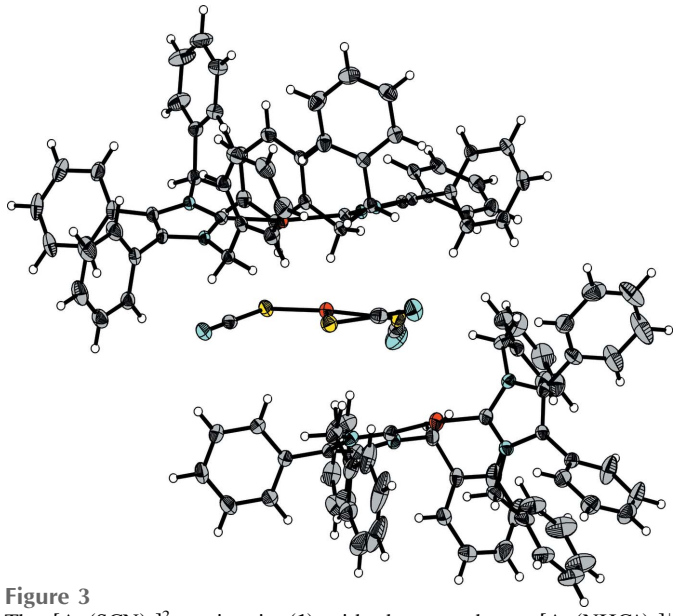


Figure 3
The $[Ag(SCN)_3]^{2-}$ anion in (**1**) with the two closest $[Ag(NHC^*)_2]^+$ cations. Displacement ellipsoids are drawn at the 50% probability level.

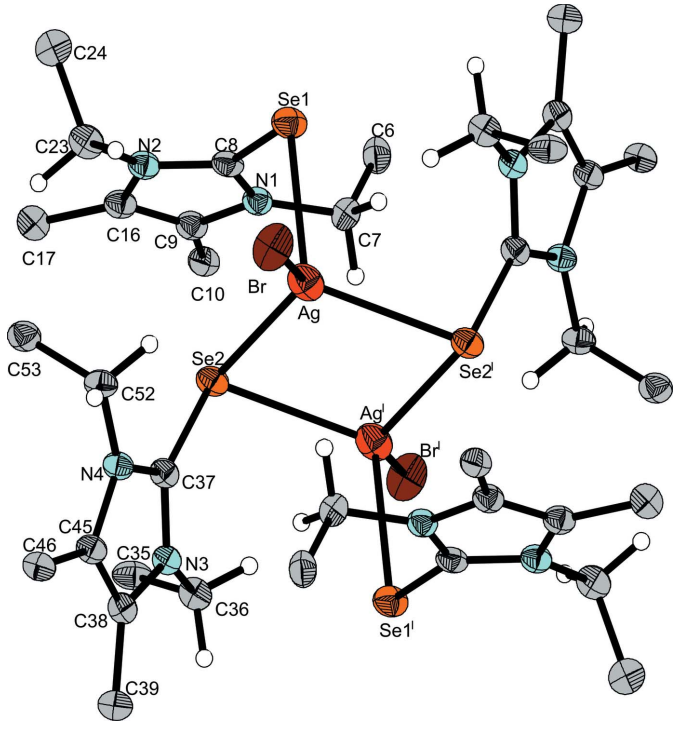


Figure 4
The molecular structure of (**2**), with phenyl groups represented by their *ipso* carbon atoms only. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry code: (I) $-x+1, -y+1, -z+1$.]

Table 2
Hydrogen-bond geometry (Å, °) for (**1**).

D—H···A	D—H	H···A	D···A	D—H···A
C31—H31···O1	0.95	2.57	3.361 (4)	141
C32—H32···N10^{i}	0.95	2.43	3.327 (4)	157
C40—H40···S1^{ii}	0.95	2.82	3.684 (2)	152

Symmetry codes: (i) $-x+2, -y+2, -z+1$; (ii) $x, y, z-1$.

or the terminal one [2.6899 (4) Å], suggesting that two AgBr(NHC*Se)$_2$ moieties are weakly attached to each other. The Ag—Se—C angles are all strongly bent (Table 1), as one would expect. The bridging and terminal NHC*Se ligand pairs, as well as the two bromide ligands, end up in pseudo-*trans* positions with respect to each other, allowing an overall compact shape of the uncharged [AgBr(NHC*Se)$_2$]$_2$ complex. Gaps in the packing are filled by dichloromethane solvent molecules, two of which were treated with the SQUEEZE option in *PLATON*.

2.3. NHC*Se—CuCN·CH$_3$CN, (3)

The structure of (**3**) is polymeric in nature and contains two distinct Cu^{I} atoms. The backbone of the structure is a linear copper–cyanide polymer $^{1}_{\infty}$[Cu1—C≡N—Cu2—], where every Cu^{I} atom is also coordinated by selenium from a terminal NHC*Se ligand (Fig. 5). The Cu—Se—C angles are in the same region as those in (**2**) (Table 1). The carbon and nitrogen atoms of the two cyanide anions can be distinguished, not only by their electron densities, but also by their different bond lengths to Cu^{I} atoms, with Cu—N shorter by ≃ 0.04 Å (Table 1). The relatively bulky NHC*Se ligands, which lead to the rare coordination number of 3 of the two Cu^{I} cations, move to opposite positions with respect to the copper cyanide polymer, allowing better packing for the overall structure

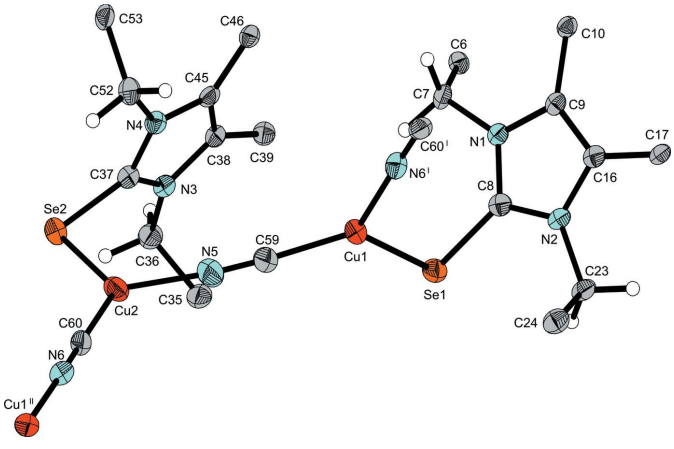


Figure 5
Section of the polymeric structure of (**3**), with displacement ellipsoids drawn at the 50% probability level. Phenyl groups are represented by their *ipso* carbons only and acetonitrile solvent molecules have been omitted for clarity. [Symmetry codes: (I) $-x+2, y+\frac{1}{2}, -z+\frac{3}{2}$; (II) $-x+2, y-\frac{1}{2}, -z+\frac{3}{2}$.]

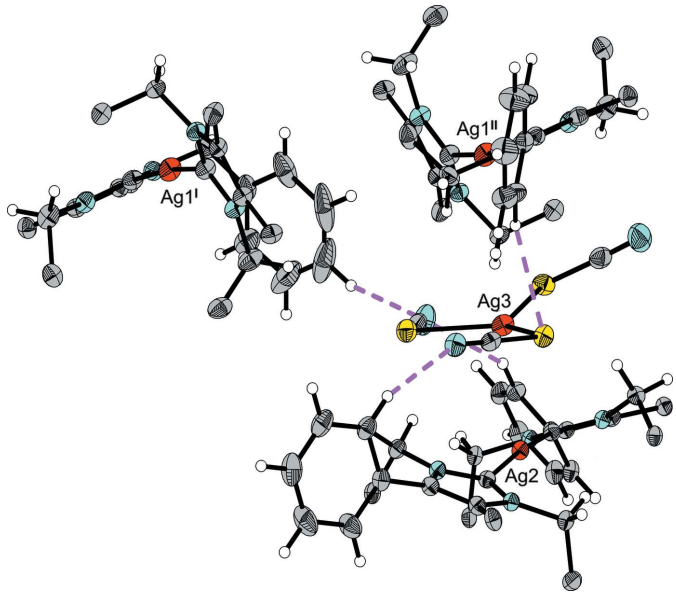


Figure 6
The [Ag(SCN)$_3$]$^{2-}$ anion in (**1**) involved in nonclassical hydrogen-bonding interactions, shown as pink dashed lines. Phenyl groups are represented by their *ipso* carbons only and displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (I) $-x+2, -y+2, -z+1$; (II) $x, y, z+1$.]

(Fig. 5). The sum of the three angles at Cu1 and Cu2 (Table 1) indicate that the coordination is practically planar at the central copper(I) atoms (the displacement of Cu1 from the least-squares Se1/N6/C5 plane is 0.099 Å and of Cu2 from the least-squares Se2/N5/C60 plane is 0.054 Å). Acetonitrile solvent molecules fill voids in the crystal packing.

All reactions reported here include cleavage of an Ag– or Cu–carbene bond, suggesting that even at room temperature (Cu) or in refluxing dichloromethane (Ag) the targeted

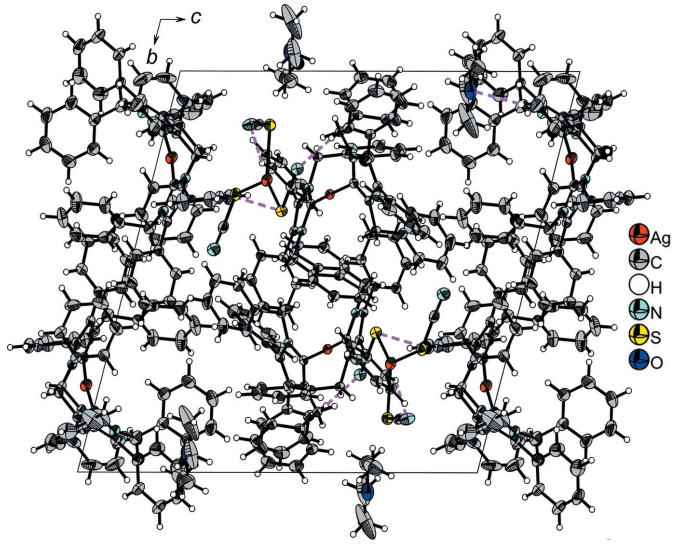


Figure 7
View of the crystal structure of (**1**) along [100]. Displacement ellipsoids are drawn at the 50% probability level and hydrogen-bonding interactions are shown as pink dashed lines.

Table 3
Experimental details.

	(1)	(2)	(3)
Crystal data			
Chemical formula	$[Ag(C_{29}H_{24}N_2)_2][Ag(NCS)_3]\cdot 2C_4H_{10}O$	$[Ag_2Br_2(C_{29}H_{24}N_2Se)_4]\cdot 6CH_2Cl_2$	$[Cu(CN)(C_{29}H_{24}N_2Se)]\cdot C_2H_3N$
M_r	2248.09	2802.96	610.07
Crystal system, space group	Triclinic, $P\overline{1}$	Triclinic, $P\overline{1}$	Monoclinic, $P2_1/c$
Temperature (K)	100	150	100
a, b, c (Å)	14.86462 (8), 19.3714 (1), 19.85451 (9)	13.6265 (1), 14.7422 (1), 16.9397 (2)	13.7704 (3), 14.3398 (3), 28.4102 (7)
α, β, γ (°)	102.7710 (4), 100.8268 (4), 99.5778 (4)	106.4172 (7), 112.2820 (8), 96.2211 (6)	90, 93.024 (2), 90
V (Å^3)	5345.84 (5)	2930.04 (5)	5602.2 (2)
Z	2	1	8
Radiation type	Cu $K\alpha$	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	5.37	2.58	2.11
Crystal size (mm)	0.32 × 0.06 × 0.04	0.37 × 0.26 × 0.20	0.35 × 0.12 × 0.11
Data collection			
Diffractometer	Rigaku SuperNova, Dual, Cu at zero, Atlas	Rigaku SuperNova, Dual, Cu at zero, Atlas	Rigaku SuperNova, Dual, Cu at zero, Atlas
Absorption correction	Gaussian (*CrysAlis PRO*; Rigaku OD, 2015)	Gaussian (*CrysAlis PRO*; Rigaku OD, 2015)	Gaussian (*CrysAlis PRO*; Rigaku OD, 2015)
T_{min}, T_{max}	0.437, 0.848	0.517, 0.664	0.643, 0.851
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	140384, 22376, 19576	119415, 12002, 10726	71725, 11392, 10122
R_{int}	0.045	0.037	0.038
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.632	0.626	0.626
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.030, 0.080, 1.03	0.035, 0.096, 1.03	0.048, 0.119, 1.06
No. of reflections	22376	12002	11392
No. of parameters	1309	654	687
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.98, −1.13	1.05, −1.49	2.04, −0.56

Computer programs: *CrysAlis PRO* (Rigaku OD, 2015), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg, 1999) and *publCIF* (Westrip, 2010).

NHC*—*M*—SeCN complexes are not very stable in solution, but are liable to Schlenk-type equilibrium exchange. It is worth mentioning that the syntheses of (**2**) and (**3**) require $SeCN^-$ acting as a selenating agent similar to selenium powder (Verlinden *et al.*, 2015) or Woollins Reagent (Bockfeld *et al.*, 2017), even under the relatively mild conditions reported here. Thus, neither thiocyanate nor selenocyanate take up their roles as unreactive substituents in these planned substitution reactions. These findings raise questions about the suitability of NHC—*M*—*X* (*M* = Cu and Ag; *X* = pseudohalide) as drugs because drug molecules need to be stable in solution under ambient conditions.

3. Supramolecular features

In (**1**), there are some weak nonclassical hydrogen bonds between the cations and the solvent molecules, as detailed in Table 2. One anion has connections to the two cations closest to it, as described above, and one to the cation of an adjacent ion triplet (Fig. 6), linking the ion triplets into a one-dimensional chain. Fig. 7 shows a view of (**1**) along [100] with these contacts shown as dashed lines.

All nonclassical hydrogen bonds in (**2**) and (**3**) are intramolecular, and we are not aware of any other noteworthy intermolecular features in these structures.

4. Database survey

To the best of our knowledge, the crystal structure of (**1**) is the first report of a salt with the tri-blade boomerang-shaped $[Ag(SCN)_3]^{2-}$ ion. The alkaline metals salts $Rb_2Ag(SCN)_3$ and $Rb_2Ag(SCN)_3$ have one-dimensional polymeric chains as anions rather than isolated $[Ag(SCN)_3]^{2-}$ (Thiele & Kehr, 1984). Hathaway *et al.* (1970) reported the spectroscopic properties of $[Cu(NH_3)_2Ag(SCN)_3]$ and indicated that they had determined its crystal structure as well. However, in this article, only the space group type ($P\overline{6}2c$) and the number of formula units (Z = 2) were given, not the crystal structure itself. From what is reported it can be gleaned that the anion must be situated on a $\overline{6}$ position, *i.e.* it is planar and adhering to threefold rotation symmetry. If this is true then this is in stark contrast to the $[Ag(SCN)_3]^{2-}$ anion reported here, where the Ag—S bond lengths and S—Ag—S and Ag—S—C bond angles cover a wide range. However, since together with the information above only a schematic drawing of the surrounding of the Cu^{II} atom was given, we cannot establish

structural details of the anion in $[Cu(NH_3)_2Ag(SCN)_3]$ with any degree of certainty.

The Ag—Se distances in (**2**) fall well within the region reported for similar compounds (Perras *et al.*, 2018; Nahra *et al.*, 2018). Remarkably, at least for the neutral compounds, the distances do not depend on whether the coordination number around the silver is 3 or 4: In *N*,*N*-dimesitylselenoimidazole–silver nitrate, the Ag—Se bond lengths range from 2.65 to 2.68 Å for the four-coordinate atom and from 2.63 to 2.71 for the three-coordinate atom (Perras *et al.*, 2018).

A comparison with the compounds reported by Kimani *et al.* (2011) shows a remarkable impact of the cyanide anion on the Cu—Se bond length compared with the corresponding halides. For threefold-coordinated Cu, the distances between Cu and nonbridging Se range from 2.33 to 2.35 Å, whereas both of them in (**3**) are about 2.39 Å (Table 1). This is closer to the Cu—μ-Se distances (2.41–2.42 Å) reported by Kimani *et al.* (2011). In other words, cyanide is the better ligand for Cu^{I} when compared with halides, and as a result relatively long Cu—Se distances are observed for cyanide derivative (**3**).

5. Synthesis and crystallization

5.1. $[NHC^*_2Ag]_2[Ag(SCN)_3]\cdot 2Et_2O$, (1)

1,3-Dibenzyl-4,5-diphenylimidazolium bromide (481 mg, 1.00 mmol), silver oxide (116 mg, 0.500 mmol) and potassium thiocyanate (107 mg, 1.10 mmol) were suspended in dichloromethane (35 ml). After stirring for 20 h under reflux, the solution was filtered and the volume of the solvent was reduced to approximately 5 ml. Pentane (40 ml) was then added and a colourless solid precipitated. The product was filtered off, washed with pentane and dried *in vacuo* (yield: 366 mg, 0.647 mmol, 65%) as a colourless powder. ^{1}H NMR (300 MHz, $CDCl_3$): δ 1.60 (*s*, 2H, H_2O), 5.49 (*s*, 4H, C_{aliph}—H), 6.90–7.43 (*m*, 20H, C_{ar}—H). IR (ATR, cm^{-1}): 3028 [$\nu(CH_{ar})$], 2924 [$\nu(CH_{aliph})$], 2053 [ν(S—C≡N)], 1445, 1348, 1021, 764, 731, 696. Elemental analysis calculated (%): C 63.61, H 4.27, N 7.42; found: C 64.52, H 4.69, N 6.64.

Diethyl ether was diffused into a saturated solution of the crude product in THF; from this solution, that was kept for 10 d at 277 K, the title compound $[NHC^*_2Ag]_2[Ag(SCN)_3]$ crystallized in the form of needles of the diethyl ether disolvate.

5.2. $(NHC^*Se)_4Ag_2Br_2\cdot 6CH_2Cl_2$, (2)

1,3-Dibenzyl-4,5-diphenylimidazolium bromide (481 mg, 1.00 mmol), silver oxide (116 mg, 0.500 mmol) and potassium selenocyanate (159 mg, 1.10 mmol) were suspended in 35 ml of dichloromethane. After stirring for 20 h under reflux, the solution was filtered and the volume of the solvent was reduced to approximately 5 ml. Then 40 ml of pentane were added and a yellow solid precipitated. The product was filtered off, washed with pentane and dried *in vacuo* (yield: 365 mg, 0.159 mmol, 64%) as a yellow powder. ^{1}H NMR (300 MHz, $CDCl_3$): δ 5.23–5.57 (*m*, 16H, C_{aliph}—H), 6.77–7.43 (*m*, 80H, C_{ar}—H). IR (ATR, cm^{-1}): 3029 [$\nu(CH_{ar})$], 2926 [$\nu(CH_{aliph})$], 1447, 1402, 764, 732, 696, 520. Elemental analysis calculated (%): C 59.08, H 4.15, N 4.71; found: C 58.39, H 3.86, N 5.08.

A saturated solution of the compound in dichloromethane was prepared at 313 K; from this solution, that was kept for 7 d at 253 K, the title compound $(NHC^*Se)_4Ag_2Br_2$ crystallized as clear pale-yellow block-like prisms of the dichloromethane hexasolvate.

5.3. NHC*Se—CuCN·CH_3CN, (3)

(1,3-Dibenzyl-4,5-diphenylimidazol-2-ylidene)copper(I) bromide (270 mg, 0.50 mmol) and potassium selenocyanate (72 mg, 0.50 mmol) were suspended in 15 ml of dichloromethane followed by 5 ml of water. After stirring for 16 h at room temperature (*ca* 295K) under nitrogen, the solutions were filtered and the two phases separated. The aqueous phase was washed with dichloromethane (2 × 10 ml) and the organic phase was washed with deionized water (2 × 10 ml). The organic phases were combined and dried over magnesium sulfate. The volume of the solvent was reduced to approximately 5 ml before 20 ml of pentane were added and a colourless solid precipitated. The product was filtered off, washed with pentane and dried *in vacuo* (yield: 121 mg, 0.212 mmol, 42%) as a colourless powder. ^{1}H NMR (300MHz, $CDCl_3$): δ 7.29–6.97 (*m*, 20H, CH_{arom}), 5.50 (*s*, 4H, $CH_{2benzyl}$). IR (ATR, cm^{-1}): 3048 (*w*), 2105 (*s*) (ν_{CN}), 1445 (*m*, *v*), 695 (*s*). M.p. 368 K. Elemental analysis calculated (%) for $C_{30}H_{25}N_3CuSe$: C 63.21, H 4.97, N 7.37; found: C 61.68, H 4.06, N 7.11.

Pentane was diffused into a saturated solution of the crude product in dichloromethane/acetonitrile 1:1 (*v*:*v*). From this solution, kept for 10 d at 277 K, the title compound $[(NHC^*Se)CuCN]_\infty$ crystallized as needles of the acetonitrile solvate.

6. Refinement details

Crystal data, data collection and structure refinement details are summarized in Table 3. H atoms were placed at calculated positions and treated as riders, with U_{iso} values set at $1.2U_{eq}$ or $1.5U_{eq}$ of their respective bonding partners.

In the crystal structure of (**1**), one of the phenyl groups was refined as partially disordered over two positions rotated against each other around the *ipso–para* axis [occupancy ratio 0.55 (2):0.45 (2)]. In the crystal structure of (**2**), one of the dichoromethane solvent molecules was refined over two positions [ratio 0.898 (4):0.102 (4)] due to positional disorder around one C—Cl bond.

The SQUEEZE procedure (Spek, 2015) in *PLATON* was used to treat regions of disordered solvent molecules in (**1**) and (**2**) which could not be modelled in terms of atomic sites. In (**1**), the number of electrons found in these regions in the unit cell, 82, was assigned to two diethyl ether solvent molecules (ideal 84 electrons). In (**2**), 84 electrons were found and assigned to two solvent molecules of dichloromethane in the unit cell (ideal 84 electrons). Since $Z = 2$ for (**1**) and $Z = 1$ for (**2**), one solvent molecule of diethyl ether in (**1**) and two

solvent molecules of dichloromethane in (**2**) are missing in the final models and the given chemical formulae and other crystal data given in Table 3 take into account these solvent molecules.

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supporting information

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Unexpected reactions of NHC*—Cu^{I} and —Ag^{I} bromides with potassium thio- or selenocyanate

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Computing details

For all structures, data collection: *CrysAlis PRO* (Rigaku OD, 2015); cell refinement: *CrysAlis PRO* (Rigaku OD, 2015); data reduction: *CrysAlis PRO* (Rigaku OD, 2015); program(s) used to solve structure: SHELXT (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015b); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Bis[bis(1,3-dibenzyl-4,5-diphenylimidazol-2-ylidene)silver(I)] tris(thiocyanato)argentate(I) diethyl ether disolvate (1)

Crystal data

$[Ag(C_{29}H_{24}N_2)_2][Ag(NCS)_3]\cdot 2C_4H_{10}O$
M_r = 2248.09
Triclinic, $P\overline{1}$
a = 14.86462 (8) Å
b = 19.3714 (1) Å
c = 19.85451 (9) Å
α = 102.7710 (4)°
β = 100.8268 (4)°
γ = 99.5778 (4)°
V = 5345.84 (5) Å^3
Z = 2
$F(000)$ = 2320
D_x = 1.397 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 59132 reflections
θ = 3.7–76.7°
μ = 5.37 mm^{-1}
T = 100 K
Needle, colourless
0.32 × 0.06 × 0.04 mm

Data collection

Rigaku SuperNova, Dual, Cu at zero, Atlas diffractometer
Radiation source: micro-focus sealed X-ray tube
Detector resolution: 10.3196 pixels mm^{-1}
ω scans
Absorption correction: gaussian (CrysAlis PRO; Rigaku OD, 2015)
T_{min} = 0.437, T_{max} = 0.848
140384 measured reflections
22376 independent reflections
19576 reflections with $I > 2\sigma(I)$
R_{int} = 0.045
θ_{max} = 76.9°, θ_{min} = 3.4°
h = −18→17
k = −24→24
l = −24→25

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.080
S = 1.03
22376 reflections
1309 parameters
0 restraints
Primary atom site location: heavy-atom method
Secondary atom site location: other
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0438P)^2 + 3.189P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.003$

$\Delta\rho_{max} = 0.98$ e Å^{-3}
$\Delta\rho_{min} = -1.13$ 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. The structure was first solved by the Patterson method as implemented in SHELXS. The three silver atoms and one sulfur atom were located. The result was subjected to the Tangens Expansion formula as implemented in SHELXS. Almost all non-hydrogen atoms were located. The remainder was found in the difference fourier map from SHELXL refinements. The PLATON SQUEEZE procedure (A. L. Spek. Acta Cryst. C71, 2015, 9-18) was used to treat regions of disordered solvent which could not be modelled in terms of atomic sites. The number of electrons found in these regions, 82, was assigned to 2 molecules of diethylether. 2 diethylethers would give 84 electrons.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Ag1	0.98105 (2)	0.78382 (2)	−0.03379 (2)	0.02968 (4)	
C1	1.21022 (18)	0.70910 (14)	−0.00838 (13)	0.0331 (5)	
H1	1.2339	0.7517	0.0297	0.040*	
C2	1.2083 (2)	0.64179 (15)	0.00485 (16)	0.0424 (6)	
H2	1.2296	0.6383	0.0519	0.051*	
C3	1.1753 (2)	0.57962 (15)	−0.05035 (18)	0.0507 (7)	
H3	1.1755	0.5334	−0.0415	0.061*	
C4	1.1422 (2)	0.58496 (15)	−0.11839 (18)	0.0519 (7)	
H4	1.1180	0.5423	−0.1562	0.062*	
C5	1.14406 (19)	0.65222 (14)	−0.13158 (13)	0.0364 (5)	
H5	1.1221	0.6555	−0.1787	0.044*	
C6	1.17778 (15)	0.71508 (12)	−0.07678 (11)	0.0252 (4)	
C7	1.17739 (17)	0.78740 (12)	−0.09409 (11)	0.0266 (4)	
H7A	1.2299	0.7994	−0.1166	0.032*	
H7B	1.1181	0.7839	−0.1284	0.032*	
N1	1.18670 (13)	0.84520 (10)	−0.03008 (9)	0.0227 (3)	
C8	1.11579 (15)	0.85001 (12)	0.00299 (11)	0.0249 (4)	
C9	1.27183 (15)	0.88709 (11)	0.01320 (11)	0.0222 (4)	
C10	1.36079 (17)	0.89170 (12)	−0.01006 (13)	0.0295 (5)	
C11	1.3764 (2)	0.92388 (17)	−0.06298 (14)	0.0426 (6)	
H11	1.3296	0.9450	−0.0850	0.051*	
C12	1.4622 (2)	0.9258 (2)	−0.08513 (16)	0.0554 (9)	
H12	1.4715	0.9461	−0.1234	0.066*	
C13	1.5306 (3)	0.8988 (2)	−0.0515 (2)	0.0630 (9)	
H13	1.5880	0.9003	−0.0662	0.076*	
C14	1.5177 (3)	0.8688 (2)	0.0043 (3)	0.0773 (13)	
H14	1.5669	0.8513	0.0285	0.093*	
C15	1.4337 (2)	0.8643 (2)	0.0246 (2)	0.0573 (9)	
H15	1.4246	0.8427	0.0620	0.069*	
C16	1.25234 (14)	0.92016 (11)	0.07505 (11)	0.0226 (4)	

C17	1.31529 (15)	0.96909 (12)	0.14136 (11)	0.0256 (4)
C18	1.31124 (18)	1.04121 (14)	0.16332 (13)	0.0344 (5)
H18	1.2679	1.0604	0.1351	0.041*
C19	1.3699 (2)	1.08602 (16)	0.22635 (14)	0.0423 (6)
H19	1.3666	1.1355	0.2406	0.051*
C20	1.4316 (2)	1.05965 (17)	0.26750 (14)	0.0467 (7)
H20	1.4726	1.0908	0.3098	0.056*
C21	1.4348 (3)	0.9874 (2)	0.24781 (18)	0.0632 (10)
H21	1.4764	0.9684	0.2776	0.076*
C22	1.3773 (2)	0.94223 (17)	0.18435 (17)	0.0533 (8)
H22	1.3808	0.8927	0.1706	0.064*
N2	1.15577 (13)	0.89728 (10)	0.06686 (9)	0.0247 (4)
C23	1.10662 (16)	0.91377 (14)	0.12398 (12)	0.0326 (5)
H23A	1.0382	0.8958	0.1046	0.039*
H23B	1.1189	0.9669	0.1437	0.039*
C24	1.13906 (18)	0.87875 (14)	0.18219 (13)	0.0343 (5)
C25	1.1708 (2)	0.92001 (16)	0.25172 (14)	0.0421 (6)
H25	1.1703	0.9702	0.2630	0.051*
C26	1.2033 (3)	0.88852 (19)	0.30501 (15)	0.0544 (8)
H26	1.2244	0.9171	0.3528	0.065*
C27	1.2051 (3)	0.8163 (2)	0.28929 (18)	0.0653 (10)
H27	1.2287	0.7951	0.3259	0.078*
C28	1.1725 (3)	0.77426 (18)	0.21979 (18)	0.0627 (10)
H28	1.1735	0.7241	0.2087	0.075*
C29	1.1384 (2)	0.80514 (15)	0.16650 (15)	0.0467 (7)
H29	1.1146	0.7760	0.1191	0.056*
C30	0.7594 (2)	0.86196 (16)	0.02635 (14)	0.0430 (6)
H30	0.7151	0.8203	0.0260	0.052*
C31	0.7872 (3)	0.9201 (2)	0.08573 (18)	0.0684 (11)
H31	0.7614	0.9181	0.1257	0.082*
C32	0.8500 (4)	0.9794 (2)	0.0880 (2)	0.0846 (17)
H32	0.8678	1.0193	0.1290	0.102*
C33	0.8881 (3)	0.98228 (17)	0.0312 (3)	0.0818 (16)
H33	0.9329	1.0242	0.0331	0.098*
C34	0.8622 (2)	0.92402 (15)	−0.03031 (18)	0.0521 (8)
H34	0.8898	0.9259	−0.0695	0.063*
C35	0.79556 (17)	0.86395 (12)	−0.03230 (12)	0.0312 (5)
C36	0.76054 (18)	0.80201 (12)	−0.09808 (11)	0.0297 (5)
H36A	0.6947	0.8014	−0.1199	0.036*
H36B	0.7986	0.8093	−0.1328	0.036*
N3	0.76572 (13)	0.73222 (10)	−0.08206 (9)	0.0238 (4)
C37	0.84843 (15)	0.71588 (12)	−0.05818 (11)	0.0252 (4)
C38	0.68993 (15)	0.67697 (11)	−0.08559 (10)	0.0220 (4)
C39	0.59068 (15)	0.67846 (11)	−0.11029 (11)	0.0233 (4)
C40	0.55652 (17)	0.68480 (13)	−0.17863 (11)	0.0288 (5)
H40	0.5977	0.6885	−0.2095	0.035*
C41	0.46292 (18)	0.68568 (15)	−0.20165 (13)	0.0358 (5)
H41	0.4404	0.6901	−0.2482	0.043*

C42	0.40217 (18)	0.68017 (16)	−0.15754 (15)	0.0404 (6)	
H42	0.3382	0.6813	−0.1734	0.049*	
C43	0.4349 (2)	0.67302 (18)	−0.08997 (15)	0.0450 (7)	
H43	0.3931	0.6687	−0.0596	0.054*	
C44	0.52835 (18)	0.67213 (15)	−0.06656 (13)	0.0344 (5)	
H44	0.5502	0.6672	−0.0201	0.041*	
C45	0.72822 (15)	0.62438 (12)	−0.06349 (11)	0.0231 (4)	
C46	0.68002 (15)	0.55211 (12)	−0.06161 (11)	0.0250 (4)	
C47A	0.6756 (10)	0.4947 (3)	−0.1191 (3)	0.0382 (19)	0.55 (2)
H47A	0.7054	0.5019	−0.1561	0.046*	0.55 (2)
C48A	0.6263 (11)	0.4262 (4)	−0.1213 (4)	0.047 (2)	0.55 (2)
H48A	0.6223	0.3858	−0.1598	0.057*	0.55 (2)
C47B	0.6300 (10)	0.4998 (4)	−0.1238 (4)	0.030 (2)	0.45 (2)
H47B	0.6306	0.5101	−0.1683	0.036*	0.45 (2)
C48B	0.5799 (10)	0.4335 (4)	−0.1225 (4)	0.035 (2)	0.45 (2)
H48B	0.5449	0.3999	−0.1657	0.042*	0.45 (2)
C49	0.5803 (2)	0.41677 (14)	−0.06271 (16)	0.0413 (6)	
H49A	0.5496	0.3695	−0.0633	0.050*	0.45 (2)
H49	0.5445	0.3710	−0.0637	0.050*	0.55 (2)
C50A	0.5907 (9)	0.4743 (5)	−0.0091 (7)	0.046 (2)	0.55 (2)
H50A	0.5638	0.4690	0.0297	0.056*	0.55 (2)
C51A	0.6397 (9)	0.5417 (5)	−0.0082 (6)	0.0385 (19)	0.55 (2)
H51A	0.6451	0.5817	0.0310	0.046*	0.55 (2)
C50B	0.6251 (10)	0.4670 (7)	0.0033 (6)	0.039 (2)	0.45 (2)
H50B	0.6214	0.4548	0.0467	0.046*	0.45 (2)
C51B	0.6748 (9)	0.5350 (6)	0.0034 (5)	0.032 (2)	0.45 (2)
H51B	0.7052	0.5696	0.0472	0.038*	0.45 (2)
N4	0.82539 (13)	0.64955 (10)	−0.04759 (9)	0.0253 (4)	
C52	0.89538 (16)	0.60961 (13)	−0.02429 (12)	0.0309 (5)	
H52A	0.9519	0.6241	−0.0418	0.037*	
H52B	0.8699	0.5572	−0.0464	0.037*	
C53	0.92407 (16)	0.62147 (12)	0.05521 (12)	0.0275 (4)	
C54	0.9906 (2)	0.58529 (14)	0.08136 (15)	0.0407 (6)	
H54	1.0179	0.5561	0.0493	0.049*	
C55	1.0175 (2)	0.59117 (17)	0.15341 (17)	0.0513 (8)	
H55	1.0625	0.5658	0.1706	0.062*	
C56	0.9789 (2)	0.6341 (2)	0.20018 (17)	0.0566 (9)	
H56	0.9965	0.6376	0.2496	0.068*	
C57	0.9145 (2)	0.6719 (2)	0.17531 (16)	0.0555 (8)	
H57	0.8892	0.7025	0.2077	0.067*	
C58	0.88663 (18)	0.66519 (17)	0.10261 (13)	0.0387 (6)	
H58	0.8418	0.6907	0.0856	0.046*	
Ag2	0.75371 (2)	0.69309 (2)	0.54662 (2)	0.01911 (4)	
C59	0.76475 (15)	0.50709 (11)	0.46307 (11)	0.0225 (4)	
H59	0.8247	0.5304	0.4598	0.027*	
C60	0.69686 (16)	0.46941 (12)	0.40157 (11)	0.0260 (4)	
H60	0.7108	0.4670	0.3564	0.031*	
C61	0.60914 (16)	0.43546 (12)	0.40584 (12)	0.0263 (4)	

H61	0.5633	0.4095	0.3638	0.032*
C62	0.58851 (16)	0.43949 (12)	0.47170 (12)	0.0274 (4)
H62	0.5282	0.4166	0.4747	0.033*
C63	0.65595 (15)	0.47693 (12)	0.53319 (11)	0.0249 (4)
H63	0.6416	0.4796	0.5782	0.030*
C64	0.74483 (14)	0.51063 (10)	0.52924 (11)	0.0198 (4)
C65	0.81645 (14)	0.54679 (11)	0.59853 (10)	0.0199 (4)
H65A	0.7839	0.5696	0.6337	0.024*
H65B	0.8430	0.5090	0.6165	0.024*
N5	0.89381 (11)	0.60198 (9)	0.59393 (8)	0.0176 (3)
C66	0.88138 (14)	0.66826 (11)	0.58793 (10)	0.0183 (4)
C67	0.98878 (14)	0.60157 (11)	0.61353 (10)	0.0180 (4)
C68	1.02285 (14)	0.53624 (11)	0.62232 (10)	0.0190 (4)
C69	0.98347 (14)	0.46886 (11)	0.57308 (11)	0.0218 (4)
H69	0.9343	0.4652	0.5334	0.026*
C70	1.01597 (16)	0.40742 (11)	0.58206 (12)	0.0255 (4)
H70	0.9884	0.3619	0.5488	0.031*
C71	1.08858 (17)	0.41245 (12)	0.63940 (13)	0.0286 (5)
H71	1.1109	0.3705	0.6453	0.034*
C72	1.12857 (17)	0.47899 (13)	0.68824 (12)	0.0288 (5)
H72	1.1782	0.4825	0.7276	0.035*
C73	1.09603 (15)	0.54048 (12)	0.67962 (11)	0.0239 (4)
H73	1.1239	0.5859	0.7131	0.029*
C74	1.03660 (14)	0.66983 (10)	0.62029 (10)	0.0176 (4)
C75	1.13793 (14)	0.70362 (10)	0.64412 (10)	0.0190 (4)
C76	1.20124 (15)	0.68387 (11)	0.60387 (11)	0.0229 (4)
H76	1.1799	0.6467	0.5607	0.027*
C77	1.29550 (15)	0.71837 (12)	0.62661 (12)	0.0262 (4)
H77	1.3383	0.7049	0.5988	0.031*
C78	1.32722 (15)	0.77236 (12)	0.68963 (13)	0.0278 (4)
H78	1.3915	0.7963	0.7047	0.033*
C79	1.26479 (16)	0.79140 (12)	0.73066 (11)	0.0265 (4)
H79	1.2868	0.8279	0.7743	0.032*
C80	1.17026 (15)	0.75747 (11)	0.70843 (11)	0.0231 (4)
H80	1.1278	0.7707	0.7367	0.028*
N6	0.96896 (11)	0.70968 (9)	0.60418 (8)	0.0174 (3)
C81	0.98813 (14)	0.78589 (10)	0.60104 (10)	0.0203 (4)
H81A	1.0433	0.8135	0.6395	0.024*
H81B	0.9337	0.8070	0.6093	0.024*
C82	1.00677 (15)	0.79387 (10)	0.53060 (11)	0.0208 (4)
C83	1.09775 (16)	0.80758 (12)	0.52096 (12)	0.0266 (4)
H83	1.1495	0.8135	0.5595	0.032*
C84	1.11334 (18)	0.81269 (13)	0.45497 (14)	0.0337 (5)
H84	1.1756	0.8219	0.4487	0.040*
C85	1.0382 (2)	0.80441 (14)	0.39856 (13)	0.0379 (6)
H85	1.0488	0.8070	0.3534	0.045*
C86	0.9477 (2)	0.79239 (15)	0.40830 (13)	0.0377 (6)
H86	0.8961	0.7876	0.3699	0.045*

C87	0.93200 (17)	0.78729 (13)	0.47376 (12)	0.0293 (5)
H87	0.8696	0.7792	0.4800	0.035*
C88	0.66481 (17)	0.64638 (13)	0.33252 (12)	0.0301 (5)
H88	0.6923	0.6888	0.3701	0.036*
C89	0.6978 (2)	0.63552 (17)	0.27051 (13)	0.0405 (6)
H89	0.7481	0.6703	0.2662	0.049*
C90	0.6575 (2)	0.57434 (18)	0.21551 (14)	0.0491 (7)
H90	0.6797	0.5672	0.1732	0.059*
C91	0.5850 (3)	0.52357 (17)	0.22198 (14)	0.0540 (8)
H91	0.5574	0.4813	0.1842	0.065*
C92	0.5522 (2)	0.53423 (14)	0.28367 (13)	0.0412 (6)
H92	0.5020	0.4993	0.2878	0.049*
C93	0.59255 (16)	0.59583 (12)	0.33951 (11)	0.0246 (4)
C94	0.55979 (15)	0.60271 (11)	0.40821 (11)	0.0214 (4)
H94A	0.4955	0.5727	0.3977	0.026*
H94B	0.6012	0.5830	0.4408	0.026*
N7	0.55944 (12)	0.67719 (9)	0.44431 (8)	0.0182 (3)
C95	0.63428 (14)	0.72101 (11)	0.49374 (10)	0.0186 (4)
C96	0.48627 (14)	0.71328 (11)	0.43243 (10)	0.0202 (4)
C97	0.38961 (14)	0.67823 (11)	0.39126 (11)	0.0230 (4)
C98	0.36889 (17)	0.63429 (14)	0.32221 (12)	0.0321 (5)
H98	0.4179	0.6280	0.2984	0.039*
C99	0.27620 (19)	0.59946 (15)	0.28787 (14)	0.0408 (6)
H99	0.2625	0.5686	0.2412	0.049*
C100	0.20452 (17)	0.60977 (14)	0.32153 (15)	0.0395 (6)
H100	0.1417	0.5856	0.2981	0.047*
C101	0.22370 (16)	0.65493 (13)	0.38890 (15)	0.0357 (5)
H101	0.1740	0.6632	0.4114	0.043*
C102	0.31620 (16)	0.68858 (12)	0.42410 (13)	0.0292 (5)
H102	0.3293	0.7189	0.4710	0.035*
C103	0.51846 (14)	0.78202 (11)	0.47479 (10)	0.0198 (4)
C104	0.46956 (14)	0.84285 (11)	0.48426 (11)	0.0230 (4)
C105	0.43043 (16)	0.85935 (12)	0.54279 (12)	0.0276 (4)
H105	0.4387	0.8338	0.5784	0.033*
C106	0.37929 (18)	0.91328 (14)	0.54867 (14)	0.0365 (5)
H106	0.3520	0.9244	0.5883	0.044*
C107	0.3679 (2)	0.95088 (15)	0.49722 (17)	0.0437 (6)
H107	0.3328	0.9877	0.5015	0.052*
C108	0.4073 (2)	0.93514 (17)	0.43954 (18)	0.0477 (7)
H108	0.3997	0.9614	0.4044	0.057*
C109	0.45788 (19)	0.88118 (14)	0.43285 (14)	0.0360 (5)
H109	0.4847	0.8703	0.3930	0.043*
N8	0.60883 (12)	0.78514 (9)	0.51169 (8)	0.0188 (3)
C110	0.67195 (14)	0.84941 (11)	0.56130 (10)	0.0212 (4)
H11A	0.7090	0.8347	0.6005	0.025*
H11B	0.6342	0.8823	0.5821	0.025*
C111	0.73840 (14)	0.89022 (11)	0.52734 (11)	0.0214 (4)
C112	0.81556 (17)	0.94234 (12)	0.57147 (12)	0.0294 (5)

H112	0.8272	0.9490	0.6214	0.035*
C113	0.87523 (19)	0.98436 (14)	0.54315 (15)	0.0394 (6)
H113	0.9270	1.0201	0.5738	0.047*
C114	0.85991 (19)	0.97460 (14)	0.47042 (16)	0.0394 (6)
H114	0.9006	1.0039	0.4511	0.047*
C115	0.78475 (18)	0.92178 (14)	0.42575 (13)	0.0333 (5)
H115	0.7748	0.9142	0.3757	0.040*
C116	0.72393 (16)	0.87995 (12)	0.45408 (12)	0.0258 (4)
H116	0.6723	0.8442	0.4233	0.031*
Ag3	0.79941 (2)	0.72828 (2)	0.71384 (2)	0.02795 (4)
S1	0.64189 (4)	0.65134 (3)	0.65701 (3)	0.02631 (10)
C117	0.57874 (15)	0.71425 (12)	0.64988 (11)	0.0240 (4)
N9	0.53253 (14)	0.75603 (11)	0.64467 (11)	0.0297 (4)
S2	0.84839 (4)	0.86528 (3)	0.74115 (3)	0.03126 (12)
C118	0.96150 (18)	0.86638 (12)	0.77086 (12)	0.0295 (5)
N10	1.04011 (16)	0.86674 (12)	0.79091 (13)	0.0412 (5)
S3	0.93489 (4)	0.69294 (3)	0.78243 (3)	0.02904 (11)
C119	0.89197 (18)	0.61118 (13)	0.79230 (12)	0.0322 (5)
N11	0.8653 (2)	0.55532 (13)	0.80169 (13)	0.0496 (6)
C120	0.9168 (4)	0.8774 (4)	0.2474 (3)	0.136 (3)
H12A	0.8818	0.8463	0.2708	0.204*
H12B	0.9833	0.8758	0.2591	0.204*
H12C	0.8922	0.8603	0.1958	0.204*
C121	0.9060 (3)	0.9548 (4)	0.2729 (2)	0.099 (2)
H12D	0.9371	0.9747	0.3239	0.119*
H12E	0.9350	0.9858	0.2458	0.119*
O1	0.81017 (17)	0.95296 (14)	0.26223 (11)	0.0551 (5)
C122	0.7881 (4)	1.0237 (2)	0.2809 (2)	0.0799 (14)
H12F	0.8157	1.0552	0.2536	0.096*
H12G	0.8141	1.0469	0.3322	0.096*
C123	0.6848 (4)	1.0135 (2)	0.2638 (3)	0.0803 (14)
H12H	0.6600	0.9920	0.2127	0.120*
H12I	0.6678	1.0606	0.2773	0.120*
H12J	0.6581	0.9812	0.2901	0.120*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.02005 (8)	0.03206 (9)	0.02983 (8)	−0.00063 (6)	0.00112 (6)	0.00219 (6)
C1	0.0323 (12)	0.0319 (12)	0.0317 (11)	0.0030 (10)	0.0026 (9)	0.0088 (9)
C2	0.0401 (15)	0.0414 (14)	0.0482 (15)	0.0082 (12)	0.0044 (12)	0.0220 (12)
C3	0.0563 (19)	0.0295 (13)	0.069 (2)	0.0084 (12)	0.0133 (15)	0.0201 (13)
C4	0.062 (2)	0.0268 (13)	0.0566 (17)	0.0042 (13)	0.0075 (15)	0.0003 (12)
C5	0.0387 (14)	0.0317 (12)	0.0320 (12)	0.0053 (10)	0.0048 (10)	−0.0007 (10)
C6	0.0200 (10)	0.0262 (10)	0.0272 (10)	0.0038 (8)	0.0049 (8)	0.0039 (8)
C7	0.0324 (12)	0.0255 (10)	0.0180 (9)	0.0041 (9)	0.0037 (8)	0.0015 (8)
N1	0.0224 (9)	0.0235 (8)	0.0191 (8)	0.0029 (7)	0.0026 (7)	0.0029 (6)
C8	0.0208 (10)	0.0271 (10)	0.0235 (10)	0.0031 (8)	0.0027 (8)	0.0033 (8)

C9	0.0197 (10)	0.0222 (9)	0.0224 (9)	0.0023 (8)	0.0028 (8)	0.0047 (7)
C10	0.0263 (11)	0.0249 (10)	0.0349 (11)	0.0015 (9)	0.0135 (9)	0.0006 (9)
C11	0.0337 (14)	0.0584 (17)	0.0352 (13)	0.0010 (12)	0.0091 (10)	0.0169 (12)
C12	0.0501 (18)	0.068 (2)	0.0377 (14)	−0.0167 (16)	0.0157 (13)	0.0104 (14)
C13	0.0454 (18)	0.060 (2)	0.093 (3)	0.0130 (16)	0.0425 (19)	0.0166 (19)
C14	0.046 (2)	0.085 (3)	0.135 (4)	0.0338 (19)	0.046 (2)	0.063 (3)
C15	0.0392 (16)	0.065 (2)	0.089 (2)	0.0229 (15)	0.0283 (16)	0.0452 (19)
C16	0.0175 (10)	0.0250 (10)	0.0227 (9)	0.0016 (8)	0.0046 (8)	0.0036 (8)
C17	0.0201 (10)	0.0302 (11)	0.0216 (9)	−0.0008 (8)	0.0038 (8)	0.0022 (8)
C18	0.0320 (12)	0.0346 (12)	0.0287 (11)	0.0054 (10)	0.0024 (9)	−0.0027 (9)
C19	0.0379 (14)	0.0408 (14)	0.0337 (13)	−0.0011 (11)	0.0046 (11)	−0.0093 (11)
C20	0.0368 (14)	0.0554 (17)	0.0295 (12)	−0.0097 (13)	−0.0041 (10)	−0.0020 (11)
C21	0.055 (2)	0.061 (2)	0.0525 (18)	0.0052 (16)	−0.0274 (15)	0.0109 (15)
C22	0.0471 (17)	0.0408 (15)	0.0533 (17)	0.0046 (13)	−0.0198 (14)	0.0044 (13)
N2	0.0189 (9)	0.0286 (9)	0.0231 (8)	0.0021 (7)	0.0052 (7)	0.0019 (7)
C23	0.0227 (11)	0.0401 (13)	0.0298 (11)	0.0012 (9)	0.0117 (9)	−0.0021 (9)
C24	0.0317 (12)	0.0361 (13)	0.0306 (11)	−0.0052 (10)	0.0163 (10)	0.0013 (9)
C25	0.0488 (16)	0.0429 (14)	0.0308 (12)	0.0014 (12)	0.0169 (11)	0.0015 (11)
C26	0.073 (2)	0.0573 (19)	0.0298 (13)	0.0016 (16)	0.0200 (14)	0.0077 (12)
C27	0.102 (3)	0.060 (2)	0.0434 (16)	0.007 (2)	0.0323 (18)	0.0267 (15)
C28	0.102 (3)	0.0379 (16)	0.0513 (17)	−0.0022 (17)	0.0335 (19)	0.0163 (13)
C29	0.0625 (19)	0.0358 (14)	0.0361 (13)	−0.0103 (13)	0.0218 (13)	0.0046 (11)
C30	0.0438 (15)	0.0458 (15)	0.0346 (13)	0.0136 (12)	0.0040 (11)	0.0024 (11)
C31	0.082 (3)	0.070 (2)	0.0405 (16)	0.041 (2)	−0.0061 (16)	−0.0142 (16)
C32	0.103 (3)	0.0426 (19)	0.070 (3)	0.036 (2)	−0.050 (3)	−0.0195 (18)
C33	0.077 (3)	0.0232 (14)	0.105 (3)	−0.0062 (15)	−0.058 (3)	0.0122 (17)
C34	0.0423 (16)	0.0340 (14)	0.0654 (19)	−0.0093 (12)	−0.0200 (14)	0.0238 (13)
C35	0.0315 (12)	0.0228 (10)	0.0330 (11)	0.0024 (9)	−0.0048 (9)	0.0076 (9)
C36	0.0367 (13)	0.0270 (11)	0.0233 (10)	0.0010 (9)	0.0017 (9)	0.0110 (8)
N3	0.0248 (9)	0.0221 (8)	0.0206 (8)	−0.0003 (7)	0.0020 (7)	0.0046 (6)
C37	0.0215 (10)	0.0283 (11)	0.0212 (9)	0.0006 (8)	0.0026 (8)	0.0024 (8)
C38	0.0223 (10)	0.0224 (10)	0.0193 (9)	0.0021 (8)	0.0032 (7)	0.0047 (7)
C39	0.0236 (10)	0.0215 (10)	0.0241 (10)	0.0051 (8)	0.0038 (8)	0.0055 (8)
C40	0.0284 (11)	0.0362 (12)	0.0222 (10)	0.0102 (9)	0.0050 (8)	0.0067 (9)
C41	0.0316 (13)	0.0481 (15)	0.0285 (11)	0.0157 (11)	0.0014 (9)	0.0106 (10)
C42	0.0241 (12)	0.0563 (16)	0.0450 (14)	0.0175 (11)	0.0054 (10)	0.0175 (12)
C43	0.0320 (14)	0.071 (2)	0.0445 (14)	0.0209 (13)	0.0181 (11)	0.0255 (14)
C44	0.0318 (13)	0.0485 (14)	0.0300 (11)	0.0148 (11)	0.0103 (9)	0.0172 (10)
C45	0.0216 (10)	0.0262 (10)	0.0205 (9)	0.0053 (8)	0.0037 (8)	0.0050 (8)
C46	0.0237 (10)	0.0252 (10)	0.0264 (10)	0.0076 (8)	0.0023 (8)	0.0087 (8)
C47A	0.051 (6)	0.030 (3)	0.032 (3)	0.004 (3)	0.008 (3)	0.0094 (19)
C48A	0.069 (7)	0.023 (3)	0.039 (3)	0.003 (3)	−0.004 (3)	0.007 (2)
C47B	0.037 (5)	0.026 (3)	0.025 (3)	0.002 (3)	0.003 (3)	0.008 (2)
C48B	0.043 (5)	0.023 (3)	0.032 (3)	0.003 (3)	0.001 (3)	0.002 (2)
C49	0.0378 (14)	0.0285 (12)	0.0535 (16)	0.0001 (10)	0.0000 (12)	0.0165 (11)
C50A	0.049 (6)	0.037 (3)	0.065 (5)	0.010 (4)	0.028 (5)	0.027 (3)
C51A	0.043 (5)	0.029 (3)	0.043 (4)	0.006 (3)	0.012 (4)	0.009 (3)
C50B	0.044 (6)	0.037 (4)	0.035 (4)	0.000 (4)	0.012 (4)	0.013 (3)

C51B	0.035 (5)	0.037 (4)	0.018 (3)	−0.007 (4)	0.003 (3)	0.008 (2)
N4	0.0211 (9)	0.0272 (9)	0.0237 (8)	0.0052 (7)	0.0012 (7)	0.0023 (7)
C52	0.0224 (11)	0.0345 (12)	0.0315 (11)	0.0105 (9)	−0.0001 (9)	0.0020 (9)
C53	0.0207 (10)	0.0269 (11)	0.0326 (11)	0.0009 (8)	0.0019 (8)	0.0099 (9)
C54	0.0360 (14)	0.0294 (12)	0.0478 (15)	0.0095 (10)	−0.0071 (11)	0.0045 (11)
C55	0.0502 (17)	0.0448 (16)	0.0539 (17)	0.0109 (13)	−0.0110 (14)	0.0216 (13)
C56	0.0475 (17)	0.090 (3)	0.0409 (15)	0.0136 (17)	0.0064 (13)	0.0389 (16)
C57	0.0427 (16)	0.099 (3)	0.0359 (14)	0.0271 (17)	0.0180 (12)	0.0252 (16)
C58	0.0291 (12)	0.0615 (17)	0.0331 (12)	0.0190 (12)	0.0101 (10)	0.0188 (12)
Ag2	0.01516 (7)	0.02111 (7)	0.02099 (7)	0.00652 (5)	0.00277 (5)	0.00464 (5)
C59	0.0174 (9)	0.0244 (10)	0.0258 (10)	0.0048 (8)	0.0069 (8)	0.0048 (8)
C60	0.0256 (11)	0.0266 (10)	0.0239 (10)	0.0059 (9)	0.0068 (8)	0.0015 (8)
C61	0.0241 (11)	0.0218 (10)	0.0271 (10)	0.0019 (8)	0.0019 (8)	0.0000 (8)
C62	0.0207 (10)	0.0269 (11)	0.0313 (11)	−0.0019 (8)	0.0057 (8)	0.0060 (9)
C63	0.0214 (10)	0.0267 (10)	0.0257 (10)	0.0010 (8)	0.0074 (8)	0.0066 (8)
C64	0.0171 (9)	0.0171 (9)	0.0247 (9)	0.0046 (7)	0.0045 (7)	0.0045 (7)
C65	0.0163 (9)	0.0213 (9)	0.0226 (9)	0.0034 (7)	0.0059 (7)	0.0063 (7)
N5	0.0148 (8)	0.0178 (8)	0.0195 (7)	0.0044 (6)	0.0031 (6)	0.0037 (6)
C66	0.0170 (9)	0.0207 (9)	0.0175 (8)	0.0058 (7)	0.0044 (7)	0.0040 (7)
C67	0.0160 (9)	0.0209 (9)	0.0172 (8)	0.0056 (7)	0.0047 (7)	0.0029 (7)
C68	0.0165 (9)	0.0198 (9)	0.0235 (9)	0.0063 (7)	0.0077 (7)	0.0072 (7)
C69	0.0182 (9)	0.0215 (9)	0.0261 (9)	0.0042 (8)	0.0064 (8)	0.0058 (8)
C70	0.0245 (11)	0.0193 (9)	0.0341 (11)	0.0055 (8)	0.0120 (9)	0.0048 (8)
C71	0.0297 (12)	0.0250 (10)	0.0395 (12)	0.0124 (9)	0.0147 (9)	0.0150 (9)
C72	0.0275 (11)	0.0328 (11)	0.0299 (11)	0.0122 (9)	0.0047 (9)	0.0138 (9)
C73	0.0236 (10)	0.0254 (10)	0.0230 (9)	0.0073 (8)	0.0044 (8)	0.0064 (8)
C74	0.0158 (9)	0.0202 (9)	0.0173 (8)	0.0067 (7)	0.0044 (7)	0.0035 (7)
C75	0.0163 (9)	0.0181 (9)	0.0222 (9)	0.0041 (7)	0.0033 (7)	0.0056 (7)
C76	0.0206 (10)	0.0190 (9)	0.0282 (10)	0.0059 (8)	0.0056 (8)	0.0035 (8)
C77	0.0198 (10)	0.0243 (10)	0.0373 (11)	0.0078 (8)	0.0109 (9)	0.0077 (9)
C78	0.0171 (10)	0.0258 (10)	0.0388 (12)	0.0025 (8)	0.0022 (8)	0.0103 (9)
C79	0.0243 (11)	0.0234 (10)	0.0258 (10)	0.0016 (8)	−0.0006 (8)	0.0021 (8)
C80	0.0204 (10)	0.0254 (10)	0.0223 (9)	0.0046 (8)	0.0055 (8)	0.0038 (8)
N6	0.0156 (8)	0.0181 (8)	0.0192 (7)	0.0057 (6)	0.0043 (6)	0.0045 (6)
C81	0.0209 (10)	0.0171 (9)	0.0227 (9)	0.0055 (7)	0.0052 (7)	0.0034 (7)
C82	0.0230 (10)	0.0157 (9)	0.0247 (9)	0.0051 (7)	0.0066 (8)	0.0054 (7)
C83	0.0250 (11)	0.0246 (10)	0.0315 (11)	0.0055 (8)	0.0071 (9)	0.0097 (8)
C84	0.0338 (13)	0.0337 (12)	0.0413 (13)	0.0085 (10)	0.0193 (10)	0.0160 (10)
C85	0.0512 (16)	0.0351 (13)	0.0322 (12)	0.0061 (11)	0.0168 (11)	0.0153 (10)
C86	0.0406 (14)	0.0409 (14)	0.0306 (12)	0.0025 (11)	0.0019 (10)	0.0170 (10)
C87	0.0255 (11)	0.0316 (11)	0.0327 (11)	0.0052 (9)	0.0051 (9)	0.0146 (9)
C88	0.0298 (12)	0.0352 (12)	0.0263 (10)	0.0080 (10)	0.0099 (9)	0.0065 (9)
C89	0.0397 (14)	0.0568 (17)	0.0314 (12)	0.0135 (12)	0.0169 (11)	0.0152 (11)
C90	0.067 (2)	0.0628 (19)	0.0240 (12)	0.0252 (16)	0.0191 (12)	0.0097 (12)
C91	0.086 (2)	0.0454 (16)	0.0249 (12)	0.0105 (16)	0.0151 (14)	−0.0025 (11)
C92	0.0588 (18)	0.0314 (13)	0.0261 (11)	0.0009 (12)	0.0077 (11)	0.0007 (9)
C93	0.0260 (11)	0.0257 (10)	0.0216 (9)	0.0085 (8)	0.0046 (8)	0.0041 (8)
C94	0.0208 (10)	0.0191 (9)	0.0238 (9)	0.0052 (7)	0.0052 (8)	0.0042 (7)

N7	0.0163 (8)	0.0189 (8)	0.0197 (7)	0.0052 (6)	0.0034 (6)	0.0050 (6)
C95	0.0173 (9)	0.0207 (9)	0.0193 (9)	0.0059 (7)	0.0058 (7)	0.0058 (7)
C96	0.0175 (9)	0.0218 (9)	0.0230 (9)	0.0069 (8)	0.0045 (7)	0.0079 (7)
C97	0.0175 (10)	0.0204 (9)	0.0300 (10)	0.0041 (8)	−0.0005 (8)	0.0096 (8)
C98	0.0248 (11)	0.0384 (13)	0.0283 (11)	0.0035 (10)	−0.0021 (9)	0.0082 (9)
C99	0.0340 (14)	0.0413 (14)	0.0355 (13)	−0.0008 (11)	−0.0102 (10)	0.0085 (11)
C100	0.0207 (11)	0.0328 (12)	0.0566 (16)	−0.0027 (9)	−0.0117 (10)	0.0182 (11)
C101	0.0169 (11)	0.0299 (12)	0.0615 (16)	0.0046 (9)	0.0062 (10)	0.0171 (11)
C102	0.0217 (11)	0.0245 (10)	0.0410 (12)	0.0052 (8)	0.0044 (9)	0.0096 (9)
C103	0.0168 (9)	0.0221 (9)	0.0206 (9)	0.0063 (7)	0.0023 (7)	0.0061 (7)
C104	0.0170 (9)	0.0224 (10)	0.0283 (10)	0.0062 (8)	0.0018 (8)	0.0051 (8)
C105	0.0250 (11)	0.0268 (11)	0.0278 (10)	0.0094 (9)	0.0019 (8)	0.0017 (8)
C106	0.0303 (12)	0.0353 (13)	0.0402 (13)	0.0149 (10)	0.0071 (10)	−0.0024 (10)
C107	0.0358 (14)	0.0348 (13)	0.0654 (18)	0.0231 (11)	0.0098 (13)	0.0130 (12)
C108	0.0467 (16)	0.0485 (16)	0.0673 (19)	0.0299 (14)	0.0192 (14)	0.0349 (15)
C109	0.0350 (13)	0.0412 (14)	0.0444 (13)	0.0202 (11)	0.0155 (11)	0.0228 (11)
N8	0.0167 (8)	0.0202 (8)	0.0192 (7)	0.0066 (6)	0.0024 (6)	0.0042 (6)
C110	0.0193 (10)	0.0212 (9)	0.0206 (9)	0.0044 (8)	0.0027 (7)	0.0021 (7)
C111	0.0193 (10)	0.0192 (9)	0.0271 (10)	0.0083 (8)	0.0054 (8)	0.0056 (7)
C112	0.0268 (11)	0.0262 (11)	0.0315 (11)	0.0031 (9)	0.0046 (9)	0.0039 (9)
C113	0.0318 (13)	0.0320 (12)	0.0484 (14)	−0.0032 (10)	0.0084 (11)	0.0066 (11)
C114	0.0359 (14)	0.0339 (13)	0.0558 (16)	0.0050 (11)	0.0217 (12)	0.0192 (11)
C115	0.0374 (13)	0.0367 (12)	0.0362 (12)	0.0163 (10)	0.0175 (10)	0.0170 (10)
C116	0.0251 (11)	0.0260 (10)	0.0286 (10)	0.0098 (8)	0.0073 (8)	0.0077 (8)
Ag3	0.02101 (8)	0.03363 (9)	0.02613 (8)	0.00446 (6)	0.00344 (6)	0.00431 (6)
S1	0.0207 (2)	0.0273 (2)	0.0305 (2)	0.00565 (19)	0.00707 (19)	0.0052 (2)
C117	0.0205 (10)	0.0260 (10)	0.0217 (9)	−0.0006 (8)	0.0063 (8)	0.0015 (8)
N9	0.0246 (9)	0.0307 (10)	0.0347 (10)	0.0072 (8)	0.0097 (8)	0.0069 (8)
S2	0.0326 (3)	0.0309 (3)	0.0323 (3)	0.0114 (2)	0.0085 (2)	0.0083 (2)
C118	0.0350 (13)	0.0242 (10)	0.0266 (10)	0.0047 (9)	0.0089 (9)	0.0006 (8)
N10	0.0338 (12)	0.0299 (11)	0.0511 (13)	0.0025 (9)	0.0049 (10)	−0.0003 (9)
S3	0.0251 (3)	0.0338 (3)	0.0254 (2)	0.0032 (2)	0.0011 (2)	0.0084 (2)
C119	0.0343 (13)	0.0339 (12)	0.0232 (10)	0.0057 (10)	0.0007 (9)	0.0032 (9)
N11	0.0614 (16)	0.0344 (12)	0.0413 (12)	−0.0008 (11)	−0.0036 (11)	0.0076 (10)
C120	0.090 (4)	0.268 (9)	0.169 (6)	0.122 (5)	0.092 (4)	0.182 (6)
C121	0.047 (2)	0.195 (6)	0.073 (3)	0.014 (3)	0.0118 (19)	0.083 (4)
O1	0.0558 (13)	0.0739 (15)	0.0417 (11)	0.0120 (11)	0.0185 (10)	0.0230 (10)
C122	0.132 (4)	0.049 (2)	0.057 (2)	−0.007 (2)	0.046 (2)	0.0105 (16)
C123	0.120 (4)	0.056 (2)	0.102 (3)	0.041 (2)	0.077 (3)	0.036 (2)

Geometric parameters (Å, º)

Ag1—C37	2.085 (2)	C60—H60	0.9500
Ag1—C8	2.091 (2)	C61—C62	1.387 (3)
C1—C2	1.383 (4)	C61—H61	0.9500
C1—C6	1.390 (3)	C62—C63	1.388 (3)
C1—H1	0.9500	C62—H62	0.9500
C2—C3	1.382 (4)	C63—C64	1.397 (3)

C2—H2	0.9500	C63—H63	0.9500
C3—C4	1.381 (5)	C64—C65	1.514 (3)
C3—H3	0.9500	C65—N5	1.465 (2)
C4—C5	1.382 (4)	C65—H65A	0.9900
C4—H4	0.9500	C65—H65B	0.9900
C5—C6	1.387 (3)	N5—C66	1.355 (3)
C5—H5	0.9500	N5—C67	1.394 (3)
C6—C7	1.515 (3)	C66—N6	1.350 (3)
C7—N1	1.463 (3)	C67—C74	1.358 (3)
C7—H7A	0.9900	C67—C68	1.472 (3)
C7—H7B	0.9900	C68—C73	1.396 (3)
N1—C8	1.348 (3)	C68—C69	1.403 (3)
N1—C9	1.393 (3)	C69—C70	1.391 (3)
C8—N2	1.350 (3)	C69—H69	0.9500
C9—C16	1.360 (3)	C70—C71	1.387 (3)
C9—C10	1.476 (3)	C70—H70	0.9500
C10—C11	1.371 (4)	C71—C72	1.390 (3)
C10—C15	1.414 (4)	C71—H71	0.9500
C11—C12	1.423 (4)	C72—C73	1.390 (3)
C11—H11	0.9500	C72—H72	0.9500
C12—C13	1.353 (5)	C73—H73	0.9500
C12—H12	0.9500	C74—N6	1.398 (2)
C13—C14	1.389 (6)	C74—C75	1.479 (3)
C13—H13	0.9500	C75—C76	1.392 (3)
C14—C15	1.378 (5)	C75—C80	1.401 (3)
C14—H14	0.9500	C76—C77	1.390 (3)
C15—H15	0.9500	C76—H76	0.9500
C16—N2	1.397 (3)	C77—C78	1.385 (3)
C16—C17	1.482 (3)	C77—H77	0.9500
C17—C22	1.382 (4)	C78—C79	1.388 (3)
C17—C18	1.383 (3)	C78—H78	0.9500
C18—C19	1.392 (3)	C79—C80	1.390 (3)
C18—H18	0.9500	C79—H79	0.9500
C19—C20	1.352 (4)	C80—H80	0.9500
C19—H19	0.9500	N6—C81	1.474 (2)
C20—C21	1.378 (5)	C81—C82	1.511 (3)
C20—H20	0.9500	C81—H81A	0.9900
C21—C22	1.394 (4)	C81—H81B	0.9900
C21—H21	0.9500	C82—C83	1.391 (3)
C22—H22	0.9500	C82—C87	1.394 (3)
N2—C23	1.467 (3)	C83—C84	1.394 (3)
C23—C24	1.508 (4)	C83—H83	0.9500
C23—H23A	0.9900	C84—C85	1.385 (4)
C23—H23B	0.9900	C84—H84	0.9500
C24—C25	1.382 (3)	C85—C86	1.385 (4)
C24—C29	1.389 (4)	C85—H85	0.9500
C25—C26	1.384 (5)	C86—C87	1.384 (3)
C25—H25	0.9500	C86—H86	0.9500

C26—C27	1.371 (5)	C87—H87	0.9500
C26—H26	0.9500	C88—C93	1.378 (3)
C27—C28	1.387 (5)	C88—C89	1.396 (3)
C27—H27	0.9500	C88—H88	0.9500
C28—C29	1.383 (5)	C89—C90	1.379 (4)
C28—H28	0.9500	C89—H89	0.9500
C29—H29	0.9500	C90—C91	1.379 (5)
C30—C35	1.376 (4)	C90—H90	0.9500
C30—C31	1.380 (4)	C91—C92	1.387 (4)
C30—H30	0.9500	C91—H91	0.9500
C31—C32	1.341 (7)	C92—C93	1.393 (3)
C31—H31	0.9500	C92—H92	0.9500
C32—C33	1.360 (8)	C93—C94	1.519 (3)
C32—H32	0.9500	C94—N7	1.463 (3)
C33—C34	1.409 (5)	C94—H94A	0.9900
C33—H33	0.9500	C94—H94B	0.9900
C34—C35	1.385 (4)	N7—C95	1.352 (3)
C34—H34	0.9500	N7—C96	1.399 (3)
C35—C36	1.503 (3)	C95—N8	1.351 (3)
C36—N3	1.466 (3)	C96—C103	1.361 (3)
C36—H36A	0.9900	C96—C97	1.477 (3)
C36—H36B	0.9900	C97—C98	1.392 (3)
N3—C37	1.347 (3)	C97—C102	1.392 (3)
N3—C38	1.398 (3)	C98—C99	1.397 (3)
C37—N4	1.346 (3)	C98—H98	0.9500
C38—C45	1.361 (3)	C99—C100	1.379 (4)
C38—C39	1.472 (3)	C99—H99	0.9500
C39—C44	1.392 (3)	C100—C101	1.375 (4)
C39—C40	1.396 (3)	C100—H100	0.9500
C40—C41	1.385 (3)	C101—C102	1.394 (3)
C40—H40	0.9500	C101—H101	0.9500
C41—C42	1.378 (4)	C102—H102	0.9500
C41—H41	0.9500	C103—N8	1.389 (3)
C42—C43	1.384 (4)	C103—C104	1.480 (3)
C42—H42	0.9500	C104—C109	1.391 (3)
C43—C44	1.384 (4)	C104—C105	1.394 (3)
C43—H43	0.9500	C105—C106	1.388 (3)
C44—H44	0.9500	C105—H105	0.9500
C45—N4	1.396 (3)	C106—C107	1.381 (4)
C45—C46	1.475 (3)	C106—H106	0.9500
C46—C51A	1.348 (9)	C107—C108	1.380 (4)
C46—C47A	1.390 (7)	C107—H107	0.9500
C46—C47B	1.399 (8)	C108—C109	1.383 (4)
C46—C51B	1.415 (9)	C108—H108	0.9500
C47A—C48A	1.392 (9)	C109—H109	0.9500
C47A—H47A	0.9500	N8—C110	1.457 (3)
C48A—C49	1.484 (12)	C110—C111	1.510 (3)
C48A—H48A	0.9500	C110—H11A	0.9900

C47B—C48B	1.382 (10)	C110—H11B	0.9900
C47B—H47B	0.9500	C111—C116	1.394 (3)
C48B—C49	1.297 (8)	C111—C112	1.396 (3)
C48B—H48B	0.9500	C112—C113	1.384 (4)
C49—C50A	1.325 (11)	C112—H112	0.9500
C49—C50B	1.415 (11)	C113—C114	1.384 (4)
C49—H49A	0.9500	C113—H113	0.9500
C49—H49	0.9500	C114—C115	1.388 (4)
C50A—C51A	1.379 (13)	C114—H114	0.9500
C50A—H50A	0.9500	C115—C116	1.393 (3)
C51A—H51A	0.9500	C115—H115	0.9500
C50B—C51B	1.399 (15)	C116—H116	0.9500
C50B—H50B	0.9500	Ag3—S1	2.4657 (5)
C51B—H51B	0.9500	Ag3—S3	2.4940 (6)
N4—C52	1.463 (3)	Ag3—S2	2.5377 (6)
C52—C53	1.510 (3)	S1—C117	1.671 (2)
C52—H52A	0.9900	C117—N9	1.154 (3)
C52—H52B	0.9900	S2—C118	1.669 (3)
C53—C58	1.384 (4)	C118—N10	1.160 (3)
C53—C54	1.392 (3)	S3—C119	1.674 (3)
C54—C55	1.385 (4)	C119—N11	1.156 (4)
C54—H54	0.9500	C120—C121	1.517 (9)
C55—C56	1.379 (5)	C120—H12A	0.9800
C55—H55	0.9500	C120—H12B	0.9800
C56—C57	1.384 (5)	C120—H12C	0.9800
C56—H56	0.9500	C121—O1	1.394 (5)
C57—C58	1.395 (4)	C121—H12D	0.9900
C57—H57	0.9500	C121—H12E	0.9900
C58—H58	0.9500	O1—C122	1.447 (5)
Ag2—C66	2.097 (2)	C122—C123	1.479 (7)
Ag2—C95	2.102 (2)	C122—H12F	0.9900
C59—C64	1.390 (3)	C122—H12G	0.9900
C59—C60	1.393 (3)	C123—H12H	0.9800
C59—H59	0.9500	C123—H12I	0.9800
C60—C61	1.386 (3)	C123—H12J	0.9800

C37—Ag1—C8	173.06 (8)	C60—C61—H61	120.1
C2—C1—C6	120.6 (2)	C62—C61—H61	120.1
C2—C1—H1	119.7	C61—C62—C63	120.0 (2)
C6—C1—H1	119.7	C61—C62—H62	120.0
C3—C2—C1	120.0 (3)	C63—C62—H62	120.0
C3—C2—H2	120.0	C62—C63—C64	120.4 (2)
C1—C2—H2	120.0	C62—C63—H63	119.8
C4—C3—C2	119.7 (3)	C64—C63—H63	119.8
C4—C3—H3	120.1	C59—C64—C63	119.32 (19)
C2—C3—H3	120.1	C59—C64—C65	123.21 (18)
C3—C4—C5	120.2 (3)	C63—C64—C65	117.42 (18)
C3—C4—H4	119.9	N5—C65—C64	114.90 (16)

C5—C4—H4	119.9	N5—C65—H65A	108.5
C4—C5—C6	120.7 (3)	C64—C65—H65A	108.5
C4—C5—H5	119.7	N5—C65—H65B	108.5
C6—C5—H5	119.7	C64—C65—H65B	108.5
C5—C6—C1	118.7 (2)	H65A—C65—H65B	107.5
C5—C6—C7	118.5 (2)	C66—N5—C67	111.26 (16)
C1—C6—C7	122.8 (2)	C66—N5—C65	121.43 (16)
N1—C7—C6	111.19 (17)	C67—N5—C65	125.21 (16)
N1—C7—H7A	109.4	N6—C66—N5	104.81 (16)
C6—C7—H7A	109.4	N6—C66—Ag2	128.78 (14)
N1—C7—H7B	109.4	N5—C66—Ag2	125.76 (14)
C6—C7—H7B	109.4	C74—C67—N5	106.39 (17)
H7A—C7—H7B	108.0	C74—C67—C68	130.61 (18)
C8—N1—C9	111.66 (17)	N5—C67—C68	122.99 (17)
C8—N1—C7	121.59 (18)	C73—C68—C69	118.72 (19)
C9—N1—C7	124.57 (18)	C73—C68—C67	120.38 (18)
N1—C8—N2	104.69 (18)	C69—C68—C67	120.90 (18)
N1—C8—Ag1	125.14 (15)	C70—C69—C68	120.41 (19)
N2—C8—Ag1	129.44 (16)	C70—C69—H69	119.8
C16—C9—N1	106.11 (18)	C68—C69—H69	119.8
C16—C9—C10	131.06 (19)	C71—C70—C69	120.2 (2)
N1—C9—C10	122.82 (19)	C71—C70—H70	119.9
C11—C10—C15	118.6 (2)	C69—C70—H70	119.9
C11—C10—C9	122.0 (2)	C70—C71—C72	119.9 (2)
C15—C10—C9	119.4 (2)	C70—C71—H71	120.0
C10—C11—C12	120.4 (3)	C72—C71—H71	120.0
C10—C11—H11	119.8	C71—C72—C73	120.1 (2)
C12—C11—H11	119.8	C71—C72—H72	120.0
C13—C12—C11	119.8 (3)	C73—C72—H72	120.0
C13—C12—H12	120.1	C72—C73—C68	120.7 (2)
C11—C12—H12	120.1	C72—C73—H73	119.7
C12—C13—C14	120.6 (3)	C68—C73—H73	119.7
C12—C13—H13	119.7	C67—C74—N6	106.25 (17)
C14—C13—H13	119.7	C67—C74—C75	131.52 (18)
C15—C14—C13	120.1 (4)	N6—C74—C75	122.10 (17)
C15—C14—H14	119.9	C76—C75—C80	119.53 (19)
C13—C14—H14	119.9	C76—C75—C74	121.65 (18)
C14—C15—C10	120.3 (3)	C80—C75—C74	118.82 (18)
C14—C15—H15	119.8	C77—C76—C75	120.21 (19)
C10—C15—H15	119.8	C77—C76—H76	119.9
C9—C16—N2	106.17 (18)	C75—C76—H76	119.9
C9—C16—C17	130.6 (2)	C78—C77—C76	120.3 (2)
N2—C16—C17	123.25 (18)	C78—C77—H77	119.9
C22—C17—C18	118.4 (2)	C76—C77—H77	119.9
C22—C17—C16	120.0 (2)	C77—C78—C79	119.8 (2)
C18—C17—C16	121.6 (2)	C77—C78—H78	120.1
C17—C18—C19	120.7 (3)	C79—C78—H78	120.1
C17—C18—H18	119.6	C78—C79—C80	120.5 (2)

C19—C18—H18	119.6	C78—C79—H79	119.8
C20—C19—C18	120.5 (3)	C80—C79—H79	119.8
C20—C19—H19	119.7	C79—C80—C75	119.7 (2)
C18—C19—H19	119.7	C79—C80—H80	120.2
C19—C20—C21	119.8 (2)	C75—C80—H80	120.2
C19—C20—H20	120.1	C66—N6—C74	111.27 (16)
C21—C20—H20	120.1	C66—N6—C81	122.92 (17)
C20—C21—C22	120.2 (3)	C74—N6—C81	125.73 (17)
C20—C21—H21	119.9	N6—C81—C82	112.59 (16)
C22—C21—H21	119.9	N6—C81—H81A	109.1
C17—C22—C21	120.3 (3)	C82—C81—H81A	109.1
C17—C22—H22	119.8	N6—C81—H81B	109.1
C21—C22—H22	119.8	C82—C81—H81B	109.1
C8—N2—C16	111.32 (18)	H81A—C81—H81B	107.8
C8—N2—C23	123.91 (19)	C83—C82—C87	118.8 (2)
C16—N2—C23	124.17 (18)	C83—C82—C81	121.23 (19)
N2—C23—C24	110.6 (2)	C87—C82—C81	119.93 (19)
N2—C23—H23A	109.5	C82—C83—C84	120.3 (2)
C24—C23—H23A	109.5	C82—C83—H83	119.8
N2—C23—H23B	109.5	C84—C83—H83	119.8
C24—C23—H23B	109.5	C85—C84—C83	120.1 (2)
H23A—C23—H23B	108.1	C85—C84—H84	119.9
C25—C24—C29	119.4 (3)	C83—C84—H84	119.9
C25—C24—C23	120.1 (2)	C86—C85—C84	119.7 (2)
C29—C24—C23	120.5 (2)	C86—C85—H85	120.1
C24—C25—C26	120.3 (3)	C84—C85—H85	120.1
C24—C25—H25	119.9	C87—C86—C85	120.2 (2)
C26—C25—H25	119.9	C87—C86—H86	119.9
C27—C26—C25	120.4 (3)	C85—C86—H86	119.9
C27—C26—H26	119.8	C86—C87—C82	120.7 (2)
C25—C26—H26	119.8	C86—C87—H87	119.7
C26—C27—C28	119.7 (3)	C82—C87—H87	119.7
C26—C27—H27	120.1	C93—C88—C89	120.3 (2)
C28—C27—H27	120.1	C93—C88—H88	119.8
C29—C28—C27	120.1 (3)	C89—C88—H88	119.8
C29—C28—H28	119.9	C90—C89—C88	120.1 (3)
C27—C28—H28	119.9	C90—C89—H89	120.0
C28—C29—C24	120.0 (3)	C88—C89—H89	120.0
C28—C29—H29	120.0	C91—C90—C89	120.0 (2)
C24—C29—H29	120.0	C91—C90—H90	120.0
C35—C30—C31	120.3 (3)	C89—C90—H90	120.0
C35—C30—H30	119.8	C90—C91—C92	120.0 (3)
C31—C30—H30	119.8	C90—C91—H91	120.0
C32—C31—C30	121.2 (4)	C92—C91—H91	120.0
C32—C31—H31	119.4	C91—C92—C93	120.4 (3)
C30—C31—H31	119.4	C91—C92—H92	119.8
C31—C32—C33	119.7 (3)	C93—C92—H92	119.8
C31—C32—H32	120.1	C88—C93—C92	119.2 (2)

C33—C32—H32	120.1	C88—C93—C94	121.89 (19)
C32—C33—C34	121.0 (4)	C92—C93—C94	118.8 (2)
C32—C33—H33	119.5	N7—C94—C93	113.90 (17)
C34—C33—H33	119.5	N7—C94—H94A	108.8
C35—C34—C33	118.4 (4)	C93—C94—H94A	108.8
C35—C34—H34	120.8	N7—C94—H94B	108.8
C33—C34—H34	120.8	C93—C94—H94B	108.8
C30—C35—C34	119.3 (3)	H94A—C94—H94B	107.7
C30—C35—C36	119.7 (2)	C95—N7—C96	111.11 (16)
C34—C35—C36	121.0 (3)	C95—N7—C94	122.37 (17)
N3—C36—C35	111.53 (17)	C96—N7—C94	126.49 (17)
N3—C36—H36A	109.3	N8—C95—N7	104.77 (17)
C35—C36—H36A	109.3	N8—C95—Ag2	125.79 (14)
N3—C36—H36B	109.3	N7—C95—Ag2	128.50 (14)
C35—C36—H36B	109.3	C103—C96—N7	106.17 (17)
H36A—C36—H36B	108.0	C103—C96—C97	128.07 (19)
C37—N3—C38	111.70 (18)	N7—C96—C97	125.00 (18)
C37—N3—C36	121.70 (19)	C98—C97—C102	118.8 (2)
C38—N3—C36	126.54 (19)	C98—C97—C96	123.2 (2)
N4—C37—N3	104.74 (18)	C102—C97—C96	118.02 (19)
N4—C37—Ag1	128.26 (16)	C97—C98—C99	120.1 (2)
N3—C37—Ag1	126.73 (16)	C97—C98—H98	119.9
C45—C38—N3	105.77 (18)	C99—C98—H98	119.9
C45—C38—C39	129.59 (19)	C100—C99—C98	120.2 (2)
N3—C38—C39	124.63 (19)	C100—C99—H99	119.9
C44—C39—C40	118.5 (2)	C98—C99—H99	119.9
C44—C39—C38	120.78 (19)	C101—C100—C99	120.2 (2)
C40—C39—C38	120.7 (2)	C101—C100—H100	119.9
C41—C40—C39	120.4 (2)	C99—C100—H100	119.9
C41—C40—H40	119.8	C100—C101—C102	119.9 (2)
C39—C40—H40	119.8	C100—C101—H101	120.1
C42—C41—C40	120.5 (2)	C102—C101—H101	120.1
C42—C41—H41	119.7	C97—C102—C101	120.7 (2)
C40—C41—H41	119.7	C97—C102—H102	119.6
C41—C42—C43	119.7 (2)	C101—C102—H102	119.6
C41—C42—H42	120.2	C96—C103—N8	106.35 (17)
C43—C42—H42	120.2	C96—C103—C104	129.11 (19)
C44—C43—C42	120.2 (2)	N8—C103—C104	124.51 (18)
C44—C43—H43	119.9	C109—C104—C105	119.6 (2)
C42—C43—H43	119.9	C109—C104—C103	120.2 (2)
C43—C44—C39	120.8 (2)	C105—C104—C103	120.07 (19)
C43—C44—H44	119.6	C106—C105—C104	119.6 (2)
C39—C44—H44	119.6	C106—C105—H105	120.2
C38—C45—N4	106.32 (18)	C104—C105—H105	120.2
C38—C45—C46	128.4 (2)	C107—C106—C105	120.3 (2)
N4—C45—C46	125.13 (19)	C107—C106—H106	119.9
C51A—C46—C47A	121.0 (5)	C105—C106—H106	119.9
C47B—C46—C51B	116.9 (5)	C108—C107—C106	120.2 (2)

C51A—C46—C45	122.4 (4)	C108—C107—H107	119.9
C47A—C46—C45	116.6 (3)	C106—C107—H107	119.9
C47B—C46—C45	121.5 (3)	C107—C108—C109	120.0 (3)
C51B—C46—C45	121.4 (4)	C107—C108—H108	120.0
C46—C47A—C48A	118.4 (6)	C109—C108—H108	120.0
C46—C47A—H47A	120.8	C108—C109—C104	120.2 (2)
C48A—C47A—H47A	120.8	C108—C109—H109	119.9
C47A—C48A—C49	119.4 (6)	C104—C109—H109	119.9
C47A—C48A—H48A	120.3	C95—N8—C103	111.58 (16)
C49—C48A—H48A	120.3	C95—N8—C110	122.79 (17)
C48B—C47B—C46	122.0 (6)	C103—N8—C110	125.57 (17)
C48B—C47B—H47B	119.0	N8—C110—C111	113.24 (16)
C46—C47B—H47B	119.0	N8—C110—H11A	108.9
C49—C48B—C47B	120.5 (6)	C111—C110—H11A	108.9
C49—C48B—H48B	119.8	N8—C110—H11B	108.9
C47B—C48B—H48B	119.8	C111—C110—H11B	108.9
C48B—C49—C50B	121.9 (6)	H11A—C110—H11B	107.7
C50A—C49—C48A	117.9 (5)	C116—C111—C112	118.8 (2)
C48B—C49—H49A	119.0	C116—C111—C110	122.77 (19)
C50B—C49—H49A	119.0	C112—C111—C110	118.43 (19)
C50A—C49—H49	121.1	C113—C112—C111	120.7 (2)
C48A—C49—H49	121.1	C113—C112—H112	119.7
C49—C50A—C51A	121.7 (8)	C111—C112—H112	119.7
C49—C50A—H50A	119.2	C114—C113—C112	120.4 (2)
C51A—C50A—H50A	119.2	C114—C113—H113	119.8
C46—C51A—C50A	121.6 (8)	C112—C113—H113	119.8
C46—C51A—H51A	119.2	C113—C114—C115	119.6 (2)
C50A—C51A—H51A	119.2	C113—C114—H114	120.2
C51B—C50B—C49	118.5 (8)	C115—C114—H114	120.2
C51B—C50B—H50B	120.7	C114—C115—C116	120.2 (2)
C49—C50B—H50B	120.7	C114—C115—H115	119.9
C50B—C51B—C46	120.0 (8)	C116—C115—H115	119.9
C50B—C51B—H51B	120.0	C115—C116—C111	120.4 (2)
C46—C51B—H51B	120.0	C115—C116—H116	119.8
C37—N4—C45	111.46 (18)	C111—C116—H116	119.8
C37—N4—C52	122.88 (19)	S1—Ag3—S3	126.936 (19)
C45—N4—C52	125.64 (19)	S1—Ag3—S2	127.68 (2)
N4—C52—C53	114.39 (19)	S3—Ag3—S2	103.957 (19)
N4—C52—H52A	108.7	C117—S1—Ag3	100.90 (7)
C53—C52—H52A	108.7	N9—C117—S1	177.8 (2)
N4—C52—H52B	108.7	C118—S2—Ag3	93.45 (8)
C53—C52—H52B	108.7	N10—C118—S2	179.4 (3)
H52A—C52—H52B	107.6	C119—S3—Ag3	105.56 (9)
C58—C53—C54	118.9 (2)	N11—C119—S3	177.1 (2)
C58—C53—C52	123.4 (2)	C121—C120—H12A	109.5
C54—C53—C52	117.7 (2)	C121—C120—H12B	109.5
C55—C54—C53	120.9 (3)	H12A—C120—H12B	109.5
C55—C54—H54	119.5	C121—C120—H12C	109.5

C53—C54—H54	119.5	H12A—C120—H12C	109.5
C56—C55—C54	119.7 (3)	H12B—C120—H12C	109.5
C56—C55—H55	120.1	O1—C121—C120	107.2 (4)
C54—C55—H55	120.1	O1—C121—H12D	110.3
C55—C56—C57	120.1 (3)	C120—C121—H12D	110.3
C55—C56—H56	119.9	O1—C121—H12E	110.3
C57—C56—H56	119.9	C120—C121—H12E	110.3
C56—C57—C58	120.0 (3)	H12D—C121—H12E	108.5
C56—C57—H57	120.0	C121—O1—C122	113.9 (4)
C58—C57—H57	120.0	O1—C122—C123	107.7 (3)
C53—C58—C57	120.3 (3)	O1—C122—H12F	110.2
C53—C58—H58	119.9	C123—C122—H12F	110.2
C57—C58—H58	119.9	O1—C122—H12G	110.2
C66—Ag2—C95	172.01 (7)	C123—C122—H12G	110.2
C64—C59—C60	120.02 (19)	H12F—C122—H12G	108.5
C64—C59—H59	120.0	C122—C123—H12H	109.5
C60—C59—H59	120.0	C122—C123—H12I	109.5
C61—C60—C59	120.4 (2)	H12H—C123—H12I	109.5
C61—C60—H60	119.8	C122—C123—H12J	109.5
C59—C60—H60	119.8	H12H—C123—H12J	109.5
C60—C61—C62	119.8 (2)	H12I—C123—H12J	109.5

C6—C1—C2—C3	1.1 (4)	C46—C45—N4—C52	−2.1 (3)
C1—C2—C3—C4	−1.6 (5)	C37—N4—C52—C53	92.3 (3)
C2—C3—C4—C5	1.6 (5)	C45—N4—C52—C53	−89.6 (3)
C3—C4—C5—C6	−1.0 (5)	N4—C52—C53—C58	1.2 (3)
C4—C5—C6—C1	0.4 (4)	N4—C52—C53—C54	−179.9 (2)
C4—C5—C6—C7	−179.4 (3)	C58—C53—C54—C55	1.6 (4)
C2—C1—C6—C5	−0.5 (4)	C52—C53—C54—C55	−177.4 (3)
C2—C1—C6—C7	179.4 (2)	C53—C54—C55—C56	−0.7 (5)
C5—C6—C7—N1	162.3 (2)	C54—C55—C56—C57	−1.0 (5)
C1—C6—C7—N1	−17.5 (3)	C55—C56—C57—C58	1.7 (5)
C6—C7—N1—C8	−72.3 (3)	C54—C53—C58—C57	−0.8 (4)
C6—C7—N1—C9	89.5 (2)	C52—C53—C58—C57	178.1 (3)
C9—N1—C8—N2	2.0 (2)	C56—C57—C58—C53	−0.8 (5)
C7—N1—C8—N2	165.95 (18)	C64—C59—C60—C61	0.2 (3)
C9—N1—C8—Ag1	−169.00 (15)	C59—C60—C61—C62	0.5 (3)
C7—N1—C8—Ag1	−5.1 (3)	C60—C61—C62—C63	−0.6 (3)
C8—N1—C9—C16	−1.1 (2)	C61—C62—C63—C64	−0.1 (3)
C7—N1—C9—C16	−164.48 (19)	C60—C59—C64—C63	−0.8 (3)
C8—N1—C9—C10	−179.9 (2)	C60—C59—C64—C65	176.41 (19)
C7—N1—C9—C10	16.8 (3)	C62—C63—C64—C59	0.8 (3)
C16—C9—C10—C11	−111.4 (3)	C62—C63—C64—C65	−176.6 (2)
N1—C9—C10—C11	67.0 (3)	C59—C64—C65—N5	23.7 (3)
C16—C9—C10—C15	66.5 (4)	C63—C64—C65—N5	−158.98 (18)
N1—C9—C10—C15	−115.1 (3)	C64—C65—N5—C66	74.7 (2)
C15—C10—C11—C12	3.5 (4)	C64—C65—N5—C67	−123.2 (2)
C9—C10—C11—C12	−178.5 (2)	C67—N5—C66—N6	−0.3 (2)

C10—C11—C12—C13	−3.1 (5)	C65—N5—C66—N6	164.03 (16)
C11—C12—C13—C14	0.3 (6)	C67—N5—C66—Ag2	171.15 (13)
C12—C13—C14—C15	2.0 (7)	C65—N5—C66—Ag2	−24.5 (2)
C13—C14—C15—C10	−1.5 (7)	C66—N5—C67—C74	0.4 (2)
C11—C10—C15—C14	−1.3 (5)	C65—N5—C67—C74	−163.23 (17)
C9—C10—C15—C14	−179.3 (4)	C66—N5—C67—C68	−178.55 (17)
N1—C9—C16—N2	−0.3 (2)	C65—N5—C67—C68	17.8 (3)
C10—C9—C16—N2	178.3 (2)	C74—C67—C68—C73	43.9 (3)
N1—C9—C16—C17	177.8 (2)	N5—C67—C68—C73	−137.5 (2)
C10—C9—C16—C17	−3.7 (4)	C74—C67—C68—C69	−135.4 (2)
C9—C16—C17—C22	−69.5 (4)	N5—C67—C68—C69	43.3 (3)
N2—C16—C17—C22	108.2 (3)	C73—C68—C69—C70	1.0 (3)
C9—C16—C17—C18	113.1 (3)	C67—C68—C69—C70	−179.74 (19)
N2—C16—C17—C18	−69.2 (3)	C68—C69—C70—C71	−0.8 (3)
C22—C17—C18—C19	1.6 (4)	C69—C70—C71—C72	0.4 (3)
C16—C17—C18—C19	179.0 (2)	C70—C71—C72—C73	−0.1 (3)
C17—C18—C19—C20	−0.4 (4)	C71—C72—C73—C68	0.3 (3)
C18—C19—C20—C21	−1.6 (5)	C69—C68—C73—C72	−0.8 (3)
C19—C20—C21—C22	2.5 (6)	C67—C68—C73—C72	180.00 (19)
C18—C17—C22—C21	−0.7 (5)	N5—C67—C74—N6	−0.3 (2)
C16—C17—C22—C21	−178.1 (3)	C68—C67—C74—N6	178.52 (19)
C20—C21—C22—C17	−1.3 (6)	N5—C67—C74—C75	175.57 (19)
N1—C8—N2—C16	−2.2 (2)	C68—C67—C74—C75	−5.6 (4)
Ag1—C8—N2—C16	168.31 (16)	C67—C74—C75—C76	68.8 (3)
N1—C8—N2—C23	−173.7 (2)	N6—C74—C75—C76	−115.9 (2)
Ag1—C8—N2—C23	−3.2 (3)	C67—C74—C75—C80	−112.0 (2)
C9—C16—N2—C8	1.6 (3)	N6—C74—C75—C80	63.3 (3)
C17—C16—N2—C8	−176.6 (2)	C80—C75—C76—C77	−1.3 (3)
C9—C16—N2—C23	173.0 (2)	C74—C75—C76—C77	177.84 (19)
C17—C16—N2—C23	−5.2 (3)	C75—C76—C77—C78	0.3 (3)
C8—N2—C23—C24	106.1 (2)	C76—C77—C78—C79	0.8 (3)
C16—N2—C23—C24	−64.3 (3)	C77—C78—C79—C80	−1.0 (3)
N2—C23—C24—C25	126.8 (2)	C78—C79—C80—C75	0.0 (3)
N2—C23—C24—C29	−52.5 (3)	C76—C75—C80—C79	1.1 (3)
C29—C24—C25—C26	1.2 (4)	C74—C75—C80—C79	−178.06 (19)
C23—C24—C25—C26	−178.0 (3)	N5—C66—N6—C74	0.1 (2)
C24—C25—C26—C27	0.6 (5)	Ag2—C66—N6—C74	−170.99 (13)
C25—C26—C27—C28	−1.3 (6)	N5—C66—N6—C81	177.12 (16)
C26—C27—C28—C29	0.2 (6)	Ag2—C66—N6—C81	6.0 (3)
C27—C28—C29—C24	1.6 (5)	C67—C74—N6—C66	0.1 (2)
C25—C24—C29—C28	−2.3 (4)	C75—C74—N6—C66	−176.22 (17)
C23—C24—C29—C28	176.9 (3)	C67—C74—N6—C81	−176.79 (17)
C35—C30—C31—C32	−0.4 (5)	C75—C74—N6—C81	6.9 (3)
C30—C31—C32—C33	−0.8 (6)	C66—N6—C81—C82	−93.6 (2)
C31—C32—C33—C34	0.5 (5)	C74—N6—C81—C82	83.0 (2)
C32—C33—C34—C35	1.1 (5)	N6—C81—C82—C83	−94.5 (2)
C31—C30—C35—C34	2.0 (4)	N6—C81—C82—C87	85.3 (2)
C31—C30—C35—C36	−176.5 (3)	C87—C82—C83—C84	−1.7 (3)

C33—C34—C35—C30	−2.3 (4)	C81—C82—C83—C84	178.2 (2)
C33—C34—C35—C36	176.2 (3)	C82—C83—C84—C85	0.2 (4)
C30—C35—C36—N3	−52.4 (3)	C83—C84—C85—C86	1.2 (4)
C34—C35—C36—N3	129.1 (2)	C84—C85—C86—C87	−1.2 (4)
C35—C36—N3—C37	−65.3 (3)	C85—C86—C87—C82	−0.2 (4)
C35—C36—N3—C38	111.4 (2)	C83—C82—C87—C86	1.7 (3)
C38—N3—C37—N4	1.0 (2)	C81—C82—C87—C86	−178.1 (2)
C36—N3—C37—N4	178.19 (18)	C93—C88—C89—C90	0.7 (4)
C38—N3—C37—Ag1	−173.48 (14)	C88—C89—C90—C91	−0.5 (5)
C36—N3—C37—Ag1	3.7 (3)	C89—C90—C91—C92	0.4 (5)
C37—N3—C38—C45	−0.6 (2)	C90—C91—C92—C93	−0.4 (5)
C36—N3—C38—C45	−177.58 (19)	C89—C88—C93—C92	−0.7 (4)
C37—N3—C38—C39	−179.36 (19)	C89—C88—C93—C94	175.1 (2)
C36—N3—C38—C39	3.6 (3)	C91—C92—C93—C88	0.5 (4)
C45—C38—C39—C44	59.2 (3)	C91—C92—C93—C94	−175.4 (3)
N3—C38—C39—C44	−122.3 (2)	C88—C93—C94—N7	38.4 (3)
C45—C38—C39—C40	−119.5 (3)	C92—C93—C94—N7	−145.8 (2)
N3—C38—C39—C40	59.0 (3)	C93—C94—N7—C95	−91.0 (2)
C44—C39—C40—C41	0.8 (4)	C93—C94—N7—C96	87.2 (2)
C38—C39—C40—C41	179.6 (2)	C96—N7—C95—N8	−1.4 (2)
C39—C40—C41—C42	−0.1 (4)	C94—N7—C95—N8	177.10 (16)
C40—C41—C42—C43	−0.6 (4)	C96—N7—C95—Ag2	167.96 (14)
C41—C42—C43—C44	0.6 (5)	C94—N7—C95—Ag2	−13.6 (3)
C42—C43—C44—C39	0.1 (5)	C95—N7—C96—C103	1.5 (2)
C40—C39—C44—C43	−0.8 (4)	C94—N7—C96—C103	−176.87 (18)
C38—C39—C44—C43	−179.5 (2)	C95—N7—C96—C97	−169.15 (19)
N3—C38—C45—N4	−0.1 (2)	C94—N7—C96—C97	12.5 (3)
C39—C38—C45—N4	178.6 (2)	C103—C96—C97—C98	137.9 (2)
N3—C38—C45—C46	−175.4 (2)	N7—C96—C97—C98	−53.6 (3)
C39—C38—C45—C46	3.3 (4)	C103—C96—C97—C102	−43.7 (3)
C38—C45—C46—C51A	−82.0 (7)	N7—C96—C97—C102	124.9 (2)
N4—C45—C46—C51A	103.5 (7)	C102—C97—C98—C99	−2.2 (3)
C38—C45—C46—C47A	96.2 (7)	C96—C97—C98—C99	176.3 (2)
N4—C45—C46—C47A	−78.3 (7)	C97—C98—C99—C100	1.5 (4)
C38—C45—C46—C47B	63.6 (8)	C98—C99—C100—C101	0.6 (4)
N4—C45—C46—C47B	−110.8 (7)	C99—C100—C101—C102	−2.0 (4)
C38—C45—C46—C51B	−110.3 (8)	C98—C97—C102—C101	0.7 (3)
N4—C45—C46—C51B	75.2 (8)	C96—C97—C102—C101	−177.8 (2)
C51A—C46—C47A—C48A	1.6 (9)	C100—C101—C102—C97	1.3 (4)
C47B—C46—C47A—C48A	−69.1 (10)	N7—C96—C103—N8	−1.0 (2)
C51B—C46—C47A—C48A	28.6 (9)	C97—C96—C103—N8	169.28 (19)
C45—C46—C47A—C48A	−176.6 (5)	N7—C96—C103—C104	−178.8 (2)
C46—C47A—C48A—C49	0.2 (10)	C97—C96—C103—C104	−8.5 (4)
C51A—C46—C47B—C48B	−26.2 (9)	C96—C103—C104—C109	−76.7 (3)
C47A—C46—C47B—C48B	95.3 (12)	N8—C103—C104—C109	105.8 (3)
C51B—C46—C47B—C48B	−1.8 (10)	C96—C103—C104—C105	99.7 (3)
C45—C46—C47B—C48B	−176.0 (6)	N8—C103—C104—C105	−77.8 (3)
C46—C47B—C48B—C49	−2.2 (12)	C109—C104—C105—C106	0.8 (3)

C47B—C48B—C49—C50A	30.1 (10)	C103—C104—C105—C106	−175.7 (2)
C47B—C48B—C49—C50B	5.1 (11)	C104—C105—C106—C107	−0.6 (4)
C47B—C48B—C49—C48A	−77.0 (11)	C105—C106—C107—C108	0.0 (4)
C47A—C48A—C49—C48B	84.6 (11)	C106—C107—C108—C109	0.5 (5)
C47A—C48A—C49—C50A	−2.2 (9)	C107—C108—C109—C104	−0.3 (5)
C47A—C48A—C49—C50B	−28.6 (9)	C105—C104—C109—C108	−0.3 (4)
C48B—C49—C50A—C51A	−29.5 (10)	C103—C104—C109—C108	176.1 (2)
C50B—C49—C50A—C51A	89 (2)	N7—C95—N8—C103	0.7 (2)
C48A—C49—C50A—C51A	2.3 (10)	Ag2—C95—N8—C103	−168.99 (14)
C47A—C46—C51A—C50A	−1.5 (9)	N7—C95—N8—C110	−176.58 (17)
C47B—C46—C51A—C50A	27.0 (9)	Ag2—C95—N8—C110	13.7 (3)
C51B—C46—C51A—C50A	−88.1 (18)	C96—C103—N8—C95	0.2 (2)
C45—C46—C51A—C50A	176.6 (6)	C104—C103—N8—C95	178.16 (19)
C49—C50A—C51A—C46	−0.6 (11)	C96—C103—N8—C110	177.40 (18)
C48B—C49—C50B—C51B	−3.8 (12)	C104—C103—N8—C110	−4.6 (3)
C50A—C49—C50B—C51B	−77.2 (19)	C95—N8—C110—C111	82.2 (2)
C48A—C49—C50B—C51B	28.1 (10)	C103—N8—C110—C111	−94.7 (2)
C49—C50B—C51B—C46	−0.4 (13)	N8—C110—C111—C116	16.9 (3)
C51A—C46—C51B—C50B	77.3 (16)	N8—C110—C111—C112	−165.55 (19)
C47A—C46—C51B—C50B	−29.3 (10)	C116—C111—C112—C113	1.7 (3)
C47B—C46—C51B—C50B	3.0 (11)	C110—C111—C112—C113	−175.9 (2)
C45—C46—C51B—C50B	177.2 (7)	C111—C112—C113—C114	−0.9 (4)
N3—C37—N4—C45	−1.1 (2)	C112—C113—C114—C115	−0.7 (4)
Ag1—C37—N4—C45	173.29 (15)	C113—C114—C115—C116	1.4 (4)
N3—C37—N4—C52	177.28 (18)	C114—C115—C116—C111	−0.6 (4)
Ag1—C37—N4—C52	−8.4 (3)	C112—C111—C116—C115	−0.9 (3)
C38—C45—N4—C37	0.8 (2)	C110—C111—C116—C115	176.6 (2)
C46—C45—N4—C37	176.21 (19)	C120—C121—O1—C122	−177.1 (3)
C38—C45—N4—C52	−177.54 (19)	C121—O1—C122—C123	177.5 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C31—H31···O1	0.95	2.57	3.361 (4)	141
C32—H32···N10^{i}	0.95	2.43	3.327 (4)	157
C40—H40···S1^{ii}	0.95	2.82	3.684 (2)	152

Symmetry codes: (i) −*x*+2, −*y*+2, −*z*+1; (ii) *x*, *y*, *z*−1.

Bis(*μ*-1,3-dibenzyl-4,5-diphenyl-2-selenoimidazole-*κ*^{2}*Se*:*Se*)bis[bromido(1,3-dibenzyl-4,5-diphenyl-2-selenoimidazole-*κSe*)silver(I)] dichloromethane hexasolvate (2)

Crystal data

$[Ag_2Br_2(C_{29}H_{24}N_2Se)_4]\cdot 6CH_2Cl_2$
M_r = 2802.96
Triclinic, $P\overline{1}$
a = 13.6265 (1) Å
b = 14.7422 (1) Å
c = 16.9397 (2) Å
α = 106.4172 (7)°
β = 112.2820 (8)°
γ = 96.2211 (6)°
V = 2930.04 (5) Å^3
Z = 1
F(000) = 1400

D_x = 1.589 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 42526 reflections
θ = 3.0–26.4°
μ = 2.58 mm^{-1}
T = 150 K
Prism, clear pale yellow
0.37 × 0.26 × 0.20 mm

Data collection

Rigaku SuperNova, Dual, Cu at zero, Atlas diffractometer
Radiation source: micro-focus sealed X-ray tube
Detector resolution: 10.3196 pixels mm^{-1}
ω scans
Absorption correction: gaussian (CrysAlis PRO; Rigaku OD, 2015)
T_{min} = 0.517, T_{max} = 0.664
119415 measured reflections
12002 independent reflections
10726 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
θ_{max} = 26.4°, θ_{min} = 2.8°
h = −17→17
k = −18→18
l = −21→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.096
S = 1.03
12002 reflections
654 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0468P)^2 + 5.4618P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 1.05 e Å^{-3}
$\Delta\rho_{min}$ = −1.48 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. The PLATON SQUEEZE procedure (A. L. Spek. Acta Cryst. C71, 2015, 9-18) was used to treat regions of disordered solvent which could not be modelled in terms of atomic sites. The number of electrons found in these regions, 84, was assigned to 2 molecules of dichloromethane. 2 dichloromethanes would give 84 electrons.

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

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.2991 (3)	0.2585 (2)	0.5958 (2)	0.0303 (6)	
H1	0.3686	0.2453	0.6224	0.036*	
C2	0.2264 (3)	0.2008 (3)	0.5078 (2)	0.0390 (8)	
H2	0.2460	0.1483	0.4743	0.047*	
C3	0.1255 (3)	0.2194 (3)	0.4687 (3)	0.0476 (9)	
H3	0.0752	0.1796	0.4083	0.057*	
C4	0.0978 (3)	0.2950 (3)	0.5167 (3)	0.0530 (10)	
H4	0.0283	0.3078	0.4894	0.064*	
C5	0.1709 (3)	0.3540 (3)	0.6060 (3)	0.0422 (8)	
H5	0.1509	0.4065	0.6390	0.051*	
C6	0.2721 (2)	0.3356 (2)	0.6459 (2)	0.0281 (6)	
C7	0.3529 (2)	0.3973 (2)	0.7424 (2)	0.0277 (6)	
H7A	0.3201	0.4477	0.7680	0.033*	

H7B	0.3677	0.3555	0.7801	0.033*
N1	0.45650 (19)	0.44492 (16)	0.74753 (15)	0.0228 (5)
C8	0.5529 (2)	0.42207 (19)	0.78510 (18)	0.0227 (5)
Se1	0.57786 (3)	0.32825 (2)	0.83916 (2)	0.02863 (8)
C9	0.4711 (2)	0.52088 (19)	0.71564 (18)	0.0232 (5)
C10	0.3796 (2)	0.5572 (2)	0.66477 (19)	0.0246 (6)
C11	0.3552 (3)	0.5471 (2)	0.5752 (2)	0.0351 (7)
H11	0.3998	0.5197	0.5481	0.042*
C12	0.2666 (3)	0.5764 (3)	0.5246 (2)	0.0444 (9)
H12	0.2507	0.5691	0.4632	0.053*
C13	0.2019 (3)	0.6158 (3)	0.5630 (3)	0.0462 (9)
H13	0.1414	0.6362	0.5283	0.055*
C14	0.2241 (4)	0.6259 (3)	0.6511 (3)	0.0519 (10)
H14	0.1781	0.6521	0.6771	0.062*
C15	0.3137 (3)	0.5981 (3)	0.7029 (2)	0.0412 (8)
H15	0.3300	0.6070	0.7647	0.049*
C16	0.5788 (2)	0.54519 (19)	0.73583 (18)	0.0227 (5)
C17	0.6406 (2)	0.6262 (2)	0.72556 (19)	0.0252 (6)
C18	0.6984 (3)	0.6095 (2)	0.6728 (2)	0.0329 (7)
H18	0.6978	0.5446	0.6418	0.039*
C19	0.7568 (3)	0.6868 (3)	0.6651 (3)	0.0418 (8)
H19	0.7959	0.6749	0.6288	0.050*
C20	0.7583 (3)	0.7811 (3)	0.7102 (3)	0.0441 (8)
H20	0.7991	0.8341	0.7055	0.053*
C21	0.7003 (3)	0.7986 (2)	0.7623 (3)	0.0436 (8)
H21	0.7011	0.8638	0.7929	0.052*
C22	0.6411 (3)	0.7217 (2)	0.7702 (2)	0.0331 (7)
H22	0.6011	0.7340	0.8058	0.040*
N2	0.62857 (19)	0.48262 (16)	0.77814 (15)	0.0220 (5)
C23	0.7469 (2)	0.4912 (2)	0.82079 (19)	0.0267 (6)
H23A	0.7644	0.4699	0.8739	0.032*
H23B	0.7852	0.5608	0.8439	0.032*
C24	0.7915 (2)	0.4329 (2)	0.75860 (19)	0.0273 (6)
C25	0.7432 (3)	0.3347 (2)	0.7062 (2)	0.0311 (6)
H25	0.6773	0.3042	0.7050	0.037*
C26	0.7911 (3)	0.2812 (3)	0.6557 (2)	0.0387 (7)
H26	0.7580	0.2142	0.6206	0.046*
C27	0.8863 (3)	0.3247 (3)	0.6561 (2)	0.0393 (8)
H27	0.9187	0.2875	0.6216	0.047*
C28	0.9342 (3)	0.4220 (3)	0.7065 (2)	0.0413 (8)
H28	0.9996	0.4524	0.7069	0.050*
C29	0.8862 (3)	0.4759 (3)	0.7571 (2)	0.0351 (7)
H29	0.9190	0.5432	0.7912	0.042*
C30	0.5585 (3)	0.1771 (3)	1.0909 (2)	0.0491 (9)
H30	0.6202	0.2240	1.1018	0.059*
C31	0.5587 (4)	0.1424 (4)	1.1588 (3)	0.0648 (13)
H31	0.6199	0.1666	1.2167	0.078*
C32	0.4709 (4)	0.0730 (3)	1.1427 (3)	0.0563 (12)

H32	0.4721	0.0474	1.1885	0.068*
C33	0.3819 (4)	0.0412 (3)	1.0607 (3)	0.0651 (13)
H33	0.3199	−0.0052	1.0498	0.078*
C34	0.3818 (4)	0.0765 (3)	0.9930 (3)	0.0558 (11)
H34	0.3197	0.0531	0.9356	0.067*
C35	0.4684 (3)	0.1437 (2)	1.00705 (19)	0.0283 (6)
C36	0.4722 (2)	0.1824 (2)	0.93410 (18)	0.0236 (5)
H36A	0.5324	0.2419	0.9626	0.028*
H36B	0.4878	0.1331	0.8900	0.028*
N3	0.36874 (18)	0.20544 (16)	0.88532 (14)	0.0195 (4)
C37	0.3351 (2)	0.28258 (19)	0.92241 (17)	0.0208 (5)
Se2	0.41926 (2)	0.38665 (2)	1.03116 (2)	0.02432 (7)
C38	0.2820 (2)	0.14190 (19)	0.80476 (17)	0.0208 (5)
C39	0.2888 (2)	0.0524 (2)	0.74254 (18)	0.0222 (5)
C40	0.3653 (2)	0.0541 (2)	0.7071 (2)	0.0280 (6)
H40	0.4178	0.1129	0.7258	0.034*
C41	0.3649 (3)	−0.0308 (2)	0.6440 (2)	0.0344 (7)
H41	0.4175	−0.0297	0.6199	0.041*
C42	0.2887 (3)	−0.1161 (2)	0.6165 (2)	0.0348 (7)
H42	0.2887	−0.1736	0.5733	0.042*
C43	0.2124 (3)	−0.1183 (2)	0.6515 (2)	0.0315 (7)
H43	0.1601	−0.1773	0.6325	0.038*
C44	0.2119 (2)	−0.0345 (2)	0.71439 (19)	0.0261 (6)
H44	0.1592	−0.0362	0.7383	0.031*
C45	0.1938 (2)	0.18073 (19)	0.79410 (18)	0.0217 (5)
C46	0.0815 (2)	0.14143 (19)	0.72006 (18)	0.0224 (5)
C47	0.0640 (2)	0.1324 (2)	0.63145 (19)	0.0273 (6)
H47	0.1229	0.1550	0.6194	0.033*
C48	−0.0397 (3)	0.0901 (2)	0.5609 (2)	0.0336 (7)
H48	−0.0521	0.0847	0.5004	0.040*
C49	−0.1246 (3)	0.0560 (2)	0.5781 (2)	0.0359 (7)
H49	−0.1954	0.0268	0.5294	0.043*
C50	−0.1075 (3)	0.0638 (2)	0.6657 (2)	0.0358 (7)
H50	−0.1664	0.0395	0.6769	0.043*
C51	−0.0047 (2)	0.1073 (2)	0.7372 (2)	0.0301 (6)
H51	0.0068	0.1136	0.7976	0.036*
N4	0.22814 (18)	0.26809 (16)	0.86718 (15)	0.0210 (4)
C52	0.1591 (2)	0.3352 (2)	0.87987 (19)	0.0236 (5)
H52A	0.1031	0.3288	0.8193	0.028*
H52B	0.2048	0.4028	0.9088	0.028*
C53	0.1023 (2)	0.3184 (2)	0.93731 (19)	0.0262 (6)
C54	0.1310 (3)	0.2618 (2)	0.9917 (2)	0.0325 (7)
H54	0.1874	0.2290	0.9922	0.039*
C55	0.0770 (3)	0.2531 (3)	1.0453 (2)	0.0434 (8)
H55	0.0962	0.2139	1.0820	0.052*
C56	−0.0046 (3)	0.3012 (3)	1.0454 (3)	0.0464 (9)
H56	−0.0407	0.2956	1.0827	0.056*
C57	−0.0336 (3)	0.3573 (3)	0.9915 (3)	0.0463 (9)

H57	−0.0898	0.3903	0.9914	0.056*	
C58	0.0191 (3)	0.3656 (3)	0.9375 (2)	0.0375 (7)	
H58	−0.0017	0.4040	0.9001	0.045*	
Ag	0.59867 (2)	0.44437 (2)	1.00177 (2)	0.03306 (7)	
Br	0.77487 (3)	0.41077 (3)	1.11754 (2)	0.04318 (9)	
C59	0.4858 (4)	0.7506 (4)	0.5306 (3)	0.0671 (13)	
H59A	0.5389	0.7634	0.5941	0.081*	
H59B	0.4115	0.7398	0.5281	0.081*	
Cl1	0.49731 (8)	0.64544 (7)	0.45851 (6)	0.0459 (2)	
Cl2	0.50991 (12)	0.85328 (9)	0.50091 (11)	0.0817 (4)	
C60	0.7655 (4)	0.1514 (3)	0.8195 (3)	0.0628 (12)	
H60A	0.7439	0.1961	0.8623	0.075*	0.898 (4)
H60B	0.8157	0.1914	0.8058	0.075*	0.898 (4)
H60C	0.7912	0.2167	0.8192	0.075*	0.102 (4)
H60D	0.8253	0.1173	0.8271	0.075*	0.102 (4)
Cl3	0.64844 (9)	0.08367 (10)	0.71812 (10)	0.0764 (4)	
Cl4A	0.83340 (11)	0.07387 (9)	0.87093 (9)	0.0670 (5)	0.898 (4)
Cl4B	0.7203 (18)	0.1617 (16)	0.9129 (15)	0.120 (7)*	0.102 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0294 (15)	0.0298 (15)	0.0306 (15)	0.0035 (12)	0.0132 (13)	0.0099 (12)
C2	0.0415 (19)	0.0386 (18)	0.0322 (17)	−0.0023 (14)	0.0181 (15)	0.0073 (14)
C3	0.041 (2)	0.055 (2)	0.0329 (18)	−0.0089 (17)	0.0050 (16)	0.0178 (17)
C4	0.0272 (18)	0.057 (2)	0.064 (3)	0.0042 (16)	0.0014 (17)	0.032 (2)
C5	0.0316 (17)	0.0375 (18)	0.056 (2)	0.0100 (14)	0.0151 (16)	0.0194 (16)
C6	0.0261 (15)	0.0273 (14)	0.0339 (16)	0.0040 (11)	0.0143 (13)	0.0138 (12)
C7	0.0294 (15)	0.0283 (14)	0.0292 (15)	0.0058 (12)	0.0173 (13)	0.0094 (12)
N1	0.0287 (12)	0.0201 (11)	0.0191 (11)	0.0052 (9)	0.0111 (10)	0.0054 (9)
C8	0.0306 (15)	0.0183 (12)	0.0171 (12)	0.0058 (11)	0.0103 (11)	0.0030 (10)
Se1	0.04242 (18)	0.02315 (14)	0.02676 (15)	0.01194 (12)	0.01801 (13)	0.01214 (12)
C9	0.0297 (15)	0.0211 (13)	0.0175 (12)	0.0055 (11)	0.0101 (11)	0.0053 (10)
C10	0.0269 (14)	0.0212 (13)	0.0252 (14)	0.0067 (11)	0.0115 (12)	0.0068 (11)
C11	0.0392 (18)	0.0455 (18)	0.0283 (16)	0.0242 (15)	0.0173 (14)	0.0147 (14)
C12	0.048 (2)	0.054 (2)	0.0320 (17)	0.0304 (18)	0.0127 (16)	0.0164 (16)
C13	0.041 (2)	0.047 (2)	0.057 (2)	0.0287 (17)	0.0187 (18)	0.0240 (18)
C14	0.061 (2)	0.057 (2)	0.068 (3)	0.042 (2)	0.045 (2)	0.032 (2)
C15	0.059 (2)	0.0440 (19)	0.0388 (18)	0.0285 (17)	0.0317 (17)	0.0190 (15)
C16	0.0283 (14)	0.0220 (13)	0.0169 (12)	0.0072 (11)	0.0090 (11)	0.0060 (10)
C17	0.0267 (14)	0.0259 (14)	0.0211 (13)	0.0065 (11)	0.0067 (11)	0.0107 (11)
C18	0.0386 (17)	0.0327 (16)	0.0321 (16)	0.0095 (13)	0.0182 (14)	0.0134 (13)
C19	0.044 (2)	0.047 (2)	0.048 (2)	0.0112 (16)	0.0277 (17)	0.0258 (17)
C20	0.0414 (19)	0.0384 (18)	0.056 (2)	0.0012 (15)	0.0201 (17)	0.0258 (17)
C21	0.051 (2)	0.0247 (16)	0.050 (2)	0.0044 (14)	0.0191 (18)	0.0113 (15)
C22	0.0392 (17)	0.0256 (15)	0.0346 (17)	0.0069 (13)	0.0166 (14)	0.0102 (13)
N2	0.0263 (12)	0.0204 (11)	0.0182 (11)	0.0069 (9)	0.0085 (9)	0.0063 (9)
C23	0.0255 (14)	0.0277 (14)	0.0185 (13)	0.0042 (11)	0.0031 (11)	0.0059 (11)

C24	0.0247 (14)	0.0347 (15)	0.0221 (14)	0.0121 (12)	0.0058 (11)	0.0133 (12)
C25	0.0315 (16)	0.0305 (15)	0.0330 (16)	0.0108 (12)	0.0140 (13)	0.0120 (13)
C26	0.0450 (19)	0.0378 (17)	0.0352 (17)	0.0201 (15)	0.0166 (15)	0.0127 (14)
C27	0.0399 (18)	0.054 (2)	0.0351 (17)	0.0282 (16)	0.0193 (15)	0.0210 (16)
C28	0.0298 (17)	0.062 (2)	0.0378 (18)	0.0155 (16)	0.0146 (15)	0.0229 (17)
C29	0.0288 (16)	0.0428 (18)	0.0293 (16)	0.0059 (13)	0.0086 (13)	0.0128 (14)
C30	0.038 (2)	0.080 (3)	0.0338 (18)	0.0264 (19)	0.0095 (16)	0.0301 (19)
C31	0.064 (3)	0.106 (4)	0.040 (2)	0.045 (3)	0.017 (2)	0.046 (2)
C32	0.104 (4)	0.054 (2)	0.041 (2)	0.054 (3)	0.041 (2)	0.0347 (19)
C33	0.096 (4)	0.051 (2)	0.046 (2)	−0.004 (2)	0.030 (2)	0.024 (2)
C34	0.070 (3)	0.050 (2)	0.0279 (18)	−0.0117 (19)	0.0063 (18)	0.0170 (16)
C35	0.0396 (17)	0.0255 (14)	0.0216 (14)	0.0170 (12)	0.0115 (13)	0.0096 (11)
C36	0.0210 (13)	0.0240 (13)	0.0201 (13)	0.0064 (10)	0.0026 (11)	0.0080 (11)
N3	0.0195 (11)	0.0202 (11)	0.0158 (10)	0.0044 (8)	0.0049 (9)	0.0060 (9)
C37	0.0234 (13)	0.0202 (12)	0.0154 (12)	0.0034 (10)	0.0061 (10)	0.0054 (10)
Se2	0.02608 (15)	0.02286 (14)	0.01577 (13)	0.00262 (11)	0.00472 (11)	0.00219 (10)
C38	0.0199 (13)	0.0222 (13)	0.0154 (12)	0.0030 (10)	0.0035 (10)	0.0062 (10)
C39	0.0215 (13)	0.0240 (13)	0.0156 (12)	0.0093 (10)	0.0020 (10)	0.0062 (10)
C40	0.0247 (14)	0.0323 (15)	0.0244 (14)	0.0096 (12)	0.0077 (12)	0.0093 (12)
C41	0.0331 (16)	0.0427 (18)	0.0276 (15)	0.0167 (14)	0.0142 (13)	0.0084 (13)
C42	0.0388 (17)	0.0315 (16)	0.0228 (15)	0.0169 (13)	0.0053 (13)	0.0012 (12)
C43	0.0307 (16)	0.0229 (14)	0.0270 (15)	0.0073 (12)	0.0012 (12)	0.0041 (12)
C44	0.0258 (14)	0.0253 (14)	0.0221 (13)	0.0068 (11)	0.0053 (11)	0.0080 (11)
C45	0.0233 (13)	0.0209 (13)	0.0164 (12)	0.0044 (10)	0.0055 (11)	0.0049 (10)
C46	0.0202 (13)	0.0210 (13)	0.0200 (13)	0.0074 (10)	0.0036 (11)	0.0050 (10)
C47	0.0294 (15)	0.0276 (14)	0.0213 (14)	0.0084 (12)	0.0071 (12)	0.0082 (11)
C48	0.0373 (17)	0.0317 (16)	0.0198 (14)	0.0104 (13)	0.0013 (13)	0.0064 (12)
C49	0.0260 (15)	0.0278 (15)	0.0321 (16)	0.0048 (12)	−0.0040 (13)	0.0031 (13)
C50	0.0234 (15)	0.0359 (17)	0.0383 (18)	0.0030 (12)	0.0079 (13)	0.0083 (14)
C51	0.0265 (15)	0.0343 (16)	0.0253 (15)	0.0063 (12)	0.0093 (12)	0.0076 (12)
N4	0.0216 (11)	0.0202 (11)	0.0175 (11)	0.0054 (9)	0.0059 (9)	0.0046 (9)
C52	0.0249 (14)	0.0214 (13)	0.0221 (13)	0.0094 (11)	0.0080 (11)	0.0057 (11)
C53	0.0246 (14)	0.0258 (14)	0.0197 (13)	0.0034 (11)	0.0065 (11)	0.0014 (11)
C54	0.0337 (16)	0.0324 (16)	0.0297 (16)	0.0061 (13)	0.0127 (13)	0.0107 (13)
C55	0.047 (2)	0.045 (2)	0.0382 (19)	0.0003 (16)	0.0190 (16)	0.0175 (16)
C56	0.042 (2)	0.051 (2)	0.0402 (19)	−0.0052 (16)	0.0238 (17)	0.0052 (16)
C57	0.0378 (19)	0.050 (2)	0.048 (2)	0.0116 (16)	0.0242 (17)	0.0057 (17)
C58	0.0346 (17)	0.0434 (19)	0.0366 (18)	0.0158 (14)	0.0170 (15)	0.0125 (15)
Ag	0.03885 (14)	0.03004 (12)	0.02210 (12)	0.00221 (10)	0.00806 (10)	0.00678 (9)
Br	0.03466 (18)	0.0598 (2)	0.03813 (19)	0.01376 (16)	0.01402 (15)	0.02296 (16)
C59	0.078 (3)	0.079 (3)	0.044 (2)	0.035 (3)	0.031 (2)	0.008 (2)
Cl1	0.0467 (5)	0.0523 (5)	0.0417 (5)	0.0182 (4)	0.0221 (4)	0.0143 (4)
Cl2	0.0795 (8)	0.0507 (6)	0.1100 (11)	0.0188 (6)	0.0553 (8)	0.0001 (6)
C60	0.056 (3)	0.046 (2)	0.070 (3)	0.0032 (19)	0.023 (2)	0.006 (2)
Cl3	0.0393 (6)	0.0724 (8)	0.0863 (9)	0.0018 (5)	0.0126 (6)	0.0080 (6)
Cl4A	0.0709 (9)	0.0580 (8)	0.0583 (8)	−0.0081 (6)	0.0150 (6)	0.0272 (6)

Geometric parameters (Å, º)

C1—C2	1.381 (5)	C33—C34	1.387 (5)
C1—C6	1.390 (4)	C33—H33	0.9500
C1—H1	0.9500	C34—C35	1.352 (5)
C2—C3	1.379 (5)	C34—H34	0.9500
C2—H2	0.9500	C35—C36	1.515 (4)
C3—C4	1.362 (6)	C36—N3	1.471 (3)
C3—H3	0.9500	C36—H36A	0.9900
C4—C5	1.400 (6)	C36—H36B	0.9900
C4—H4	0.9500	N3—C37	1.351 (3)
C5—C6	1.383 (5)	N3—C38	1.397 (3)
C5—H5	0.9500	C37—N4	1.353 (3)
C6—C7	1.512 (4)	C37—Se2	1.866 (3)
C7—N1	1.466 (4)	Se2—Ag^{i}	2.7187 (4)
C7—H7A	0.9900	Se2—Ag	2.7677 (4)
C7—H7B	0.9900	C38—C45	1.359 (4)
N1—C8	1.352 (4)	C38—C39	1.475 (4)
N1—C9	1.400 (3)	C39—C40	1.386 (4)
C8—N2	1.351 (4)	C39—C44	1.397 (4)
C8—Se1	1.857 (3)	C40—C41	1.395 (4)
Se1—Ag	2.6899 (4)	C40—H40	0.9500
C9—C16	1.354 (4)	C41—C42	1.377 (5)
C9—C10	1.475 (4)	C41—H41	0.9500
C10—C11	1.384 (4)	C42—C43	1.380 (5)
C10—C15	1.386 (4)	C42—H42	0.9500
C11—C12	1.384 (4)	C43—C44	1.387 (4)
C11—H11	0.9500	C43—H43	0.9500
C12—C13	1.368 (5)	C44—H44	0.9500
C12—H12	0.9500	C45—N4	1.392 (3)
C13—C14	1.365 (6)	C45—C46	1.481 (4)
C13—H13	0.9500	C46—C51	1.389 (4)
C14—C15	1.389 (5)	C46—C47	1.392 (4)
C14—H14	0.9500	C47—C48	1.387 (4)
C15—H15	0.9500	C47—H47	0.9500
C16—N2	1.402 (3)	C48—C49	1.374 (5)
C16—C17	1.476 (4)	C48—H48	0.9500
C17—C18	1.389 (4)	C49—C50	1.380 (5)
C17—C22	1.396 (4)	C49—H49	0.9500
C18—C19	1.384 (5)	C50—C51	1.386 (4)
C18—H18	0.9500	C50—H50	0.9500
C19—C20	1.377 (5)	C51—H51	0.9500
C19—H19	0.9500	N4—C52	1.465 (3)
C20—C21	1.384 (5)	C52—C53	1.507 (4)
C20—H20	0.9500	C52—H52A	0.9900
C21—C22	1.387 (5)	C52—H52B	0.9900
C21—H21	0.9500	C53—C54	1.389 (4)
C22—H22	0.9500	C53—C58	1.395 (4)

N2—C23	1.469 (4)	C54—C55	1.392 (5)
C23—C24	1.518 (4)	C54—H54	0.9500
C23—H23A	0.9900	C55—C56	1.383 (6)
C23—H23B	0.9900	C55—H55	0.9500
C24—C29	1.387 (4)	C56—C57	1.378 (6)
C24—C25	1.393 (4)	C56—H56	0.9500
C25—C26	1.391 (5)	C57—C58	1.381 (5)
C25—H25	0.9500	C57—H57	0.9500
C26—C27	1.381 (5)	C58—H58	0.9500
C26—H26	0.9500	Ag—Br	2.6631 (4)
C27—C28	1.377 (5)	Ag—Se2^{i}	2.7186 (4)
C27—H27	0.9500	C59—Cl1	1.746 (4)
C28—C29	1.395 (5)	C59—Cl2	1.761 (6)
C28—H28	0.9500	C59—H59A	0.9900
C29—H29	0.9500	C59—H59B	0.9900
C30—C31	1.384 (6)	C60—Cl3	1.760 (5)
C30—C35	1.385 (5)	C60—Cl4A	1.762 (5)
C30—H30	0.9500	C60—Cl4B	1.88 (2)
C31—C32	1.372 (7)	C60—H60A	0.9900
C31—H31	0.9500	C60—H60B	0.9900
C32—C33	1.360 (7)	C60—H60C	0.9900
C32—H32	0.9500	C60—H60D	0.9900

C2—C1—C6	120.9 (3)	C35—C34—H34	119.4
C2—C1—H1	119.5	C33—C34—H34	119.4
C6—C1—H1	119.5	C34—C35—C30	118.8 (3)
C3—C2—C1	119.9 (3)	C34—C35—C36	122.7 (3)
C3—C2—H2	120.0	C30—C35—C36	118.4 (3)
C1—C2—H2	120.0	N3—C36—C35	112.0 (2)
C4—C3—C2	119.9 (3)	N3—C36—H36A	109.2
C4—C3—H3	120.0	C35—C36—H36A	109.2
C2—C3—H3	120.0	N3—C36—H36B	109.2
C3—C4—C5	120.7 (3)	C35—C36—H36B	109.2
C3—C4—H4	119.7	H36A—C36—H36B	107.9
C5—C4—H4	119.7	C37—N3—C38	109.6 (2)
C6—C5—C4	119.8 (4)	C37—N3—C36	123.6 (2)
C6—C5—H5	120.1	C38—N3—C36	125.3 (2)
C4—C5—H5	120.1	N3—C37—N4	106.8 (2)
C5—C6—C1	118.7 (3)	N3—C37—Se2	126.4 (2)
C5—C6—C7	121.4 (3)	N4—C37—Se2	126.8 (2)
C1—C6—C7	119.8 (3)	C37—Se2—Ag^{i}	108.43 (8)
N1—C7—C6	112.7 (2)	C37—Se2—Ag	100.72 (8)
N1—C7—H7A	109.1	Ag^{i}—Se2—Ag	73.649 (11)
C6—C7—H7A	109.1	C45—C38—N3	106.9 (2)
N1—C7—H7B	109.1	C45—C38—C39	127.7 (2)
C6—C7—H7B	109.1	N3—C38—C39	125.4 (2)
H7A—C7—H7B	107.8	C40—C39—C44	119.5 (3)
C8—N1—C9	109.8 (2)	C40—C39—C38	121.4 (3)

C8—N1—C7	124.5 (2)	C44—C39—C38	118.9 (3)
C9—N1—C7	125.7 (2)	C39—C40—C41	119.9 (3)
N2—C8—N1	106.8 (2)	C39—C40—H40	120.1
N2—C8—Se1	126.4 (2)	C41—C40—H40	120.1
N1—C8—Se1	126.8 (2)	C42—C41—C40	120.3 (3)
C8—Se1—Ag	94.72 (8)	C42—C41—H41	119.9
C16—C9—N1	106.7 (2)	C40—C41—H41	119.9
C16—C9—C10	130.3 (3)	C41—C42—C43	120.2 (3)
N1—C9—C10	122.8 (3)	C41—C42—H42	119.9
C11—C10—C15	118.5 (3)	C43—C42—H42	119.9
C11—C10—C9	119.6 (3)	C42—C43—C44	120.2 (3)
C15—C10—C9	121.9 (3)	C42—C43—H43	119.9
C10—C11—C12	120.7 (3)	C44—C43—H43	119.9
C10—C11—H11	119.6	C43—C44—C39	120.0 (3)
C12—C11—H11	119.6	C43—C44—H44	120.0
C13—C12—C11	120.1 (3)	C39—C44—H44	120.0
C13—C12—H12	120.0	C38—C45—N4	106.9 (2)
C11—C12—H12	120.0	C38—C45—C46	128.4 (2)
C14—C13—C12	120.2 (3)	N4—C45—C46	124.7 (2)
C14—C13—H13	119.9	C51—C46—C47	119.9 (3)
C12—C13—H13	119.9	C51—C46—C45	120.6 (3)
C13—C14—C15	120.2 (3)	C47—C46—C45	119.3 (3)
C13—C14—H14	119.9	C48—C47—C46	119.7 (3)
C15—C14—H14	119.9	C48—C47—H47	120.2
C10—C15—C14	120.3 (3)	C46—C47—H47	120.2
C10—C15—H15	119.8	C49—C48—C47	120.2 (3)
C14—C15—H15	119.8	C49—C48—H48	119.9
C9—C16—N2	107.2 (2)	C47—C48—H48	119.9
C9—C16—C17	129.5 (3)	C48—C49—C50	120.4 (3)
N2—C16—C17	123.1 (2)	C48—C49—H49	119.8
C18—C17—C22	119.4 (3)	C50—C49—H49	119.8
C18—C17—C16	121.6 (3)	C49—C50—C51	120.2 (3)
C22—C17—C16	119.0 (3)	C49—C50—H50	119.9
C19—C18—C17	120.5 (3)	C51—C50—H50	119.9
C19—C18—H18	119.8	C50—C51—C46	119.6 (3)
C17—C18—H18	119.8	C50—C51—H51	120.2
C20—C19—C18	120.0 (3)	C46—C51—H51	120.2
C20—C19—H19	120.0	C37—N4—C45	109.7 (2)
C18—C19—H19	120.0	C37—N4—C52	125.6 (2)
C19—C20—C21	120.1 (3)	C45—N4—C52	124.7 (2)
C19—C20—H20	120.0	N4—C52—C53	114.1 (2)
C21—C20—H20	120.0	N4—C52—H52A	108.7
C20—C21—C22	120.4 (3)	C53—C52—H52A	108.7
C20—C21—H21	119.8	N4—C52—H52B	108.7
C22—C21—H21	119.8	C53—C52—H52B	108.7
C21—C22—C17	119.6 (3)	H52A—C52—H52B	107.6
C21—C22—H22	120.2	C54—C53—C58	118.9 (3)
C17—C22—H22	120.2	C54—C53—C52	123.7 (3)

C8—N2—C16	109.5 (2)	C58—C53—C52	117.3 (3)
C8—N2—C23	124.8 (2)	C53—C54—C55	119.9 (3)
C16—N2—C23	125.1 (2)	C53—C54—H54	120.0
N2—C23—C24	115.0 (2)	C55—C54—H54	120.0
N2—C23—H23A	108.5	C56—C55—C54	120.4 (3)
C24—C23—H23A	108.5	C56—C55—H55	119.8
N2—C23—H23B	108.5	C54—C55—H55	119.8
C24—C23—H23B	108.5	C57—C56—C55	120.0 (3)
H23A—C23—H23B	107.5	C57—C56—H56	120.0
C29—C24—C25	118.5 (3)	C55—C56—H56	120.0
C29—C24—C23	119.8 (3)	C56—C57—C58	120.0 (3)
C25—C24—C23	121.6 (3)	C56—C57—H57	120.0
C26—C25—C24	120.2 (3)	C58—C57—H57	120.0
C26—C25—H25	119.9	C57—C58—C53	120.8 (3)
C24—C25—H25	119.9	C57—C58—H58	119.6
C27—C26—C25	120.7 (3)	C53—C58—H58	119.6
C27—C26—H26	119.7	Br—Ag—Se1	102.274 (13)
C25—C26—H26	119.7	Br—Ag—Se2^{i}	126.883 (14)
C28—C27—C26	119.8 (3)	Se1—Ag—Se2^{i}	100.026 (11)
C28—C27—H27	120.1	Br—Ag—Se2	109.628 (12)
C26—C27—H27	120.1	Se1—Ag—Se2	110.623 (12)
C27—C28—C29	119.7 (3)	Se2^{i}—Ag—Se2	106.352 (11)
C27—C28—H28	120.2	Cl1—C59—Cl2	112.3 (3)
C29—C28—H28	120.2	Cl1—C59—H59A	109.1
C24—C29—C28	121.2 (3)	Cl2—C59—H59A	109.1
C24—C29—H29	119.4	Cl1—C59—H59B	109.1
C28—C29—H29	119.4	Cl2—C59—H59B	109.1
C31—C30—C35	120.1 (4)	H59A—C59—H59B	107.9
C31—C30—H30	119.9	Cl3—C60—Cl4A	110.9 (2)
C35—C30—H30	119.9	Cl3—C60—Cl4B	104.9 (7)
C32—C31—C30	120.2 (4)	Cl3—C60—H60A	109.5
C32—C31—H31	119.9	Cl4A—C60—H60A	109.5
C30—C31—H31	119.9	Cl3—C60—H60B	109.5
C33—C32—C31	119.5 (4)	Cl4A—C60—H60B	109.5
C33—C32—H32	120.2	H60A—C60—H60B	108.0
C31—C32—H32	120.2	Cl3—C60—H60C	110.8
C32—C33—C34	120.0 (4)	Cl4B—C60—H60C	110.8
C32—C33—H33	120.0	Cl3—C60—H60D	110.8
C34—C33—H33	120.0	Cl4B—C60—H60D	110.8
C35—C34—C33	121.2 (4)	H60C—C60—H60D	108.8

C6—C1—C2—C3	0.0 (5)	C30—C31—C32—C33	−2.3 (7)
C1—C2—C3—C4	0.3 (5)	C31—C32—C33—C34	2.0 (7)
C2—C3—C4—C5	−0.3 (6)	C32—C33—C34—C35	−1.0 (8)
C3—C4—C5—C6	0.1 (6)	C33—C34—C35—C30	0.1 (6)
C4—C5—C6—C1	0.2 (5)	C33—C34—C35—C36	178.7 (4)
C4—C5—C6—C7	−179.6 (3)	C31—C30—C35—C34	−0.4 (6)
C2—C1—C6—C5	−0.2 (5)	C31—C30—C35—C36	−179.0 (4)

C2—C1—C6—C7	179.6 (3)	C34—C35—C36—N3	44.2 (4)
C5—C6—C7—N1	−120.5 (3)	C30—C35—C36—N3	−137.3 (3)
C1—C6—C7—N1	59.7 (4)	C35—C36—N3—C37	72.1 (3)
C6—C7—N1—C8	−111.0 (3)	C35—C36—N3—C38	−92.7 (3)
C6—C7—N1—C9	69.7 (3)	C38—N3—C37—N4	0.8 (3)
C9—N1—C8—N2	0.4 (3)	C36—N3—C37—N4	−166.1 (2)
C7—N1—C8—N2	−179.0 (2)	C38—N3—C37—Se2	178.82 (19)
C9—N1—C8—Se1	178.68 (19)	C36—N3—C37—Se2	11.9 (4)
C7—N1—C8—Se1	−0.7 (4)	N3—C37—Se2—Ag^{i}	128.8 (2)
N2—C8—Se1—Ag	94.9 (2)	N4—C37—Se2—Ag^{i}	−53.6 (2)
N1—C8—Se1—Ag	−83.1 (2)	N3—C37—Se2—Ag	52.6 (2)
C8—N1—C9—C16	−1.0 (3)	N4—C37—Se2—Ag	−129.7 (2)
C7—N1—C9—C16	178.4 (2)	C37—N3—C38—C45	−1.2 (3)
C8—N1—C9—C10	175.2 (2)	C36—N3—C38—C45	165.5 (2)
C7—N1—C9—C10	−5.5 (4)	C37—N3—C38—C39	176.5 (3)
C16—C9—C10—C11	59.5 (4)	C36—N3—C38—C39	−16.9 (4)
N1—C9—C10—C11	−115.8 (3)	C45—C38—C39—C40	123.0 (3)
C16—C9—C10—C15	−123.2 (4)	N3—C38—C39—C40	−54.1 (4)
N1—C9—C10—C15	61.6 (4)	C45—C38—C39—C44	−52.8 (4)
C15—C10—C11—C12	−0.5 (5)	N3—C38—C39—C44	130.1 (3)
C9—C10—C11—C12	176.9 (3)	C44—C39—C40—C41	−0.1 (4)
C10—C11—C12—C13	0.0 (6)	C38—C39—C40—C41	−176.0 (3)
C11—C12—C13—C14	−0.3 (6)	C39—C40—C41—C42	0.2 (5)
C12—C13—C14—C15	1.2 (7)	C40—C41—C42—C43	−0.3 (5)
C11—C10—C15—C14	1.4 (5)	C41—C42—C43—C44	0.2 (5)
C9—C10—C15—C14	−176.0 (3)	C42—C43—C44—C39	−0.1 (4)
C13—C14—C15—C10	−1.8 (6)	C40—C39—C44—C43	0.1 (4)
N1—C9—C16—N2	1.2 (3)	C38—C39—C44—C43	176.0 (2)
C10—C9—C16—N2	−174.6 (3)	N3—C38—C45—N4	1.0 (3)
N1—C9—C16—C17	−173.6 (3)	C39—C38—C45—N4	−176.5 (3)
C10—C9—C16—C17	10.6 (5)	N3—C38—C45—C46	−179.5 (3)
C9—C16—C17—C18	−121.8 (3)	C39—C38—C45—C46	2.9 (5)
N2—C16—C17—C18	64.1 (4)	C38—C45—C46—C51	111.2 (3)
C9—C16—C17—C22	58.3 (4)	N4—C45—C46—C51	−69.5 (4)
N2—C16—C17—C22	−115.7 (3)	C38—C45—C46—C47	−64.2 (4)
C22—C17—C18—C19	0.6 (5)	N4—C45—C46—C47	115.2 (3)
C16—C17—C18—C19	−179.3 (3)	C51—C46—C47—C48	0.7 (4)
C17—C18—C19—C20	0.2 (5)	C45—C46—C47—C48	176.1 (3)
C18—C19—C20—C21	−0.8 (6)	C46—C47—C48—C49	−1.0 (4)
C19—C20—C21—C22	0.5 (6)	C47—C48—C49—C50	0.3 (5)
C20—C21—C22—C17	0.3 (5)	C48—C49—C50—C51	0.7 (5)
C18—C17—C22—C21	−0.9 (5)	C49—C50—C51—C46	−1.0 (5)
C16—C17—C22—C21	179.0 (3)	C47—C46—C51—C50	0.3 (4)
N1—C8—N2—C16	0.4 (3)	C45—C46—C51—C50	−175.0 (3)
Se1—C8—N2—C16	−177.93 (19)	N3—C37—N4—C45	−0.1 (3)
N1—C8—N2—C23	171.8 (2)	Se2—C37—N4—C45	−178.15 (19)
Se1—C8—N2—C23	−6.5 (4)	N3—C37—N4—C52	−178.2 (2)
C9—C16—N2—C8	−1.0 (3)	Se2—C37—N4—C52	3.8 (4)

C17—C16—N2—C8	174.2 (2)	C38—C45—N4—C37	−0.6 (3)
C9—C16—N2—C23	−172.4 (2)	C46—C45—N4—C37	180.0 (2)
C17—C16—N2—C23	2.8 (4)	C38—C45—N4—C52	177.5 (2)
C8—N2—C23—C24	97.6 (3)	C46—C45—N4—C52	−2.0 (4)
C16—N2—C23—C24	−92.3 (3)	C37—N4—C52—C53	−89.4 (3)
N2—C23—C24—C29	134.4 (3)	C45—N4—C52—C53	92.9 (3)
N2—C23—C24—C25	−49.4 (4)	N4—C52—C53—C54	14.8 (4)
C29—C24—C25—C26	1.5 (4)	N4—C52—C53—C58	−167.5 (3)
C23—C24—C25—C26	−174.7 (3)	C58—C53—C54—C55	−0.1 (5)
C24—C25—C26—C27	−0.6 (5)	C52—C53—C54—C55	177.5 (3)
C25—C26—C27—C28	−0.3 (5)	C53—C54—C55—C56	−0.5 (5)
C26—C27—C28—C29	0.2 (5)	C54—C55—C56—C57	0.7 (6)
C25—C24—C29—C28	−1.7 (5)	C55—C56—C57—C58	−0.1 (6)
C23—C24—C29—C28	174.7 (3)	C56—C57—C58—C53	−0.5 (5)
C27—C28—C29—C24	0.8 (5)	C54—C53—C58—C57	0.7 (5)
C35—C30—C31—C32	1.5 (7)	C52—C53—C58—C57	−177.2 (3)

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+2.

catena-Poly[[[(1,3-dibenzyl-4,5-diphenyl-2-selenoimidazole-κSe)copper(I)]-μ-cyanido-κ^2C:*N*] acetonitrile monosolvate] (3)

Crystal data

$[Cu(CN)(C_{29}H_{24}N_2Se)]\cdot C_2H_3N$
M_r = 610.07
Monoclinic, $P2_1/c$
a = 13.7704 (3) Å
b = 14.3398 (3) Å
c = 28.4102 (7) Å
β = 93.024 (2)°
V = 5602.2 (2) Å^3
Z = 8
$F(000)$ = 2480
D_x = 1.447 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 23662 reflections
θ = 3.0–26.3°
μ = 2.11 mm^{-1}
T = 100 K
Rod, colourless
0.35 × 0.12 × 0.11 mm

Data collection

Rigaku SuperNova, Dual, Cu at zero, Atlas diffractometer
Radiation source: micro-focus sealed X-ray tube
Detector resolution: 10.3196 pixels mm^{-1}
ω scans
Absorption correction: gaussian (CrysAlis PRO; Rigaku OD, 2015)
T_{min} = 0.643, T_{max} = 0.851
71725 measured reflections
11392 independent reflections
10122 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
θ_{max} = 26.4°, θ_{min} = 2.8°
h = −17→17
k = −17→17
l = −34→35

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.119
S = 1.06
11392 reflections
687 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.045P)^2 + 17.9881P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$

$\Delta\rho_{max} = 2.04$ e Å^{-3}
$\Delta\rho_{min} = -0.56$ 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.7661 (3)	0.8105 (3)	0.56492 (13)	0.0266 (8)
H1	0.8151	0.7909	0.5448	0.032*
C2	0.6869 (3)	0.8612 (3)	0.54673 (14)	0.0324 (9)
H2	0.6819	0.8758	0.5141	0.039*
C3	0.6153 (3)	0.8906 (3)	0.57562 (15)	0.0332 (9)
H3	0.5620	0.9265	0.5631	0.040*
C4	0.6218 (3)	0.8673 (3)	0.62283 (15)	0.0343 (9)
H4	0.5720	0.8859	0.6427	0.041*
C5	0.7008 (3)	0.8171 (3)	0.64125 (13)	0.0253 (7)
H5	0.7051	0.8019	0.6738	0.030*
C6	0.7738 (2)	0.7886 (2)	0.61249 (12)	0.0189 (7)
C7	0.8551 (2)	0.7292 (2)	0.63438 (12)	0.0204 (7)
H7A	0.8727	0.7532	0.6664	0.024*
H7B	0.8310	0.6646	0.6377	0.024*
N1	0.9424 (2)	0.72729 (19)	0.60732 (9)	0.0183 (6)
C8	0.9750 (2)	0.6511 (2)	0.58509 (11)	0.0200 (7)
C9	1.0034 (2)	0.8028 (2)	0.60041 (11)	0.0174 (6)
C10	0.9878 (2)	0.8956 (2)	0.62140 (11)	0.0177 (6)
C11	0.9911 (2)	0.9067 (2)	0.67034 (12)	0.0218 (7)
H11	1.0039	0.8545	0.6903	0.026*
C12	0.9757 (3)	0.9937 (3)	0.68992 (13)	0.0262 (8)
H12	0.9773	1.0007	0.7232	0.031*
C13	0.9580 (3)	1.0703 (3)	0.66121 (14)	0.0281 (8)
H13	0.9476	1.1298	0.6747	0.034*
C14	0.9554 (3)	1.0602 (3)	0.61274 (14)	0.0284 (8)
H14	0.9438	1.1130	0.5930	0.034*
C15	0.9697 (3)	0.9730 (2)	0.59275 (12)	0.0237 (7)
H15	0.9671	0.9663	0.5594	0.028*
C16	1.0749 (2)	0.7722 (2)	0.57321 (11)	0.0188 (7)
C17	1.1600 (2)	0.8218 (2)	0.55600 (11)	0.0180 (6)
C18	1.1500 (3)	0.8798 (3)	0.51648 (13)	0.0301 (8)
H18	1.0883	0.8867	0.5003	0.036*
C19	1.2298 (3)	0.9274 (3)	0.50083 (15)	0.0357 (9)
H19	1.2227	0.9667	0.4739	0.043*
C20	1.3199 (3)	0.9176 (3)	0.52444 (14)	0.0313 (8)
H20	1.3743	0.9508	0.5139	0.038*

C21	1.3312 (3)	0.8598 (3)	0.56325 (13)	0.0281 (8)
H21	1.3933	0.8525	0.5790	0.034*
C22	1.2508 (3)	0.8122 (3)	0.57926 (12)	0.0235 (7)
H22	1.2582	0.7730	0.6062	0.028*
N2	1.0562 (2)	0.67822 (19)	0.56411 (9)	0.0195 (6)
C23	1.1121 (3)	0.6179 (2)	0.53376 (12)	0.0224 (7)
H23A	1.1495	0.6576	0.5127	0.027*
H23B	1.0663	0.5800	0.5137	0.027*
C24	1.1821 (3)	0.5528 (3)	0.56083 (13)	0.0253 (7)
C25	1.2045 (3)	0.5611 (3)	0.60863 (13)	0.0269 (8)
H25	1.1780	0.6111	0.6257	0.032*
C26	1.2657 (3)	0.4965 (3)	0.63204 (15)	0.0384 (10)
H26	1.2812	0.5033	0.6648	0.046*
C27	1.3040 (3)	0.4226 (4)	0.60772 (16)	0.0453 (11)
H27	1.3435	0.3774	0.6239	0.054*
C28	1.2840 (3)	0.4152 (3)	0.55930 (16)	0.0464 (11)
H28	1.3121	0.3661	0.5421	0.056*
C29	1.2230 (3)	0.4793 (3)	0.53623 (15)	0.0390 (10)
H29	1.2089	0.4733	0.5033	0.047*
Se1	0.92117 (3)	0.53117 (2)	0.58409 (2)	0.02398 (10)
Cu1	0.95522 (3)	0.49927 (3)	0.66587 (2)	0.02577 (11)
C59	0.9042 (3)	0.3973 (3)	0.69925 (13)	0.0282 (8)
N5	0.8749 (2)	0.3390 (2)	0.72193 (12)	0.0322 (7)
Cu2	0.82825 (3)	0.24571 (3)	0.76454 (2)	0.02719 (12)
Se2	0.66152 (3)	0.27327 (3)	0.77892 (2)	0.02914 (10)
C30	0.5614 (4)	0.3668 (4)	0.59119 (16)	0.0474 (11)
H30	0.5037	0.4033	0.5905	0.057*
C31	0.6036 (5)	0.3434 (5)	0.54929 (18)	0.0644 (16)
H31	0.5758	0.3649	0.5200	0.077*
C32	0.6879 (4)	0.2878 (4)	0.55079 (18)	0.0641 (17)
H32	0.7136	0.2659	0.5224	0.077*
C33	0.7316 (5)	0.2661 (5)	0.5926 (2)	0.084 (2)
H33	0.7924	0.2347	0.5937	0.101*
C34	0.6894 (4)	0.2887 (4)	0.63443 (18)	0.0614 (16)
H34	0.7205	0.2706	0.6636	0.074*
C35	0.6040 (3)	0.3366 (3)	0.63423 (13)	0.0280 (8)
C36	0.5573 (3)	0.3625 (3)	0.67936 (13)	0.0262 (8)
H36A	0.4960	0.3965	0.6714	0.031*
H36B	0.5404	0.3047	0.6961	0.031*
N3	0.6190 (2)	0.4204 (2)	0.71106 (10)	0.0216 (6)
C37	0.6612 (3)	0.3937 (2)	0.75286 (12)	0.0232 (7)
C38	0.6364 (2)	0.5153 (2)	0.70361 (12)	0.0199 (7)
C39	0.6004 (2)	0.5646 (2)	0.66026 (12)	0.0208 (7)
C40	0.6554 (3)	0.5642 (3)	0.62088 (13)	0.0283 (8)
H40	0.7164	0.5330	0.6219	0.034*
C41	0.6218 (3)	0.6090 (3)	0.57994 (14)	0.0364 (10)
H41	0.6600	0.6091	0.5531	0.044*
C42	0.5336 (3)	0.6530 (3)	0.57830 (15)	0.0427 (11)

H42	0.5104	0.6835	0.5502	0.051*
C43	0.4786 (3)	0.6529 (4)	0.61719 (19)	0.0559 (14)
H43	0.4170	0.6831	0.6157	0.067*
C44	0.5114 (3)	0.6097 (3)	0.65840 (16)	0.0430 (11)
H44	0.4732	0.6109	0.6853	0.052*
C45	0.6898 (2)	0.5460 (2)	0.74189 (12)	0.0194 (7)
C46	0.7299 (2)	0.6395 (2)	0.75337 (11)	0.0194 (7)
C47	0.8295 (3)	0.6547 (2)	0.75481 (12)	0.0233 (7)
H47	0.8723	0.6051	0.7480	0.028*
C48	0.8669 (3)	0.7425 (3)	0.76618 (12)	0.0276 (8)
H48	0.9352	0.7525	0.7673	0.033*
C49	0.8050 (3)	0.8150 (3)	0.77590 (13)	0.0313 (9)
H49	0.8305	0.8750	0.7836	0.038*
C50	0.7054 (3)	0.7999 (3)	0.77436 (13)	0.0314 (8)
H50	0.6629	0.8497	0.7811	0.038*
C51	0.6676 (3)	0.7132 (3)	0.76306 (12)	0.0251 (7)
H51	0.5993	0.7035	0.7619	0.030*
N4	0.7045 (2)	0.4698 (2)	0.77188 (10)	0.0214 (6)
C52	0.7539 (3)	0.4747 (2)	0.81887 (12)	0.0235 (7)
H52A	0.8209	0.4984	0.8159	0.028*
H52B	0.7586	0.4112	0.8325	0.028*
C53	0.7010 (3)	0.5374 (2)	0.85174 (12)	0.0223 (7)
C54	0.5996 (3)	0.5417 (3)	0.84997 (13)	0.0292 (8)
H54	0.5627	0.5049	0.8277	0.035*
C55	0.5525 (3)	0.5998 (3)	0.88072 (15)	0.0381 (10)
H55	0.4835	0.6028	0.8793	0.046*
C56	0.6058 (3)	0.6533 (3)	0.91339 (16)	0.0426 (10)
H56	0.5736	0.6932	0.9342	0.051*
C57	0.7057 (3)	0.6483 (3)	0.91558 (15)	0.0411 (10)
H57	0.7424	0.6846	0.9381	0.049*
C58	0.7534 (3)	0.5903 (3)	0.88486 (13)	0.0302 (8)
H58	0.8224	0.5871	0.8867	0.036*
C60	0.9083 (3)	0.1490 (2)	0.79035 (12)	0.0238 (7)
N6	0.9596 (2)	0.0943 (2)	0.80625 (11)	0.0280 (7)
N7	0.5766 (3)	0.4987 (3)	0.24282 (14)	0.0445 (9)
C61	0.6400 (3)	0.4766 (3)	0.22229 (16)	0.0365 (9)
C62	0.7238 (4)	0.4507 (4)	0.1964 (2)	0.0624 (16)
H62A	0.7024	0.4155	0.1682	0.094*
H62B	0.7677	0.4121	0.2164	0.094*
H62C	0.7581	0.5072	0.1871	0.094*
N8	0.9405 (3)	0.7629 (3)	0.47523 (14)	0.0484 (10)
C63	0.9333 (3)	0.7302 (3)	0.43914 (15)	0.0340 (9)
C64	0.9265 (4)	0.6919 (3)	0.39148 (16)	0.0476 (11)
H64A	0.8753	0.7245	0.3727	0.071*
H64B	0.9109	0.6253	0.3929	0.071*
H64C	0.9888	0.7001	0.3769	0.071*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0223 (18)	0.035 (2)	0.0229 (18)	0.0024 (15)	0.0034 (14)	0.0067 (15)
C2	0.030 (2)	0.039 (2)	0.028 (2)	−0.0039 (17)	−0.0033 (16)	0.0129 (17)
C3	0.0228 (19)	0.029 (2)	0.047 (2)	0.0033 (15)	−0.0051 (17)	0.0048 (17)
C4	0.0237 (19)	0.038 (2)	0.041 (2)	0.0055 (16)	0.0071 (17)	−0.0092 (18)
C5	0.0246 (18)	0.0293 (19)	0.0222 (18)	0.0007 (14)	0.0043 (14)	−0.0037 (14)
C6	0.0183 (16)	0.0174 (15)	0.0212 (16)	−0.0028 (12)	0.0018 (13)	−0.0007 (13)
C7	0.0200 (16)	0.0244 (17)	0.0173 (16)	0.0015 (13)	0.0062 (13)	0.0041 (13)
N1	0.0178 (14)	0.0198 (14)	0.0172 (13)	0.0013 (11)	0.0015 (11)	0.0004 (11)
C8	0.0218 (17)	0.0209 (16)	0.0170 (16)	0.0032 (13)	−0.0014 (13)	0.0002 (13)
C9	0.0169 (16)	0.0216 (16)	0.0135 (15)	0.0027 (12)	−0.0005 (12)	0.0018 (12)
C10	0.0155 (15)	0.0195 (16)	0.0184 (16)	0.0019 (12)	0.0037 (12)	−0.0004 (12)
C11	0.0187 (16)	0.0263 (17)	0.0204 (17)	0.0001 (13)	0.0004 (13)	−0.0008 (14)
C12	0.0219 (18)	0.0318 (19)	0.0251 (18)	−0.0009 (14)	0.0047 (14)	−0.0084 (15)
C13	0.0225 (18)	0.0231 (18)	0.039 (2)	0.0000 (14)	0.0069 (16)	−0.0098 (16)
C14	0.0283 (19)	0.0226 (18)	0.035 (2)	0.0040 (15)	0.0062 (16)	0.0042 (15)
C15	0.0266 (18)	0.0240 (17)	0.0207 (17)	0.0031 (14)	0.0040 (14)	0.0003 (14)
C16	0.0223 (17)	0.0209 (16)	0.0131 (15)	0.0050 (13)	−0.0019 (12)	0.0016 (12)
C17	0.0193 (16)	0.0207 (16)	0.0144 (15)	0.0036 (13)	0.0035 (12)	−0.0014 (12)
C18	0.0244 (18)	0.040 (2)	0.0260 (19)	0.0019 (16)	0.0010 (15)	0.0080 (16)
C19	0.032 (2)	0.043 (2)	0.033 (2)	−0.0007 (18)	0.0044 (17)	0.0143 (18)
C20	0.0261 (19)	0.032 (2)	0.037 (2)	−0.0038 (16)	0.0085 (16)	0.0020 (17)
C21	0.0207 (18)	0.033 (2)	0.031 (2)	0.0021 (15)	0.0011 (15)	−0.0050 (16)
C22	0.0243 (18)	0.0279 (18)	0.0185 (16)	0.0024 (14)	0.0021 (14)	0.0005 (14)
N2	0.0196 (14)	0.0224 (14)	0.0165 (14)	0.0035 (11)	0.0022 (11)	−0.0019 (11)
C23	0.0254 (18)	0.0247 (17)	0.0172 (16)	0.0039 (14)	0.0035 (14)	−0.0032 (13)
C24	0.0227 (18)	0.0296 (19)	0.0235 (18)	0.0052 (14)	0.0008 (14)	−0.0017 (15)
C25	0.0266 (19)	0.0305 (19)	0.0237 (18)	0.0027 (15)	0.0015 (14)	−0.0045 (15)
C26	0.035 (2)	0.053 (3)	0.026 (2)	0.0072 (19)	−0.0058 (17)	−0.0002 (18)
C27	0.038 (2)	0.057 (3)	0.040 (2)	0.016 (2)	−0.0028 (19)	0.009 (2)
C28	0.048 (3)	0.050 (3)	0.041 (2)	0.025 (2)	0.000 (2)	−0.004 (2)
C29	0.046 (2)	0.044 (2)	0.027 (2)	0.017 (2)	−0.0013 (18)	−0.0035 (18)
Se1	0.02574 (19)	0.02198 (18)	0.02412 (19)	−0.00181 (13)	0.00024 (14)	−0.00282 (13)
Cu1	0.0309 (2)	0.0204 (2)	0.0263 (2)	−0.00198 (17)	0.00483 (18)	0.00115 (17)
C59	0.036 (2)	0.0238 (18)	0.0250 (19)	−0.0014 (15)	0.0041 (16)	−0.0006 (15)
N5	0.0349 (18)	0.0259 (17)	0.0360 (18)	0.0016 (14)	0.0032 (14)	0.0023 (14)
Cu2	0.0365 (3)	0.0186 (2)	0.0263 (2)	0.00050 (18)	0.00004 (19)	0.00181 (17)
Se2	0.0374 (2)	0.02157 (18)	0.0290 (2)	−0.00150 (15)	0.00708 (16)	0.00452 (14)
C30	0.043 (3)	0.065 (3)	0.035 (2)	−0.007 (2)	−0.001 (2)	−0.007 (2)
C31	0.072 (4)	0.090 (4)	0.031 (3)	−0.021 (3)	0.002 (2)	−0.013 (3)
C32	0.066 (4)	0.089 (4)	0.039 (3)	−0.022 (3)	0.024 (3)	−0.037 (3)
C33	0.076 (4)	0.116 (6)	0.060 (4)	0.047 (4)	0.015 (3)	−0.030 (4)
C34	0.065 (3)	0.083 (4)	0.036 (3)	0.034 (3)	0.002 (2)	−0.013 (3)
C35	0.033 (2)	0.0274 (19)	0.0243 (18)	−0.0089 (15)	0.0049 (15)	−0.0091 (15)
C36	0.0266 (19)	0.0271 (18)	0.0253 (18)	−0.0062 (15)	0.0028 (15)	−0.0051 (15)
N3	0.0247 (15)	0.0220 (14)	0.0185 (14)	−0.0006 (12)	0.0041 (12)	−0.0025 (11)

C37	0.0268 (18)	0.0210 (17)	0.0224 (17)	0.0010 (14)	0.0070 (14)	−0.0007 (14)
C38	0.0188 (16)	0.0213 (16)	0.0202 (17)	0.0006 (13)	0.0056 (13)	−0.0002 (13)
C39	0.0215 (17)	0.0225 (16)	0.0181 (16)	−0.0036 (13)	−0.0009 (13)	−0.0023 (13)
C40	0.033 (2)	0.0285 (19)	0.0243 (18)	−0.0025 (15)	0.0062 (15)	−0.0016 (15)
C41	0.054 (3)	0.036 (2)	0.0202 (19)	−0.0099 (19)	0.0053 (18)	−0.0018 (16)
C42	0.052 (3)	0.044 (2)	0.030 (2)	−0.014 (2)	−0.018 (2)	0.0143 (19)
C43	0.033 (2)	0.069 (3)	0.065 (3)	0.012 (2)	−0.003 (2)	0.035 (3)
C44	0.033 (2)	0.057 (3)	0.040 (2)	0.015 (2)	0.0140 (19)	0.020 (2)
C45	0.0185 (16)	0.0216 (16)	0.0188 (16)	0.0041 (13)	0.0068 (13)	−0.0007 (13)
C46	0.0248 (17)	0.0213 (16)	0.0123 (15)	0.0006 (13)	0.0010 (13)	0.0010 (12)
C47	0.0267 (18)	0.0257 (18)	0.0175 (16)	0.0010 (14)	0.0017 (14)	0.0015 (13)
C48	0.030 (2)	0.032 (2)	0.0205 (17)	−0.0070 (16)	0.0002 (15)	0.0021 (15)
C49	0.049 (2)	0.0245 (19)	0.0204 (18)	−0.0069 (17)	−0.0023 (16)	0.0005 (14)
C50	0.044 (2)	0.0229 (18)	0.0271 (19)	0.0058 (16)	0.0042 (17)	−0.0024 (15)
C51	0.0247 (18)	0.0271 (18)	0.0235 (18)	0.0025 (14)	0.0032 (14)	−0.0005 (14)
N4	0.0261 (15)	0.0209 (14)	0.0174 (14)	0.0020 (12)	0.0027 (11)	0.0013 (11)
C52	0.0244 (18)	0.0251 (17)	0.0209 (17)	0.0003 (14)	−0.0015 (14)	0.0051 (14)
C53	0.0267 (18)	0.0249 (17)	0.0155 (16)	−0.0027 (14)	0.0035 (13)	0.0037 (13)
C54	0.0261 (19)	0.036 (2)	0.0251 (19)	−0.0069 (16)	0.0014 (15)	−0.0022 (16)
C55	0.028 (2)	0.054 (3)	0.032 (2)	0.0029 (19)	0.0047 (17)	−0.0054 (19)
C56	0.048 (3)	0.044 (2)	0.038 (2)	−0.002 (2)	0.014 (2)	−0.0121 (19)
C57	0.046 (3)	0.046 (2)	0.032 (2)	−0.018 (2)	0.0035 (19)	−0.0149 (19)
C58	0.029 (2)	0.036 (2)	0.0264 (19)	−0.0104 (16)	0.0034 (15)	−0.0013 (16)
C60	0.0297 (19)	0.0225 (17)	0.0195 (17)	−0.0037 (15)	0.0045 (14)	0.0009 (14)
N6	0.0349 (18)	0.0267 (16)	0.0229 (16)	−0.0004 (14)	0.0078 (13)	−0.0035 (13)
N7	0.037 (2)	0.047 (2)	0.050 (2)	−0.0062 (17)	0.0076 (18)	0.0022 (18)
C61	0.031 (2)	0.037 (2)	0.042 (2)	−0.0038 (18)	−0.0033 (19)	0.0119 (18)
C62	0.044 (3)	0.064 (3)	0.081 (4)	0.023 (3)	0.020 (3)	0.030 (3)
N8	0.042 (2)	0.072 (3)	0.032 (2)	−0.003 (2)	−0.0019 (17)	−0.0028 (19)
C63	0.032 (2)	0.036 (2)	0.034 (2)	0.0025 (17)	−0.0027 (17)	0.0068 (18)
C64	0.064 (3)	0.040 (2)	0.038 (2)	0.012 (2)	0.003 (2)	−0.005 (2)

Geometric parameters (Å, º)

C1—C6	1.386 (5)	C30—H30	0.9500
C1—C2	1.388 (5)	C31—C32	1.407 (9)
C1—H1	0.9500	C31—H31	0.9500
C2—C3	1.382 (6)	C32—C33	1.340 (9)
C2—H2	0.9500	C32—H32	0.9500
C3—C4	1.381 (6)	C33—C34	1.389 (7)
C3—H3	0.9500	C33—H33	0.9500
C4—C5	1.384 (5)	C34—C35	1.360 (6)
C4—H4	0.9500	C34—H34	0.9500
C5—C6	1.391 (5)	C35—C36	1.512 (5)
C5—H5	0.9500	C36—N3	1.464 (4)
C6—C7	1.513 (5)	C36—H36A	0.9900
C7—N1	1.461 (4)	C36—H36B	0.9900
C7—H7A	0.9900	N3—C37	1.350 (5)

C7—H7B	0.9900	N3—C38	1.399 (4)
N1—C8	1.351 (4)	C37—N4	1.343 (5)
N1—C9	1.391 (4)	C38—C45	1.354 (5)
C8—N2	1.351 (4)	C38—C39	1.483 (5)
C8—Se1	1.872 (3)	C39—C40	1.383 (5)
C9—C16	1.356 (5)	C39—C44	1.385 (5)
C9—C10	1.478 (4)	C40—C41	1.387 (6)
C10—C15	1.391 (5)	C40—H40	0.9500
C10—C11	1.398 (5)	C41—C42	1.367 (7)
C11—C12	1.386 (5)	C41—H41	0.9500
C11—H11	0.9500	C42—C43	1.372 (7)
C12—C13	1.382 (5)	C42—H42	0.9500
C12—H12	0.9500	C43—C44	1.379 (6)
C13—C14	1.383 (5)	C43—H43	0.9500
C13—H13	0.9500	C44—H44	0.9500
C14—C15	1.391 (5)	C45—N4	1.394 (4)
C14—H14	0.9500	C45—C46	1.480 (5)
C15—H15	0.9500	C46—C47	1.387 (5)
C16—N2	1.393 (4)	C46—C51	1.397 (5)
C16—C17	1.478 (5)	C47—C48	1.391 (5)
C17—C22	1.389 (5)	C47—H47	0.9500
C17—C18	1.398 (5)	C48—C49	1.382 (6)
C18—C19	1.386 (6)	C48—H48	0.9500
C18—H18	0.9500	C49—C50	1.386 (6)
C19—C20	1.386 (6)	C49—H49	0.9500
C19—H19	0.9500	C50—C51	1.380 (5)
C20—C21	1.382 (6)	C50—H50	0.9500
C20—H20	0.9500	C51—H51	0.9500
C21—C22	1.398 (5)	N4—C52	1.468 (4)
C21—H21	0.9500	C52—C53	1.512 (5)
C22—H22	0.9500	C52—H52A	0.9900
N2—C23	1.468 (4)	C52—H52B	0.9900
C23—C24	1.521 (5)	C53—C58	1.382 (5)
C23—H23A	0.9900	C53—C54	1.395 (5)
C23—H23B	0.9900	C54—C55	1.392 (6)
C24—C25	1.382 (5)	C54—H54	0.9500
C24—C29	1.399 (5)	C55—C56	1.384 (6)
C25—C26	1.397 (6)	C55—H55	0.9500
C25—H25	0.9500	C56—C57	1.375 (6)
C26—C27	1.384 (6)	C56—H56	0.9500
C26—H26	0.9500	C57—C58	1.395 (6)
C27—C28	1.393 (6)	C57—H57	0.9500
C27—H27	0.9500	C58—H58	0.9500
C28—C29	1.386 (6)	C60—N6	1.134 (5)
C28—H28	0.9500	N6—Cu1^{ii}	1.939 (3)
C29—H29	0.9500	N7—C61	1.121 (6)
Se1—Cu1	2.3900 (6)	C61—C62	1.450 (7)
Cu1—C59	1.898 (4)	C62—H62A	0.9800

Cu1—N6^{i}	1.939 (3)	C62—H62B	0.9800
C59—N5	1.141 (5)	C62—H62C	0.9800
N5—Cu2	1.937 (3)	N8—C63	1.127 (6)
Cu2—C60	1.895 (4)	C63—C64	1.460 (6)
Cu2—Se2	2.3861 (6)	C64—H64A	0.9800
Se2—C37	1.879 (3)	C64—H64B	0.9800
C30—C31	1.393 (7)	C64—H64C	0.9800
C30—C35	1.397 (6)		

C6—C1—C2	120.0 (3)	C30—C31—C32	119.4 (5)
C6—C1—H1	120.0	C30—C31—H31	120.3
C2—C1—H1	120.0	C32—C31—H31	120.3
C3—C2—C1	120.7 (4)	C33—C32—C31	119.3 (5)
C3—C2—H2	119.7	C33—C32—H32	120.3
C1—C2—H2	119.7	C31—C32—H32	120.3
C4—C3—C2	119.4 (4)	C32—C33—C34	121.0 (6)
C4—C3—H3	120.3	C32—C33—H33	119.5
C2—C3—H3	120.3	C34—C33—H33	119.5
C3—C4—C5	120.2 (4)	C35—C34—C33	121.0 (5)
C3—C4—H4	119.9	C35—C34—H34	119.5
C5—C4—H4	119.9	C33—C34—H34	119.5
C4—C5—C6	120.6 (3)	C34—C35—C30	118.9 (4)
C4—C5—H5	119.7	C34—C35—C36	121.8 (4)
C6—C5—H5	119.7	C30—C35—C36	119.2 (4)
C1—C6—C5	119.1 (3)	N3—C36—C35	113.7 (3)
C1—C6—C7	123.1 (3)	N3—C36—H36A	108.8
C5—C6—C7	117.8 (3)	C35—C36—H36A	108.8
N1—C7—C6	113.9 (3)	N3—C36—H36B	108.8
N1—C7—H7A	108.8	C35—C36—H36B	108.8
C6—C7—H7A	108.8	H36A—C36—H36B	107.7
N1—C7—H7B	108.8	C37—N3—C38	109.9 (3)
C6—C7—H7B	108.8	C37—N3—C36	126.1 (3)
H7A—C7—H7B	107.7	C38—N3—C36	123.8 (3)
C8—N1—C9	110.2 (3)	N4—C37—N3	106.5 (3)
C8—N1—C7	124.4 (3)	N4—C37—Se2	126.6 (3)
C9—N1—C7	125.4 (3)	N3—C37—Se2	126.9 (3)
N2—C8—N1	106.0 (3)	C45—C38—N3	106.6 (3)
N2—C8—Se1	126.5 (2)	C45—C38—C39	130.9 (3)
N1—C8—Se1	127.5 (3)	N3—C38—C39	122.5 (3)
C16—C9—N1	106.8 (3)	C40—C39—C44	119.5 (3)
C16—C9—C10	130.3 (3)	C40—C39—C38	119.8 (3)
N1—C9—C10	122.9 (3)	C44—C39—C38	120.7 (3)
C15—C10—C11	119.1 (3)	C39—C40—C41	120.2 (4)
C15—C10—C9	120.5 (3)	C39—C40—H40	119.9
C11—C10—C9	120.4 (3)	C41—C40—H40	119.9
C12—C11—C10	120.3 (3)	C42—C41—C40	120.0 (4)
C12—C11—H11	119.9	C42—C41—H41	120.0
C10—C11—H11	119.9	C40—C41—H41	120.0

C13—C12—C11	120.3 (3)	C41—C42—C43	120.0 (4)
C13—C12—H12	119.9	C41—C42—H42	120.0
C11—C12—H12	119.9	C43—C42—H42	120.0
C12—C13—C14	119.9 (3)	C42—C43—C44	120.9 (4)
C12—C13—H13	120.0	C42—C43—H43	119.6
C14—C13—H13	120.0	C44—C43—H43	119.6
C13—C14—C15	120.3 (3)	C43—C44—C39	119.5 (4)
C13—C14—H14	119.9	C43—C44—H44	120.3
C15—C14—H14	119.9	C39—C44—H44	120.3
C10—C15—C14	120.2 (3)	C38—C45—N4	106.9 (3)
C10—C15—H15	119.9	C38—C45—C46	130.8 (3)
C14—C15—H15	119.9	N4—C45—C46	122.4 (3)
C9—C16—N2	106.7 (3)	C47—C46—C51	119.4 (3)
C9—C16—C17	130.1 (3)	C47—C46—C45	120.4 (3)
N2—C16—C17	123.1 (3)	C51—C46—C45	120.1 (3)
C22—C17—C18	119.3 (3)	C46—C47—C48	120.2 (3)
C22—C17—C16	120.3 (3)	C46—C47—H47	119.9
C18—C17—C16	120.4 (3)	C48—C47—H47	119.9
C19—C18—C17	120.3 (3)	C49—C48—C47	120.2 (4)
C19—C18—H18	119.9	C49—C48—H48	119.9
C17—C18—H18	119.9	C47—C48—H48	119.9
C18—C19—C20	119.9 (4)	C48—C49—C50	119.7 (4)
C18—C19—H19	120.0	C48—C49—H49	120.2
C20—C19—H19	120.0	C50—C49—H49	120.2
C21—C20—C19	120.5 (4)	C51—C50—C49	120.6 (4)
C21—C20—H20	119.8	C51—C50—H50	119.7
C19—C20—H20	119.8	C49—C50—H50	119.7
C20—C21—C22	119.7 (3)	C50—C51—C46	119.9 (3)
C20—C21—H21	120.2	C50—C51—H51	120.0
C22—C21—H21	120.2	C46—C51—H51	120.0
C17—C22—C21	120.3 (3)	C37—N4—C45	110.1 (3)
C17—C22—H22	119.8	C37—N4—C52	125.4 (3)
C21—C22—H22	119.8	C45—N4—C52	124.3 (3)
C8—N2—C16	110.2 (3)	N4—C52—C53	112.0 (3)
C8—N2—C23	124.1 (3)	N4—C52—H52A	109.2
C16—N2—C23	125.5 (3)	C53—C52—H52A	109.2
N2—C23—C24	113.8 (3)	N4—C52—H52B	109.2
N2—C23—H23A	108.8	C53—C52—H52B	109.2
C24—C23—H23A	108.8	H52A—C52—H52B	107.9
N2—C23—H23B	108.8	C58—C53—C54	119.1 (3)
C24—C23—H23B	108.8	C58—C53—C52	119.7 (3)
H23A—C23—H23B	107.7	C54—C53—C52	121.2 (3)
C25—C24—C29	118.7 (3)	C55—C54—C53	120.2 (4)
C25—C24—C23	123.1 (3)	C55—C54—H54	119.9
C29—C24—C23	118.1 (3)	C53—C54—H54	119.9
C24—C25—C26	120.6 (4)	C56—C55—C54	120.3 (4)
C24—C25—H25	119.7	C56—C55—H55	119.9
C26—C25—H25	119.7	C54—C55—H55	119.9

C27—C26—C25	120.4 (4)	C57—C56—C55	119.7 (4)
C27—C26—H26	119.8	C57—C56—H56	120.2
C25—C26—H26	119.8	C55—C56—H56	120.2
C26—C27—C28	119.4 (4)	C56—C57—C58	120.4 (4)
C26—C27—H27	120.3	C56—C57—H57	119.8
C28—C27—H27	120.3	C58—C57—H57	119.8
C29—C28—C27	119.9 (4)	C53—C58—C57	120.4 (4)
C29—C28—H28	120.0	C53—C58—H58	119.8
C27—C28—H28	120.0	C57—C58—H58	119.8
C28—C29—C24	120.9 (4)	N6—C60—Cu2	176.7 (3)
C28—C29—H29	119.6	C60—N6—Cu1^{ii}	178.6 (3)
C24—C29—H29	119.6	N7—C61—C62	178.0 (5)
C8—Se1—Cu1	95.96 (10)	C61—C62—H62A	109.5
C59—Cu1—N6^{i}	124.68 (14)	C61—C62—H62B	109.5
C59—Cu1—Se1	125.06 (12)	H62A—C62—H62B	109.5
N6^{i}—Cu1—Se1	110.25 (9)	C61—C62—H62C	109.5
N5—C59—Cu1	175.6 (3)	H62A—C62—H62C	109.5
C59—N5—Cu2	175.7 (3)	H62B—C62—H62C	109.5
C60—Cu2—N5	122.84 (15)	N8—C63—C64	177.2 (5)
C60—Cu2—Se2	126.88 (11)	C63—C64—H64A	109.5
N5—Cu2—Se2	110.28 (10)	C63—C64—H64B	109.5
C37—Se2—Cu2	93.84 (11)	H64A—C64—H64B	109.5
C31—C30—C35	119.8 (5)	C63—C64—H64C	109.5
C31—C30—H30	120.1	H64A—C64—H64C	109.5
C35—C30—H30	120.1	H64B—C64—H64C	109.5

C6—C1—C2—C3	0.3 (6)	C35—C30—C31—C32	1.3 (8)
C1—C2—C3—C4	−1.5 (6)	C30—C31—C32—C33	−6.6 (9)
C2—C3—C4—C5	1.7 (6)	C31—C32—C33—C34	7.2 (11)
C3—C4—C5—C6	−0.7 (6)	C32—C33—C34—C35	−2.3 (11)
C2—C1—C6—C5	0.8 (5)	C33—C34—C35—C30	−3.1 (9)
C2—C1—C6—C7	176.6 (3)	C33—C34—C35—C36	−179.5 (6)
C4—C5—C6—C1	−0.5 (5)	C31—C30—C35—C34	3.5 (7)
C4—C5—C6—C7	−176.6 (3)	C31—C30—C35—C36	−180.0 (4)
C1—C6—C7—N1	22.7 (5)	C34—C35—C36—N3	58.9 (6)
C5—C6—C7—N1	−161.4 (3)	C30—C35—C36—N3	−117.5 (4)
C6—C7—N1—C8	−112.7 (3)	C35—C36—N3—C37	−110.2 (4)
C6—C7—N1—C9	66.9 (4)	C35—C36—N3—C38	75.0 (4)
C9—N1—C8—N2	−0.1 (4)	C38—N3—C37—N4	0.2 (4)
C7—N1—C8—N2	179.5 (3)	C36—N3—C37—N4	−175.2 (3)
C9—N1—C8—Se1	178.8 (2)	C38—N3—C37—Se2	−178.8 (2)
C7—N1—C8—Se1	−1.5 (5)	C36—N3—C37—Se2	5.8 (5)
C8—N1—C9—C16	0.2 (4)	Cu2—Se2—C37—N4	−72.0 (3)
C7—N1—C9—C16	−179.5 (3)	Cu2—Se2—C37—N3	106.7 (3)
C8—N1—C9—C10	−178.5 (3)	C37—N3—C38—C45	−0.3 (4)
C7—N1—C9—C10	1.8 (5)	C36—N3—C38—C45	175.2 (3)
C16—C9—C10—C15	63.8 (5)	C37—N3—C38—C39	179.0 (3)
N1—C9—C10—C15	−117.8 (4)	C36—N3—C38—C39	−5.5 (5)

C16—C9—C10—C11	−116.2 (4)	C45—C38—C39—C40	92.5 (5)
N1—C9—C10—C11	62.2 (4)	N3—C38—C39—C40	−86.6 (4)
C15—C10—C11—C12	0.5 (5)	C45—C38—C39—C44	−88.8 (5)
C9—C10—C11—C12	−179.5 (3)	N3—C38—C39—C44	92.1 (5)
C10—C11—C12—C13	−0.7 (5)	C44—C39—C40—C41	0.4 (6)
C11—C12—C13—C14	0.1 (5)	C38—C39—C40—C41	179.1 (3)
C12—C13—C14—C15	0.6 (6)	C39—C40—C41—C42	−0.7 (6)
C11—C10—C15—C14	0.2 (5)	C40—C41—C42—C43	0.2 (7)
C9—C10—C15—C14	−179.8 (3)	C41—C42—C43—C44	0.6 (8)
C13—C14—C15—C10	−0.7 (6)	C42—C43—C44—C39	−0.9 (8)
N1—C9—C16—N2	−0.1 (3)	C40—C39—C44—C43	0.4 (7)
C10—C9—C16—N2	178.4 (3)	C38—C39—C44—C43	−178.3 (4)
N1—C9—C16—C17	−178.4 (3)	N3—C38—C45—N4	0.3 (4)
C10—C9—C16—C17	0.1 (6)	C39—C38—C45—N4	−178.9 (3)
C9—C16—C17—C22	98.5 (4)	N3—C38—C45—C46	179.5 (3)
N2—C16—C17—C22	−79.5 (4)	C39—C38—C45—C46	0.3 (6)
C9—C16—C17—C18	−80.8 (5)	C38—C45—C46—C47	−111.4 (4)
N2—C16—C17—C18	101.2 (4)	N4—C45—C46—C47	67.7 (4)
C22—C17—C18—C19	−0.2 (6)	C38—C45—C46—C51	68.9 (5)
C16—C17—C18—C19	179.1 (4)	N4—C45—C46—C51	−112.1 (4)
C17—C18—C19—C20	0.0 (6)	C51—C46—C47—C48	0.5 (5)
C18—C19—C20—C21	0.7 (6)	C45—C46—C47—C48	−179.2 (3)
C19—C20—C21—C22	−1.1 (6)	C46—C47—C48—C49	−0.3 (5)
C18—C17—C22—C21	−0.1 (5)	C47—C48—C49—C50	0.1 (5)
C16—C17—C22—C21	−179.4 (3)	C48—C49—C50—C51	−0.2 (6)
C20—C21—C22—C17	0.8 (5)	C49—C50—C51—C46	0.4 (6)
N1—C8—N2—C16	0.0 (4)	C47—C46—C51—C50	−0.6 (5)
Se1—C8—N2—C16	−178.9 (2)	C45—C46—C51—C50	179.1 (3)
N1—C8—N2—C23	−176.4 (3)	N3—C37—N4—C45	0.0 (4)
Se1—C8—N2—C23	4.6 (5)	Se2—C37—N4—C45	178.9 (2)
C9—C16—N2—C8	0.0 (4)	N3—C37—N4—C52	175.7 (3)
C17—C16—N2—C8	178.5 (3)	Se2—C37—N4—C52	−5.3 (5)
C9—C16—N2—C23	176.4 (3)	C38—C45—N4—C37	−0.1 (4)
C17—C16—N2—C23	−5.1 (5)	C46—C45—N4—C37	−179.4 (3)
C8—N2—C23—C24	−81.7 (4)	C38—C45—N4—C52	−175.9 (3)
C16—N2—C23—C24	102.4 (4)	C46—C45—N4—C52	4.8 (5)
N2—C23—C24—C25	−11.3 (5)	C37—N4—C52—C53	−113.1 (4)
N2—C23—C24—C29	166.4 (4)	C45—N4—C52—C53	62.0 (4)
C29—C24—C25—C26	−0.9 (6)	N4—C52—C53—C58	−145.1 (3)
C23—C24—C25—C26	176.9 (4)	N4—C52—C53—C54	36.2 (5)
C24—C25—C26—C27	−0.8 (7)	C58—C53—C54—C55	1.1 (6)
C25—C26—C27—C28	2.5 (7)	C52—C53—C54—C55	179.8 (4)
C26—C27—C28—C29	−2.6 (8)	C53—C54—C55—C56	−0.3 (6)
C27—C28—C29—C24	1.0 (8)	C54—C55—C56—C57	−0.4 (7)
C25—C24—C29—C28	0.8 (7)	C55—C56—C57—C58	0.5 (7)
C23—C24—C29—C28	−177.1 (4)	C54—C53—C58—C57	−1.0 (6)

N2—C8—Se1—Cu1	111.9 (3)	C52—C53—C58—C57	−179.8 (4)
N1—C8—Se1—Cu1	−66.9 (3)	C56—C57—C58—C53	0.3 (7)

Symmetry codes: (i) −*x*+2, *y*+1/2, −*z*+3/2; (ii) −*x*+2, *y*−1/2, −*z*+3/2.