

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

Hexakis(μ_3 -2-hydroxynaphthalene-1-carboxaldehyde thiosemicarbazone- $\kappa^3N^2:S:S$)hexasilver(I) *N,N*-dimethylformamide tetrasolvate

Qiaozhen Sun,^{a*} Liyuan Chai,^b Hui Liu^b and Junke Wang^a

^aDepartment of Materials Chemistry, School of Materials Science and Engineering, Key Laboratory of Nonferrous Metal of the Ministry of Education, Central South University, Changsha 410083, People's Republic of China, and ^bChinese National Engineering Research Center for Control & Treatment of Heavy Metal Pollution (CNERC-CTHMP), Environmental Engineering Institute, School of Metallurgical Science and Engineering, Central South University, Changsha 410083, People's Republic of China

Correspondence e-mail: rosesunqz@yahoo.com.cn

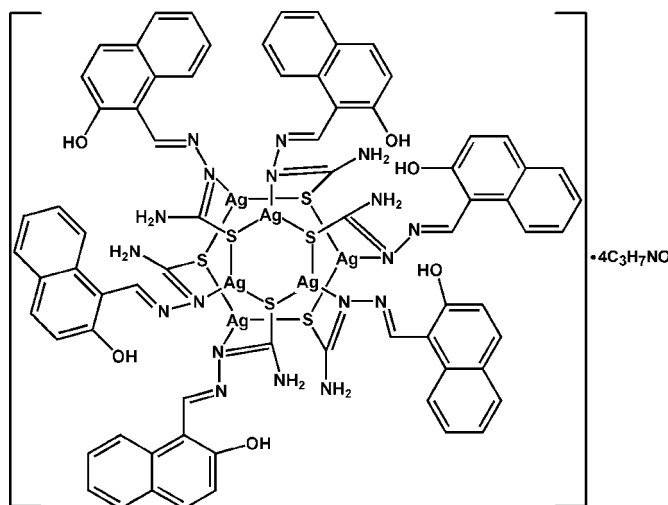
Received 9 November 2012; accepted 8 December 2012

Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(C-C) = 0.007$ Å; disorder in solvent or counterion; R factor = 0.046; wR factor = 0.145; data-to-parameter ratio = 15.1.

In the title compound, $[Ag_6(C_{12}H_{10}N_3OS)_6] \cdot 4C_3H_7NO$, the hexanuclear complex molecule lies about an inversion center. The six Ag atoms form a distorted octahedron, with $Ag \cdots Ag$ distances in the range 2.933 (1)–3.401 (1) Å. Each Ag atom is surrounded by one N atom and two thiolate S atoms from two deprotonated 2-hydroxy-1-naphthaldehyde thiosemicarbazone ligands. Each ligand coordinates three Ag atoms *via* a bridging thiolate S atom and a monodentate N atom, thus two Ag_3S_3 hexagonal rings are linked together. Two dimethylformamide solvent molecules are located in four sets of sites with half-occupancy and form $O \cdots H-N$ hydrogen bonds to the complex molecule. Intramolecular $O-H \cdots N$ hydrogen bonds are also present. The discrete hexanuclear clusters are further linked through $\pi-\pi$ interactions into layers parallel to (001), the shortest distance between the centroids of aromatic rings being 3.698 (2) Å.

Related literature

For the structure and luminescent properties of d^{10} metal complexes, see: Brito *et al.* (2011); Forward *et al.* (1995). For structures of related complexes with thiosemicarbazone Schiff base ligands, see: Ashfield *et al.* (2004); Castiñeiras & Pedrido (2009); Li *et al.* (2010); Onodera *et al.* (2007); Pedrido *et al.* (2009); Sun (2011); Sun *et al.* (2012); Sun & Chai (2012); Xu *et al.* (2011). For bond-length data, see: Han *et al.* (2004).



Experimental

Crystal data

 $[Ag_6(C_{12}H_{10}N_3OS)_6] \cdot 4C_3H_7NO$ $M_r = 2405.34$ Monoclinic, $C2/c$ $a = 24.604$ (3) Å $b = 18.877$ (3) Å $c = 24.816$ (3) Å $\beta = 94.763$ (3)° $V = 11486$ (3) Å³ $Z = 4$ Mo $K\alpha$ radiation $\mu = 1.17$ mm⁻¹ $T = 293$ K

0.22 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD

diffractometer

Absorption correction: multi-scan

(SADABS; Sheldrick, 1996)

 $T_{\min} = 0.238$, $T_{\max} = 0.373$

28454 measured reflections

10056 independent reflections

7829 reflections with $I > 2s(I)$ $R_{\text{int}} = 0.042$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.046$ $wR(F^2) = 0.145$ $S = 1.08$

10056 reflections

667 parameters

63 restraints

H-atom parameters constrained

 $\Delta\rho_{\max} = 0.92$ e Å⁻³ $\Delta\rho_{\min} = -0.42$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$N3-H3B \cdots O4$	0.86	1.98	2.835 (8)	175
$N6-H6B \cdots O6^i$	0.86	2.00	2.845 (7)	166
$N9-H9A \cdots O5^{ii}$	0.86	2.31	3.049 (8)	145
$N9-H9B \cdots O7$	0.86	2.02	2.870 (6)	172
$O1-H1B \cdots N1$	0.82	1.86	2.588 (5)	147
$O2-H2B \cdots N4$	0.82	1.85	2.583 (4)	148
$O3-H3C \cdots N7$	0.82	1.86	2.587 (5)	147

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

The authors acknowledge financial support from the National Science and Technology Support Program (2012BAC12B03), the Postdoctoral Science Foundation of Central South University and the Fundamental Research Funds for the Central Universities (No. 2012QNZT001).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: YK2079).

References

- Ashfield, L. J., Cowley, A. R., Dilworth, J. R. & Donnelly, P. S. (2004). *Inorg. Chem.* **43**, 4121–4123.
- Brito, I., Vallejos, J., Cárdenas, A., López-Rodríguez, M., Bolte, M. & Llanos, J. (2011). *Inorg. Chem. Commun.* **14**, 897–901.
- Bruker (2000). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Castiñeiras, A. & Pedrido, R. (2009). *Inorg. Chem.* **48**, 4847–4855.
- Forward, J. M., Bohmann, D., Fackler, J. P. & Staples, R. J. (1995). *Inorg. Chem.* **34**, 6330–6336.
- Han, W., Yi, L., Liu, Z. Q., Gu, W., Yan, S. P., Cheng, P., Liao, D. Z. & Jiang, Z. H. (2004). *Eur. J. Inorg. Chem.* pp. 2130–2136.
- Li, M. X., Zhang, D., Zhang, L. Z. & Niu, J. Y. (2010). *Inorg. Chem. Commun.* **13**, 1268–1271.
- Onodera, K., Kasuga, N. C., Takashima, T., Hara, A., Amano, A., Murakami, H. & Nomiya, K. (2007). *Dalton Trans.* pp. 3646–3652.
- Pedrido, R., Romero, M. J., Bermejo, M. R., Martínez-Calvo, M., González-Noya, A. M. & Zaragoza, G. (2009). *Dalton Trans.* pp. 8329–8340.
- Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
- Sheldrick, G. M. (2008). *Acta Cryst. A* **64**, 112–122.
- Sun, Q. Z. (2011). *Chin. J. Struct. Chem.* **30**, 1355–1360.
- Sun, Q. Z. & Chai, L. Y. (2012). *Chin. J. Struct. Chem.* **31**, 408–414.
- Sun, Q. Z., Liao, S. Y., Chai, L. Y., Xu, X. W., Yao, J. J. & Fang, Q. J. L. (2012). *Chin. J. Struct. Chem.* **31**, 1229–1234.
- Xu, C. Y., Sun, Q. Z., Chen, P. & Chai, L. Y. (2011). *Chin. J. Struct. Chem.* **30**, 951–956.

supplementary materials

Acta Cryst. (2013). E69, m50–m51 [doi:10.1107/S1600536812050155]

Hexakis(μ_3 -2-hydroxynaphthalene-1-carboxaldehyde thiosemicarbazonato- $\kappa^3N^2:S:S$)hexasilver(I) *N,N*-dimethylformamide tetrasolvate

Qiaozhen Sun, Liyuan Chai, Hui Liu and Junke Wang

Comment

Transition metal-chalcogen compounds, especially for d^{10} metal complexes, have attracted a great deal of attention for their interesting structures and excellent luminescent properties (Brito *et al.*, 2011; Forward *et al.*, 1995). Of which many coordination complexes with thiosemicarbazone Schiff base ligands have been reported (Ashfield *et al.*, 2004; Castiñeiras & Pedrido, 2009; Li *et al.*, 2010; Onodera *et al.*, 2007; Pedrido *et al.*, 2009). As a part of our studies on this class of compounds (Sun, 2011; Sun *et al.*, 2012; Sun & Chai, 2012; Xu *et al.*, 2011), we describe here the structure of the title compound.

The structure of the title compound is shown in Fig. 1. It contains an Ag_6 hexanuclear cluster with the $Ag\cdots Ag$ distances varying from 2.93 Å to 3.40 Å (Fig. 2), which is shorter than the sum of van der Waals radii of two silver atoms (3.44 Å) (Han *et al.*, 2004). In the cluster, each Ag(I) ion is surrounded by one nitrogen atom and two thiolate sulfur atoms from two deprotonated ligands L^5 . Each ligand coordinates to three Ag(I) ions using a bridged thiolate sulfur atom and a monodentate nitrogen atom, from which two Ag_3S_3 hexagonal rings are linked together to give the overall Ferris wheel structure.

There are intramolecular hydrogen bonds of $O\cdots H\cdots N$ type. Besides this, solvent DMF molecules are linked to the hexanuclear cluster *via* $O\cdots H\cdots N$ hydrogen bonds.

Packing of the title compound (Fig. 3) is facilitated through π - π stacking interactions between aromatic rings I, II [defined by the atoms C(1), C(2), C(3), C(4), C(9) and C(10) and the atoms C(13), C(14), C(15), C(16), C(21) and C(22), respectively] and the symmetry related ones (ring centroid distances: 3.78 Å and 3.70 Å, respectively).

Experimental

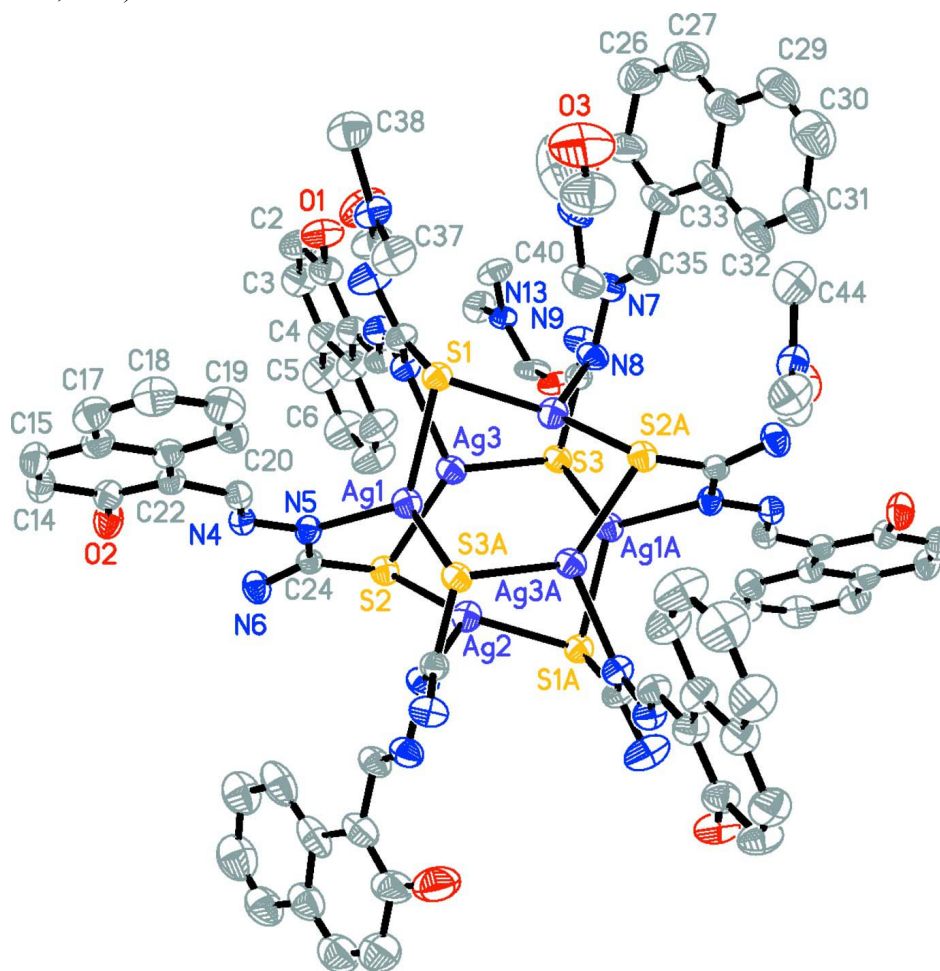
Triethylamine (25 μ L, 0.175 mmol) was added to a solution of L^5 (0.175 mmol, 0.043 g) in 3 ml DMF. After stirring for 30 min, a DMF solution (2 ml) of $AgNO_3$ (0.175 mmol, 0.030 g) was added. Block yellow crystals were formed by standing the solution in air for two months. Anal. Calcd for $C_{84}H_{88}Ag_6N_{22}O_{10}S_6$: C, 41.9; H, 3.7; N, 12.8. Found: C, 41.9; H, 3.6; N, 12.8.

Refinement

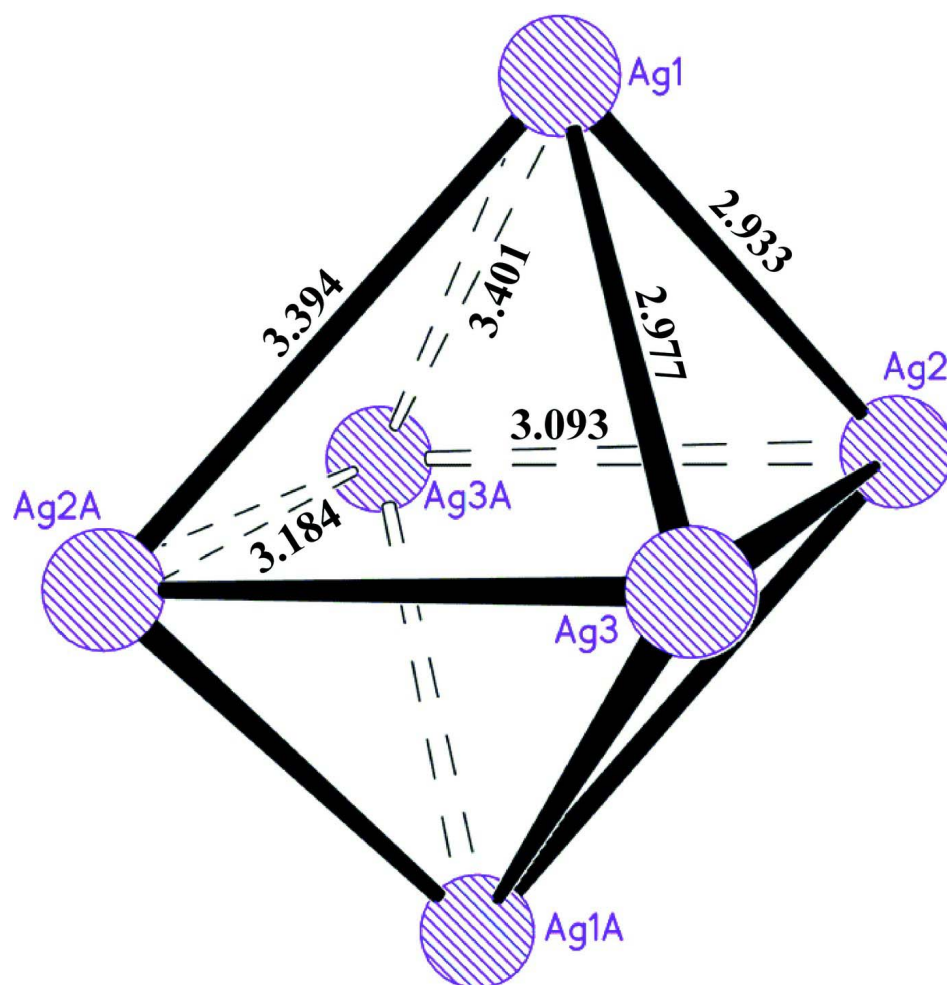
In the compound, all the DMF molecules were found to be disordered, and the s.o.f. for the four disordered molecules were fixed at 0.5. All of the non-hydrogen atoms were refined with anisotropic thermal displacement parameters. The H atoms were placed in calculated positions using the riding model approximation with C—H distances of 0.93–0.96 Å, O—H distances of 0.82 Å and N—H distances of 0.86 Å. $U_{iso}(H)$ were set to 1.2Ueq (C, N) or 1.5Ueq (C, O).

Computing details

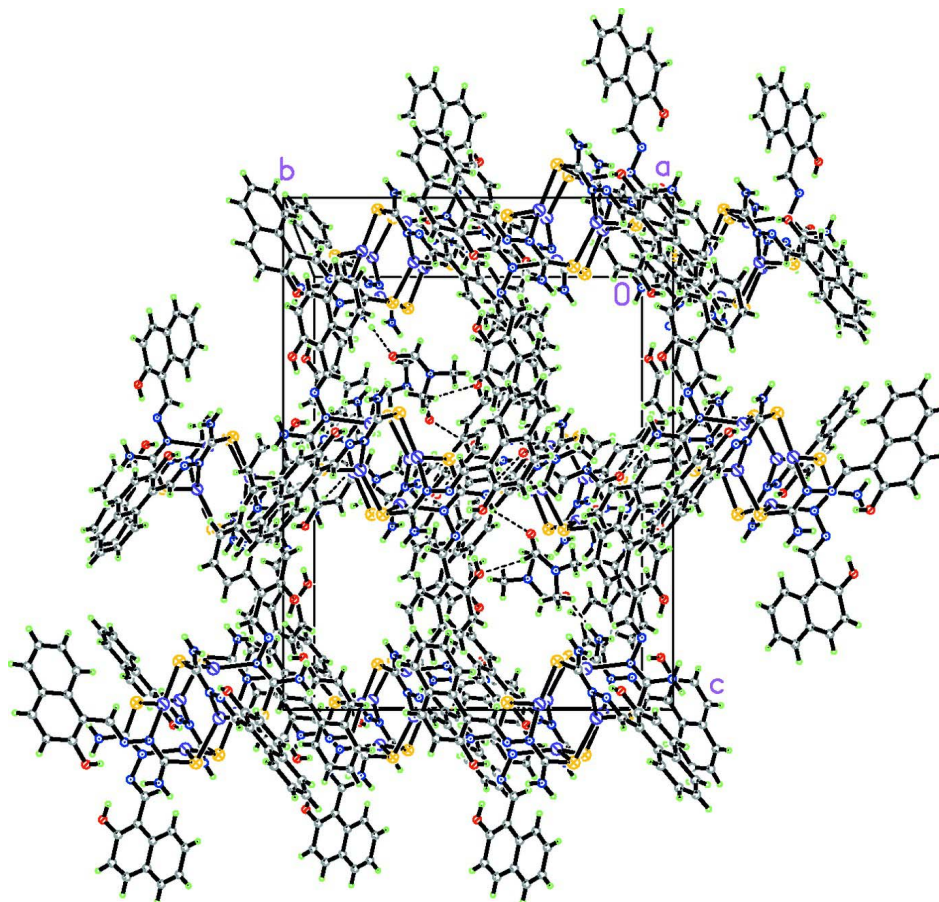
Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINTE* (Bruker, 2000); data reduction: *SAINTE* (Bruker, 2000); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

**Figure 1**

The structure of title compound showing the atom-numbering scheme with H atoms omitted for clarity. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (i) $-x + 0.5, -y + 1.5, -z + 2$]

**Figure 2**

Ag₆ octahedron in the title compound


Figure 3

Packing diagram of the title compound, viewed along the *a* axis direction.

Hexakis(μ_3 -2-hydroxynaphthalene-1-carboxaldehyde thiosemicarbazonato- $\kappa^3N^2:S:S$)hexasilver(I) *N,N'*-dimethylformamide tetrasolvate

Crystal data

[Ag₆(C₁₂H₁₀N₃OS)₆]·4C₃H₇NO

M_r = 2405.34

Monoclinic, *C2/c*

Hall symbol: -C 2yc

a = 24.604 (3) Å

b = 18.877 (3) Å

c = 24.816 (3) Å

β = 94.763 (3)°

V = 11486 (3) Å³

Z = 4

F(000) = 4816

D_x = 1.391 Mg m⁻³

Mo *K* α radiation, λ = 0.71073 Å

Cell parameters from 6309 reflections

θ = 2.2–27.2°

μ = 1.17 mm⁻¹

T = 293 K

Block, yellow

0.22 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan
(*SADABS*; Sheldrick, 1996)

T_{min} = 0.238, *T_{max}* = 0.373

28454 measured reflections

10056 independent reflections

7829 reflections with *I* > 2*s*(*I*)

$R_{\text{int}} = 0.042$
 $\theta_{\text{max}} = 25.0^\circ$, $\theta_{\text{min}} = 1.7^\circ$
 $h = -28 \rightarrow 29$

$k = -22 \rightarrow 21$
 $l = -29 \rightarrow 16$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.046$
 $wR(F^2) = 0.145$
 $S = 1.08$
 10056 reflections
 667 parameters
 63 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
 $w = 1/[\sigma^2(F_o^2) + (0.095P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.002$
 $\Delta\rho_{\text{max}} = 0.92 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.42 \text{ e } \text{\AA}^{-3}$

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Ag1	0.171626 (12)	0.813538 (16)	0.482106 (12)	0.05265 (8)	
Ag2	0.240712 (12)	0.788788 (17)	0.582419 (12)	0.05635 (9)	
Ag3	0.191030 (13)	0.661685 (16)	0.509778 (12)	0.05414 (8)	
S1	0.16540 (4)	0.75257 (5)	0.39220 (4)	0.0510 (2)	
S2	0.16228 (4)	0.70906 (5)	0.59592 (4)	0.0520 (2)	
S3	0.27035 (4)	0.57841 (5)	0.51287 (4)	0.0499 (2)	
N1	0.09822 (14)	0.57526 (18)	0.43441 (14)	0.0591 (9)	
N2	0.13114 (13)	0.63483 (17)	0.43751 (13)	0.0531 (8)	
N3	0.08875 (19)	0.6661 (3)	0.35352 (18)	0.0993 (14)	
H3A	0.0673	0.6301	0.3527	0.119*	
H3B	0.0868	0.6956	0.3271	0.119*	
N4	0.05033 (12)	0.83205 (16)	0.52337 (13)	0.0475 (8)	
N5	0.10008 (12)	0.79779 (16)	0.53377 (12)	0.0476 (8)	
N6	0.06729 (14)	0.76102 (19)	0.61488 (13)	0.0614 (9)	
H6A	0.0380	0.7858	0.6092	0.074*	
H6B	0.0725	0.7360	0.6438	0.074*	
N7	0.27039 (15)	0.5619 (2)	0.35485 (14)	0.0656 (10)	
N8	0.27440 (14)	0.59230 (18)	0.40692 (12)	0.0575 (9)	
N9	0.25925 (15)	0.47922 (19)	0.43895 (15)	0.0671 (10)	
H9A	0.2586	0.4610	0.4071	0.080*	
H9B	0.2547	0.4527	0.4664	0.080*	
O1	0.02497 (15)	0.48899 (18)	0.39190 (13)	0.0853 (10)	
H1B	0.0463	0.5224	0.3930	0.128*	

O2	-0.05009 (11)	0.86290 (17)	0.53609 (12)	0.0686 (8)
H2B	-0.0209	0.8420	0.5413	0.103*
O3	0.2174 (2)	0.4973 (3)	0.27494 (18)	0.1230 (16)
H3C	0.2245	0.5096	0.3064	0.184*
C1	0.0316 (2)	0.4524 (2)	0.4389 (2)	0.0696 (12)
C2	-0.0022 (2)	0.3926 (3)	0.4433 (2)	0.0858 (16)
H2A	-0.0264	0.3788	0.4144	0.103*
C3	0.0012 (2)	0.3550 (3)	0.4907 (2)	0.0824 (15)
H3D	-0.0213	0.3157	0.4936	0.099*
C4	0.0369 (2)	0.3736 (2)	0.5340 (2)	0.0710 (13)
C5	0.0388 (3)	0.3357 (3)	0.5855 (3)	0.0961 (18)
H5A	0.0155	0.2975	0.5892	0.115*
C6	0.0736 (3)	0.3551 (3)	0.6272 (3)	0.109 (2)
H6C	0.0739	0.3303	0.6596	0.131*
C7	0.1083 (3)	0.4100 (3)	0.6233 (2)	0.104 (2)
H7B	0.1324	0.4220	0.6527	0.125*
C8	0.1084 (2)	0.4484 (3)	0.5761 (2)	0.0873 (16)
H8B	0.1330	0.4856	0.5742	0.105*
C9	0.07184 (19)	0.4329 (2)	0.53019 (19)	0.0678 (12)
C10	0.06846 (18)	0.4728 (2)	0.48118 (18)	0.0633 (11)
C11	0.10170 (17)	0.5363 (2)	0.47600 (18)	0.0600 (11)
H11A	0.1266	0.5487	0.5047	0.072*
C12	0.12505 (16)	0.6761 (2)	0.39585 (16)	0.0529 (10)
C13	-0.04809 (15)	0.9071 (2)	0.49380 (17)	0.0547 (10)
C14	-0.09473 (17)	0.9478 (2)	0.47924 (19)	0.0659 (12)
H14A	-0.1254	0.9428	0.4984	0.079*
C15	-0.09576 (17)	0.9941 (3)	0.4380 (2)	0.0671 (12)
H15A	-0.1271	1.0207	0.4294	0.080*
C16	-0.05039 (17)	1.0030 (2)	0.40773 (17)	0.0602 (11)
C17	-0.0514 (2)	1.0516 (3)	0.36387 (19)	0.0711 (13)
H17A	-0.0823	1.0790	0.3556	0.085*
C18	-0.0087 (2)	1.0587 (3)	0.3344 (2)	0.0818 (15)
H18A	-0.0103	1.0906	0.3058	0.098*
C19	0.0376 (2)	1.0188 (3)	0.3463 (2)	0.0780 (14)
H19A	0.0667	1.0235	0.3249	0.094*
C20	0.04169 (19)	0.9720 (2)	0.38905 (18)	0.0654 (12)
H20A	0.0739	0.9468	0.3968	0.078*
C21	-0.00225 (15)	0.9620 (2)	0.42120 (16)	0.0521 (10)
C22	-0.00177 (15)	0.9137 (2)	0.46551 (15)	0.0497 (9)
C23	0.04720 (15)	0.87334 (19)	0.48270 (15)	0.0484 (9)
H23A	0.0776	0.8780	0.4630	0.058*
C24	0.10444 (14)	0.76144 (19)	0.57889 (14)	0.0435 (8)
C25	0.2510 (3)	0.5314 (4)	0.2427 (2)	0.104 (2)
C26	0.2459 (3)	0.5160 (4)	0.1857 (3)	0.1147 (18)
H26A	0.2203	0.4836	0.1712	0.138*
C27	0.2789 (3)	0.5496 (4)	0.1544 (3)	0.1144 (18)
H27A	0.2745	0.5391	0.1177	0.137*
C28	0.3180 (3)	0.5973 (3)	0.1699 (2)	0.0934 (15)
C29	0.3531 (3)	0.6318 (4)	0.1345 (2)	0.1046 (18)

H29A	0.3493	0.6213	0.0977	0.126*	
C30	0.3886 (3)	0.6755 (4)	0.1515 (3)	0.127 (2)	
H30A	0.4086	0.6988	0.1268	0.152*	
C31	0.3996 (3)	0.6910 (4)	0.2081 (3)	0.114 (2)	
H31A	0.4273	0.7223	0.2199	0.137*	
C32	0.3687 (3)	0.6590 (3)	0.2442 (2)	0.1015 (19)	
H32A	0.3757	0.6680	0.2809	0.122*	
C33	0.3264 (2)	0.6125 (3)	0.2266 (2)	0.0911 (16)	
C34	0.2898 (2)	0.5779 (3)	0.26316 (19)	0.0814 (15)	
C35	0.29397 (18)	0.5973 (3)	0.32006 (16)	0.0645 (12)	
H35A	0.3145	0.6368	0.3313	0.077*	
C36	0.26717 (15)	0.5477 (2)	0.44566 (15)	0.0488 (9)	
C37	0.1231 (5)	0.9297 (5)	0.2325 (5)	0.087 (3)	0.50
H37A	0.1419	0.9325	0.2679	0.130*	0.50
H37B	0.0973	0.9678	0.2277	0.130*	0.50
H37C	0.1489	0.9331	0.2056	0.130*	0.50
C38	0.0619 (5)	0.8437 (6)	0.1746 (5)	0.089 (3)	0.50
H38A	0.0455	0.7980	0.1785	0.133*	0.50
H38B	0.0854	0.8423	0.1456	0.133*	0.50
H38C	0.0338	0.8784	0.1667	0.133*	0.50
C39	0.0960 (4)	0.8193 (6)	0.2672 (4)	0.078 (3)	0.50
H39A	0.1113	0.8342	0.3008	0.093*	0.50
N10	0.0949 (3)	0.8634 (3)	0.2267 (3)	0.0561 (17)	0.50
O4	0.0773 (3)	0.7578 (4)	0.2628 (3)	0.095 (2)	0.50
C40	0.2559 (5)	0.7879 (6)	0.2711 (4)	0.087 (3)	0.50
H40A	0.2754	0.8308	0.2806	0.130*	0.50
H40B	0.2801	0.7482	0.2767	0.130*	0.50
H40C	0.2260	0.7828	0.2932	0.130*	0.50
C41	0.2129 (6)	0.7401 (7)	0.2012 (6)	0.161 (6)	0.50
H41A	0.2007	0.7454	0.1636	0.242*	0.50
H41B	0.1820	0.7328	0.2217	0.242*	0.50
H41C	0.2369	0.7001	0.2057	0.242*	0.50
C42	0.2428 (7)	0.8450 (8)	0.1807 (6)	0.125 (5)	0.50
H42A	0.2656	0.8799	0.1965	0.150*	0.50
N11	0.2359 (3)	0.7908 (4)	0.2164 (3)	0.0563 (18)	0.50
O5	0.2296 (5)	0.8580 (5)	0.1406 (3)	0.136 (4)	0.50
O6	0.4334 (3)	0.8328 (4)	0.2955 (3)	0.090 (2)	0.50
C43	0.4240 (4)	1.0056 (5)	0.2406 (4)	0.081 (3)	0.50
H43A	0.4350	1.0254	0.2754	0.121*	0.50
H43B	0.3889	1.0239	0.2279	0.121*	0.50
H43C	0.4502	1.0180	0.2155	0.121*	0.50
C44	0.4052 (4)	0.8921 (6)	0.1971 (4)	0.084 (3)	0.50
H44A	0.4048	0.8424	0.2051	0.126*	0.50
H44B	0.4307	0.9012	0.1707	0.126*	0.50
H44C	0.3694	0.9069	0.1832	0.126*	0.50
C45	0.4319 (4)	0.8969 (7)	0.2912 (5)	0.089 (3)	0.50
H45A	0.4389	0.9239	0.3224	0.107*	0.50
N12	0.4210 (3)	0.9304 (4)	0.2449 (2)	0.063 (2)	0.50
O7	0.2454 (2)	0.3792 (3)	0.5239 (2)	0.0587 (13)	0.50

C46	0.1547 (4)	0.2320 (4)	0.5242 (4)	0.075 (3)	0.50
H46A	0.1703	0.2201	0.5598	0.112*	0.50
H46B	0.1600	0.1934	0.5000	0.112*	0.50
H46C	0.1164	0.2410	0.5252	0.112*	0.50
C47	0.1648 (4)	0.3228 (5)	0.4527 (4)	0.073 (3)	0.50
H47A	0.1858	0.3643	0.4461	0.109*	0.50
H47B	0.1268	0.3351	0.4510	0.109*	0.50
H47C	0.1704	0.2876	0.4259	0.109*	0.50
C48	0.2207 (4)	0.3293 (4)	0.5356 (3)	0.060 (2)	0.50
H48A	0.2294	0.3111	0.5701	0.072*	0.50
N13	0.1815 (3)	0.2954 (3)	0.5052 (3)	0.0468 (15)	0.50

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.05776 (17)	0.05486 (17)	0.04597 (16)	-0.00022 (13)	0.00805 (13)	0.00734 (12)
Ag2	0.05578 (17)	0.06027 (18)	0.05285 (18)	0.00050 (13)	0.00367 (14)	0.00891 (13)
Ag3	0.06226 (18)	0.05244 (17)	0.04791 (17)	0.00372 (13)	0.00561 (14)	0.00294 (12)
S1	0.0549 (5)	0.0543 (5)	0.0438 (5)	-0.0023 (4)	0.0035 (4)	0.0061 (4)
S2	0.0564 (5)	0.0552 (5)	0.0450 (5)	0.0023 (4)	0.0079 (4)	0.0091 (4)
S3	0.0570 (5)	0.0488 (5)	0.0446 (5)	0.0013 (4)	0.0081 (4)	0.0031 (4)
N1	0.0648 (19)	0.0566 (19)	0.0556 (19)	-0.0095 (16)	0.0042 (16)	0.0038 (16)
N2	0.0554 (17)	0.0538 (18)	0.0497 (18)	-0.0064 (15)	0.0017 (14)	0.0065 (15)
N3	0.109 (3)	0.098 (3)	0.085 (3)	-0.033 (2)	-0.027 (2)	0.016 (2)
N4	0.0439 (15)	0.0487 (17)	0.0504 (17)	0.0009 (13)	0.0069 (13)	0.0001 (14)
N5	0.0439 (15)	0.0514 (17)	0.0480 (17)	0.0004 (13)	0.0064 (13)	0.0060 (13)
N6	0.0601 (19)	0.073 (2)	0.0532 (19)	0.0072 (17)	0.0165 (16)	0.0100 (16)
N7	0.079 (2)	0.068 (2)	0.0490 (19)	0.0157 (18)	0.0009 (17)	-0.0046 (17)
N8	0.071 (2)	0.063 (2)	0.0390 (17)	0.0076 (17)	0.0063 (15)	0.0032 (15)
N9	0.091 (3)	0.057 (2)	0.054 (2)	-0.0044 (18)	0.0069 (18)	-0.0029 (16)
O1	0.116 (3)	0.073 (2)	0.0638 (19)	-0.0227 (19)	-0.0104 (18)	-0.0023 (16)
O2	0.0522 (15)	0.084 (2)	0.0713 (19)	0.0015 (15)	0.0128 (14)	0.0191 (16)
O3	0.131 (3)	0.137 (4)	0.095 (3)	-0.006 (3)	-0.029 (3)	-0.024 (3)
C1	0.082 (3)	0.057 (2)	0.070 (3)	-0.012 (2)	0.007 (2)	-0.005 (2)
C2	0.105 (4)	0.064 (3)	0.086 (4)	-0.028 (3)	-0.005 (3)	-0.007 (3)
C3	0.093 (3)	0.056 (3)	0.099 (4)	-0.024 (2)	0.011 (3)	-0.001 (3)
C4	0.081 (3)	0.053 (2)	0.080 (3)	-0.011 (2)	0.012 (2)	0.006 (2)
C5	0.110 (4)	0.067 (3)	0.112 (5)	-0.018 (3)	0.013 (4)	0.020 (3)
C6	0.135 (5)	0.097 (4)	0.095 (4)	-0.015 (4)	0.008 (4)	0.041 (3)
C7	0.127 (5)	0.093 (4)	0.088 (4)	-0.028 (4)	-0.022 (3)	0.032 (3)
C8	0.093 (3)	0.075 (3)	0.091 (4)	-0.023 (3)	-0.010 (3)	0.019 (3)
C9	0.073 (3)	0.056 (2)	0.075 (3)	-0.005 (2)	0.004 (2)	0.007 (2)
C10	0.073 (3)	0.054 (2)	0.063 (3)	-0.012 (2)	0.008 (2)	0.0020 (19)
C11	0.063 (2)	0.057 (2)	0.059 (2)	-0.0090 (19)	0.000 (2)	-0.001 (2)
C12	0.057 (2)	0.053 (2)	0.047 (2)	-0.0052 (17)	-0.0048 (17)	0.0039 (17)
C13	0.048 (2)	0.057 (2)	0.058 (2)	-0.0037 (18)	0.0050 (18)	-0.0016 (18)
C14	0.047 (2)	0.071 (3)	0.080 (3)	0.001 (2)	0.010 (2)	-0.001 (2)
C15	0.050 (2)	0.069 (3)	0.081 (3)	0.011 (2)	-0.001 (2)	-0.007 (2)
C16	0.064 (2)	0.052 (2)	0.061 (2)	0.0017 (19)	-0.011 (2)	-0.0077 (19)

C17	0.075 (3)	0.064 (3)	0.072 (3)	0.004 (2)	-0.011 (2)	0.008 (2)
C18	0.106 (4)	0.068 (3)	0.069 (3)	0.001 (3)	-0.005 (3)	0.019 (2)
C19	0.091 (3)	0.079 (3)	0.064 (3)	-0.003 (3)	0.013 (3)	0.013 (2)
C20	0.070 (3)	0.067 (3)	0.060 (3)	0.003 (2)	0.012 (2)	0.006 (2)
C21	0.054 (2)	0.048 (2)	0.053 (2)	-0.0029 (17)	0.0006 (17)	-0.0022 (17)
C22	0.050 (2)	0.048 (2)	0.050 (2)	-0.0012 (16)	-0.0007 (16)	-0.0053 (16)
C23	0.0459 (18)	0.047 (2)	0.053 (2)	0.0008 (16)	0.0070 (16)	-0.0009 (17)
C24	0.0447 (17)	0.0476 (19)	0.0386 (18)	-0.0071 (15)	0.0062 (15)	-0.0008 (15)
C25	0.123 (5)	0.123 (5)	0.060 (3)	0.036 (4)	-0.021 (3)	-0.018 (3)
C26	0.119 (3)	0.127 (5)	0.093 (4)	0.025 (3)	-0.021 (2)	-0.002 (3)
C27	0.131 (3)	0.117 (3)	0.093 (3)	0.036 (3)	-0.002 (2)	-0.010 (3)
C28	0.109 (3)	0.105 (3)	0.0665 (12)	0.033 (3)	0.009 (2)	0.005 (2)
C29	0.126 (3)	0.119 (3)	0.072 (3)	0.026 (3)	0.022 (3)	0.007 (3)
C30	0.137 (4)	0.138 (4)	0.109 (4)	0.021 (3)	0.032 (3)	0.022 (3)
C31	0.123 (4)	0.118 (4)	0.103 (3)	0.020 (3)	0.025 (3)	0.017 (3)
C32	0.126 (4)	0.108 (4)	0.076 (3)	0.045 (4)	0.043 (3)	0.030 (3)
C33	0.116 (4)	0.105 (4)	0.0553 (15)	0.061 (3)	0.026 (2)	0.022 (2)
C34	0.105 (3)	0.088 (3)	0.050 (3)	0.045 (3)	0.000 (2)	0.002 (2)
C35	0.080 (3)	0.072 (3)	0.042 (2)	0.021 (2)	0.006 (2)	0.0029 (19)
C36	0.0509 (19)	0.048 (2)	0.047 (2)	0.0081 (16)	0.0000 (16)	-0.0023 (16)
C37	0.098 (7)	0.069 (6)	0.091 (7)	-0.002 (5)	-0.009 (6)	0.005 (5)
C38	0.104 (4)	0.079 (4)	0.081 (4)	0.007 (3)	-0.013 (4)	0.012 (3)
C39	0.091 (7)	0.082 (6)	0.056 (5)	0.006 (5)	-0.024 (5)	0.014 (5)
N10	0.071 (4)	0.037 (3)	0.057 (4)	0.015 (3)	-0.020 (3)	0.011 (3)
O4	0.105 (4)	0.095 (4)	0.078 (3)	-0.016 (3)	-0.027 (3)	0.037 (3)
C40	0.116 (8)	0.080 (7)	0.063 (6)	0.031 (6)	-0.002 (6)	-0.007 (5)
C41	0.162 (12)	0.139 (11)	0.189 (15)	0.098 (9)	0.052 (11)	0.082 (10)
C42	0.157 (12)	0.105 (10)	0.112 (11)	-0.033 (9)	0.004 (10)	-0.007 (8)
N11	0.079 (4)	0.050 (4)	0.041 (3)	0.008 (3)	0.015 (3)	0.004 (3)
O5	0.222 (10)	0.130 (6)	0.054 (4)	-0.029 (7)	-0.002 (5)	0.058 (4)
O6	0.115 (5)	0.103 (5)	0.055 (3)	0.005 (4)	0.030 (3)	0.049 (3)
C43	0.086 (6)	0.071 (6)	0.084 (7)	-0.016 (5)	-0.003 (5)	0.017 (5)
C44	0.092 (7)	0.084 (7)	0.076 (6)	-0.011 (5)	0.004 (5)	0.033 (5)
C45	0.082 (4)	0.104 (5)	0.082 (4)	0.000 (4)	0.014 (3)	0.004 (4)
N12	0.049 (3)	0.103 (5)	0.038 (3)	0.001 (4)	0.000 (3)	0.029 (3)
O7	0.086 (3)	0.049 (2)	0.038 (2)	-0.033 (2)	-0.010 (2)	0.0095 (19)
C46	0.081 (6)	0.048 (5)	0.096 (7)	-0.031 (4)	0.010 (5)	0.001 (5)
C47	0.078 (6)	0.060 (5)	0.076 (6)	-0.007 (4)	-0.024 (5)	-0.009 (4)
C48	0.101 (6)	0.051 (4)	0.025 (3)	-0.008 (4)	-0.005 (4)	0.007 (3)
N13	0.058 (3)	0.031 (3)	0.050 (4)	-0.010 (3)	0.002 (3)	-0.009 (2)

Geometric parameters (Å, °)

Ag1—N5	2.282 (3)	C18—C19	1.377 (7)
Ag1—S3 ⁱ	2.4869 (10)	C18—H18A	0.9300
Ag1—S1	2.5039 (10)	C19—C20	1.378 (6)
Ag1—Ag2	2.9329 (5)	C19—H19A	0.9300
Ag1—Ag3	2.9769 (6)	C20—C21	1.409 (6)
Ag2—N8 ⁱ	2.294 (3)	C20—H20A	0.9300
Ag2—S1 ⁱ	2.4699 (10)	C21—C22	1.428 (5)

Ag2—S2	2.4917 (11)	C22—C23	1.459 (5)
Ag2—Ag3 ⁱ	3.0931 (5)	C23—H23A	0.9300
Ag2—Ag3	3.1835 (5)	C25—C34	1.364 (8)
Ag3—N2	2.282 (3)	C25—C26	1.438 (8)
Ag3—S2	2.4741 (11)	C26—C27	1.330 (10)
Ag3—S3	2.5020 (10)	C26—H26A	0.9300
Ag3—Ag2 ⁱ	3.0931 (5)	C27—C28	1.350 (9)
S1—C12	1.759 (4)	C27—H27A	0.9300
S1—Ag2 ⁱ	2.4699 (10)	C28—C33	1.436 (7)
S2—C24	1.755 (4)	C28—C29	1.438 (9)
S3—C36	1.762 (4)	C29—C30	1.248 (10)
S3—Ag1 ⁱ	2.4869 (10)	C29—H29A	0.9300
N1—C11	1.264 (5)	C30—C31	1.438 (10)
N1—N2	1.384 (5)	C30—H30A	0.9300
N2—C12	1.293 (5)	C31—C32	1.363 (9)
N3—C12	1.335 (6)	C31—H31A	0.9300
N3—H3A	0.8600	C32—C33	1.403 (9)
N3—H3B	0.8600	C32—H32A	0.9300
N4—C23	1.273 (5)	C33—C34	1.480 (8)
N4—N5	1.390 (4)	C34—C35	1.454 (6)
N5—C24	1.310 (5)	C35—H35A	0.9300
N6—C24	1.330 (5)	C37—N10	1.432 (12)
N6—H6A	0.8600	C37—H37A	0.9600
N6—H6B	0.8600	C37—H37B	0.9600
N7—C35	1.270 (6)	C37—H37C	0.9600
N7—N8	1.410 (5)	C38—N10	1.516 (12)
N8—C36	1.302 (5)	C38—H38A	0.9600
N8—Ag2 ⁱ	2.294 (3)	C38—H38B	0.9600
N9—C36	1.315 (5)	C38—H38C	0.9600
N9—H9A	0.8600	C39—O4	1.250 (12)
N9—H9B	0.8600	C39—N10	1.302 (11)
O1—C1	1.354 (6)	C39—H39A	0.9300
O1—H1B	0.8200	C40—N11	1.406 (11)
O2—C13	1.345 (5)	C40—H40A	0.9600
O2—H2B	0.8200	C40—H40B	0.9600
O3—C25	1.361 (8)	C40—H40C	0.9600
O3—H3C	0.8200	C41—N11	1.159 (16)
C1—C10	1.384 (6)	C41—H41A	0.9600
C1—C2	1.411 (7)	C41—H41B	0.9600
C2—C3	1.369 (7)	C41—H41C	0.9600
C2—H2A	0.9300	C42—O5	1.052 (16)
C3—C4	1.377 (7)	C42—N11	1.372 (16)
C3—H3D	0.9300	C42—H42A	0.9300
C4—C9	1.419 (6)	O6—C45	1.215 (14)
C4—C5	1.461 (8)	C43—N12	1.425 (13)
C5—C6	1.340 (9)	C43—H43A	0.9600
C5—H5A	0.9300	C43—H43B	0.9600
C6—C7	1.352 (8)	C43—H43C	0.9600
C6—H6C	0.9300	C44—N12	1.415 (13)

C7—C8	1.377 (8)	C44—H44A	0.9600
C7—H7B	0.9300	C44—H44B	0.9600
C8—C9	1.422 (7)	C44—H44C	0.9600
C8—H8B	0.9300	C45—N12	1.320 (13)
C9—C10	1.428 (6)	C45—H45A	0.9300
C10—C11	1.463 (6)	O7—C48	1.171 (10)
C11—H11A	0.9300	C46—N13	1.463 (10)
C13—C22	1.393 (5)	C46—H46A	0.9600
C13—C14	1.404 (6)	C46—H46B	0.9600
C14—C15	1.343 (7)	C46—H46C	0.9600
C14—H14A	0.9300	C47—N13	1.428 (11)
C15—C16	1.407 (6)	C47—H47A	0.9600
C15—H15A	0.9300	C47—H47B	0.9600
C16—C17	1.423 (6)	C47—H47C	0.9600
C16—C21	1.431 (6)	C48—N13	1.338 (10)
C17—C18	1.334 (7)	C48—H48A	0.9300
C17—H17A	0.9300		
N5—Ag1—S3 ⁱ	123.04 (8)	C18—C19—C20	121.5 (5)
N5—Ag1—S1	116.61 (8)	C18—C19—H19A	119.3
S3 ⁱ —Ag1—S1	114.45 (3)	C20—C19—H19A	119.3
N5—Ag1—Ag2	85.53 (8)	C19—C20—C21	120.8 (4)
S3 ⁱ —Ag1—Ag2	78.36 (2)	C19—C20—H20A	119.6
S1—Ag1—Ag2	132.17 (3)	C21—C20—H20A	119.6
N5—Ag1—Ag3	82.03 (8)	C20—C21—C22	124.4 (4)
S3 ⁱ —Ag1—Ag3	134.25 (3)	C20—C21—C16	117.0 (4)
S1—Ag1—Ag3	76.10 (2)	C22—C21—C16	118.6 (4)
Ag2—Ag1—Ag3	65.183 (11)	C13—C22—C21	119.4 (3)
N8 ⁱ —Ag2—S1 ⁱ	115.91 (9)	C13—C22—C23	119.8 (3)
N8 ⁱ —Ag2—S2	116.15 (9)	C21—C22—C23	120.8 (3)
S1 ⁱ —Ag2—S2	119.55 (4)	N4—C23—C22	123.1 (3)
N8 ⁱ —Ag2—Ag1	81.60 (8)	N4—C23—H23A	118.5
S1 ⁱ —Ag2—Ag1	136.94 (3)	C22—C23—H23A	118.5
S2—Ag2—Ag1	79.02 (2)	N5—C24—N6	124.4 (3)
N8 ⁱ —Ag2—Ag3 ⁱ	83.84 (8)	N5—C24—S2	120.5 (3)
S1 ⁱ —Ag2—Ag3 ⁱ	74.37 (2)	N6—C24—S2	115.1 (3)
S2—Ag2—Ag3 ⁱ	139.12 (3)	O3—C25—C34	121.8 (5)
Ag1—Ag2—Ag3 ⁱ	68.654 (13)	O3—C25—C26	118.3 (6)
N8 ⁱ —Ag2—Ag3	138.11 (8)	C34—C25—C26	119.9 (6)
S1 ⁱ —Ag2—Ag3	102.31 (3)	C27—C26—C25	118.0 (7)
S2—Ag2—Ag3	49.88 (2)	C27—C26—H26A	121.0
Ag1—Ag2—Ag3	58.076 (12)	C25—C26—H26A	121.0
Ag3 ⁱ —Ag2—Ag3	90.886 (14)	C26—C27—C28	127.3 (7)
N2—Ag3—S2	123.17 (9)	C26—C27—H27A	116.3
N2—Ag3—S3	109.62 (9)	C28—C27—H27A	116.3
S2—Ag3—S3	118.61 (3)	C27—C28—C33	117.0 (6)
N2—Ag3—Ag1	87.24 (8)	C27—C28—C29	125.3 (6)
S2—Ag3—Ag1	78.42 (3)	C33—C28—C29	117.7 (6)
S3—Ag3—Ag1	136.20 (3)	C30—C29—C28	122.0 (7)

N2—Ag3—Ag2 ⁱ	80.83 (8)	C30—C29—H29A	119.0
S2—Ag3—Ag2 ⁱ	137.87 (3)	C28—C29—H29A	119.0
S3—Ag3—Ag2 ⁱ	75.09 (2)	C29—C30—C31	122.4 (8)
Ag1—Ag3—Ag2 ⁱ	67.966 (11)	C29—C30—H30A	118.8
N2—Ag3—Ag2	143.62 (8)	C31—C30—H30A	118.8
S2—Ag3—Ag2	50.37 (2)	C32—C31—C30	118.7 (7)
S3—Ag3—Ag2	101.20 (3)	C32—C31—H31A	120.7
Ag1—Ag3—Ag2	56.741 (12)	C30—C31—H31A	120.7
Ag2 ⁱ —Ag3—Ag2	89.114 (14)	C31—C32—C33	120.9 (6)
C12—S1—Ag2 ⁱ	104.32 (14)	C31—C32—H32A	119.5
C12—S1—Ag1	108.93 (14)	C33—C32—H32A	119.5
Ag2 ⁱ —S1—Ag1	86.06 (3)	C32—C33—C28	118.1 (5)
C24—S2—Ag3	106.25 (12)	C32—C33—C34	124.0 (5)
C24—S2—Ag2	104.41 (12)	C28—C33—C34	117.9 (6)
Ag3—S2—Ag2	79.74 (3)	C25—C34—C35	121.0 (5)
C36—S3—Ag1 ⁱ	107.32 (13)	C25—C34—C33	119.8 (5)
C36—S3—Ag3	101.81 (12)	C35—C34—C33	119.1 (5)
Ag1 ⁱ —S3—Ag3	85.95 (3)	N7—C35—C34	121.9 (5)
C11—N1—N2	115.3 (3)	N7—C35—H35A	119.1
C12—N2—N1	114.6 (3)	C34—C35—H35A	119.1
C12—N2—Ag3	121.3 (3)	N8—C36—N9	124.8 (4)
N1—N2—Ag3	124.1 (2)	N8—C36—S3	119.2 (3)
C12—N3—H3A	120.0	N9—C36—S3	116.0 (3)
C12—N3—H3B	120.0	N10—C37—H37A	109.5
H3A—N3—H3B	120.0	N10—C37—H37B	109.5
C23—N4—N5	115.3 (3)	H37A—C37—H37B	109.5
C24—N5—N4	114.3 (3)	N10—C37—H37C	109.5
C24—N5—Ag1	122.4 (2)	H37A—C37—H37C	109.5
N4—N5—Ag1	122.9 (2)	H37B—C37—H37C	109.5
C24—N6—H6A	120.0	N10—C38—H38A	109.5
C24—N6—H6B	120.0	N10—C38—H38B	109.5
H6A—N6—H6B	120.0	H38A—C38—H38B	109.5
C35—N7—N8	114.1 (4)	N10—C38—H38C	109.5
C36—N8—N7	114.2 (3)	H38A—C38—H38C	109.5
C36—N8—Ag2 ⁱ	121.0 (3)	H38B—C38—H38C	109.5
N7—N8—Ag2 ⁱ	120.3 (2)	O4—C39—N10	122.9 (9)
C36—N9—H9A	120.0	O4—C39—H39A	118.5
C36—N9—H9B	120.0	N10—C39—H39A	118.5
H9A—N9—H9B	120.0	C39—N10—C37	120.2 (8)
C1—O1—H1B	109.5	C39—N10—C38	118.4 (8)
C13—O2—H2B	109.5	C37—N10—C38	121.3 (7)
C25—O3—H3C	109.5	N11—C40—H40A	109.5
O1—C1—C10	122.3 (4)	N11—C40—H40B	109.5
O1—C1—C2	116.5 (4)	H40A—C40—H40B	109.5
C10—C1—C2	121.1 (5)	N11—C40—H40C	109.5
C3—C2—C1	119.2 (5)	H40A—C40—H40C	109.5
C3—C2—H2A	120.4	H40B—C40—H40C	109.5
C1—C2—H2A	120.4	N11—C41—H41A	109.5
C2—C3—C4	121.7 (5)	N11—C41—H41B	109.5

C2—C3—H3D	119.1	H41A—C41—H41B	109.5
C4—C3—H3D	119.1	N11—C41—H41C	109.5
C3—C4—C9	120.1 (4)	H41A—C41—H41C	109.5
C3—C4—C5	121.9 (5)	H41B—C41—H41C	109.5
C9—C4—C5	118.0 (5)	O5—C42—N11	137.7 (15)
C6—C5—C4	121.0 (5)	O5—C42—H42A	111.2
C6—C5—H5A	119.5	N11—C42—H42A	111.2
C4—C5—H5A	119.5	C41—N11—C42	119.4 (11)
C5—C6—C7	121.3 (6)	C41—N11—C40	113.8 (10)
C5—C6—H6C	119.3	C42—N11—C40	126.8 (9)
C7—C6—H6C	119.3	N12—C43—H43A	109.5
C6—C7—C8	120.7 (6)	N12—C43—H43B	109.5
C6—C7—H7B	119.6	H43A—C43—H43B	109.5
C8—C7—H7B	119.6	N12—C43—H43C	109.5
C7—C8—C9	121.8 (5)	H43A—C43—H43C	109.5
C7—C8—H8B	119.1	H43B—C43—H43C	109.5
C9—C8—H8B	119.1	N12—C44—H44A	109.5
C4—C9—C8	117.1 (4)	N12—C44—H44B	109.5
C4—C9—C10	118.7 (4)	H44A—C44—H44B	109.5
C8—C9—C10	124.2 (4)	N12—C44—H44C	109.5
C1—C10—C9	119.1 (4)	H44A—C44—H44C	109.5
C1—C10—C11	119.9 (4)	H44B—C44—H44C	109.5
C9—C10—C11	120.9 (4)	O6—C45—N12	123.7 (11)
N1—C11—C10	123.2 (4)	O6—C45—H45A	118.1
N1—C11—H11A	118.4	N12—C45—H45A	118.1
C10—C11—H11A	118.4	C45—N12—C44	120.4 (9)
N2—C12—N3	124.7 (4)	C45—N12—C43	122.3 (9)
N2—C12—S1	120.5 (3)	C44—N12—C43	117.2 (7)
N3—C12—S1	114.8 (3)	N13—C46—H46A	109.5
O2—C13—C22	122.2 (3)	N13—C46—H46B	109.5
O2—C13—C14	117.3 (4)	H46A—C46—H46B	109.5
C22—C13—C14	120.5 (4)	N13—C46—H46C	109.5
C15—C14—C13	121.0 (4)	H46A—C46—H46C	109.5
C15—C14—H14A	119.5	H46B—C46—H46C	109.5
C13—C14—H14A	119.5	N13—C47—H47A	109.5
C14—C15—C16	121.3 (4)	N13—C47—H47B	109.5
C14—C15—H15A	119.4	H47A—C47—H47B	109.5
C16—C15—H15A	119.4	N13—C47—H47C	109.5
C15—C16—C17	121.5 (4)	H47A—C47—H47C	109.5
C15—C16—C21	119.2 (4)	H47B—C47—H47C	109.5
C17—C16—C21	119.3 (4)	O7—C48—N13	127.4 (7)
C18—C17—C16	121.3 (4)	O7—C48—H48A	116.3
C18—C17—H17A	119.3	N13—C48—H48A	116.3
C16—C17—H17A	119.3	C48—N13—C47	118.8 (6)
C17—C18—C19	120.1 (5)	C48—N13—C46	122.1 (7)
C17—C18—H18A	119.9	C47—N13—C46	119.1 (7)
C19—C18—H18A	119.9		

Symmetry code: (i) $-x+1/2, -y+3/2, -z+1$.

Hydrogen-bond geometry (Å, °)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N3—H3B \cdots O4	0.86	1.98	2.835 (8)	175
N6—H6B \cdots O6 ⁱ	0.86	2.00	2.845 (7)	166
N9—H9A \cdots O5 ⁱⁱ	0.86	2.31	3.049 (8)	145
N9—H9B \cdots O7	0.86	2.02	2.870 (6)	172
O1—H1B \cdots N1	0.82	1.86	2.588 (5)	147
O2—H2B \cdots N4	0.82	1.85	2.583 (4)	148
O3—H3C \cdots N7	0.82	1.86	2.587 (5)	147

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