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# Hexakis($\mu_3$-2-hydroxynaphthalene-1-carboxaldehyde thiosemicarbazonato-$\kappa^3N^2$:*S*:*S*)hexasilver(I) *N*,*N*-dimethylformamide tetrasolvate

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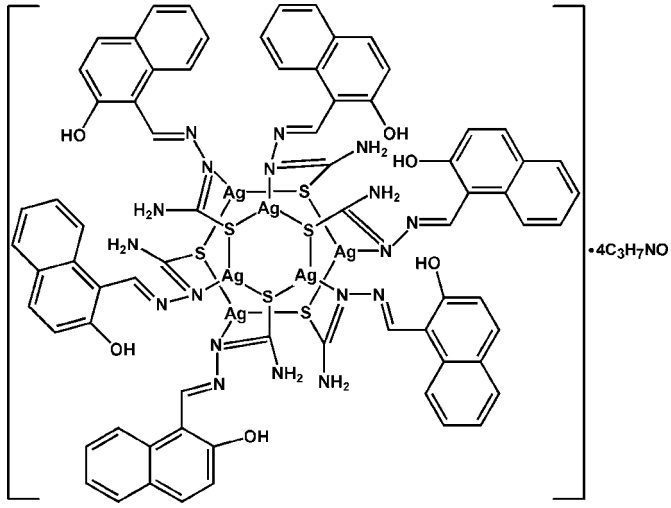
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.007 Å; disorder in solvent or counterion; $R$ factor = 0.046; $wR$ factor = 0.145; data-to-parameter ratio = 15.1.

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···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···H—N hydrogen bonds to the complex molecule. Intramolecular O—H···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 compexes 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) Å$^3$
$Z$ = 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 $I > 2s(I)$
$R_{int}$ = 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···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N3—H3$B$···O4 | 0.86 | 1.98 | 2.835 (8) | 175 |
| N6—H6$B$···O6$^{i}$ | 0.86 | 2.00 | 2.845 (7) | 166 |
| N9—H9$A$···O5$^{ii}$ | 0.86 | 2.31 | 3.049 (8) | 145 |
| N9—H9$B$···O7 | 0.86 | 2.02 | 2.870 (6) | 172 |
| O1—H1$B$···N1 | 0.82 | 1.86 | 2.588 (5) | 147 |
| O2—H2$B$···N4 | 0.82 | 1.85 | 2.583 (4) | 148 |
| O3—H3$C$···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*.

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

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Xu, C. Y., Sun, Q. Z., Chen, P. & Chai, L. Y. (2011). *Chin. J. Struct. Chem.* **30**, 951–956.

# supporting information

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## Hexakis($\mu_3$-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**

### S1. 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···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—H···N type. Besides this, solvent DMF molecules are linked to the hexanuclear cluster *via* O···H—N hydrogen bonds.

Packing of the title compound (Fig. 3) is facilitated through $\pi$–$\pi$ 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).

### S2. Experimental

Triethylamine (25 $\mu$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.

### S3. 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).

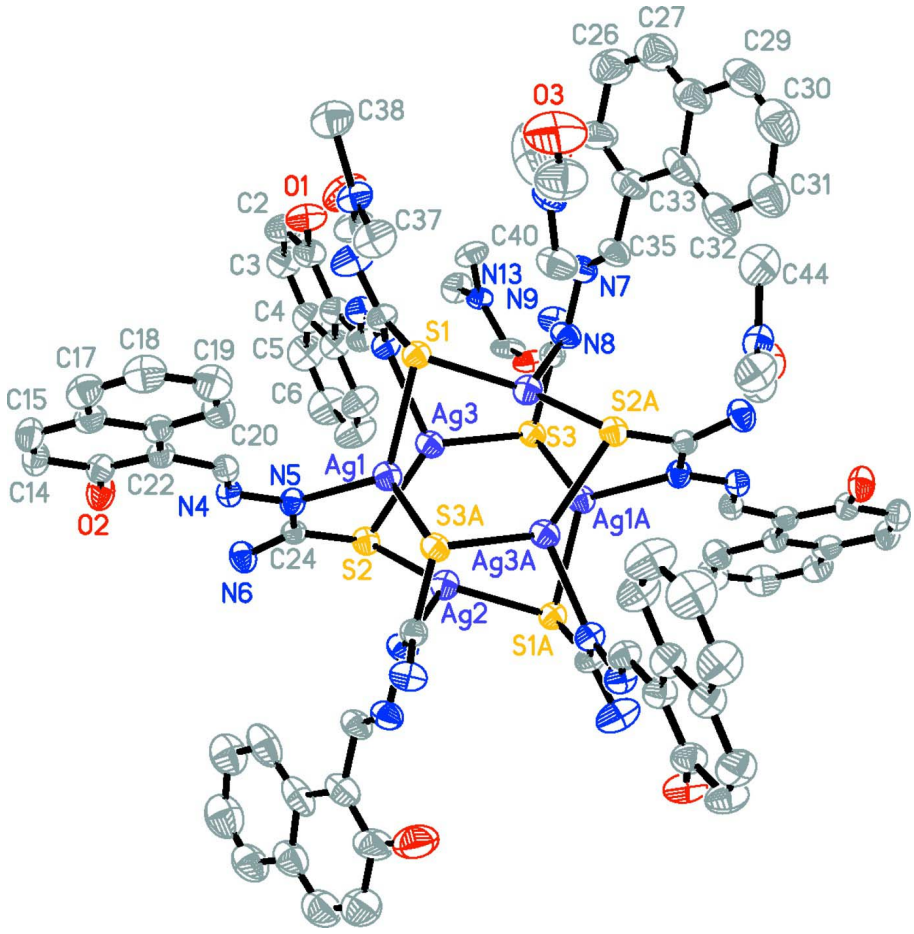


**Figure 1**

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]

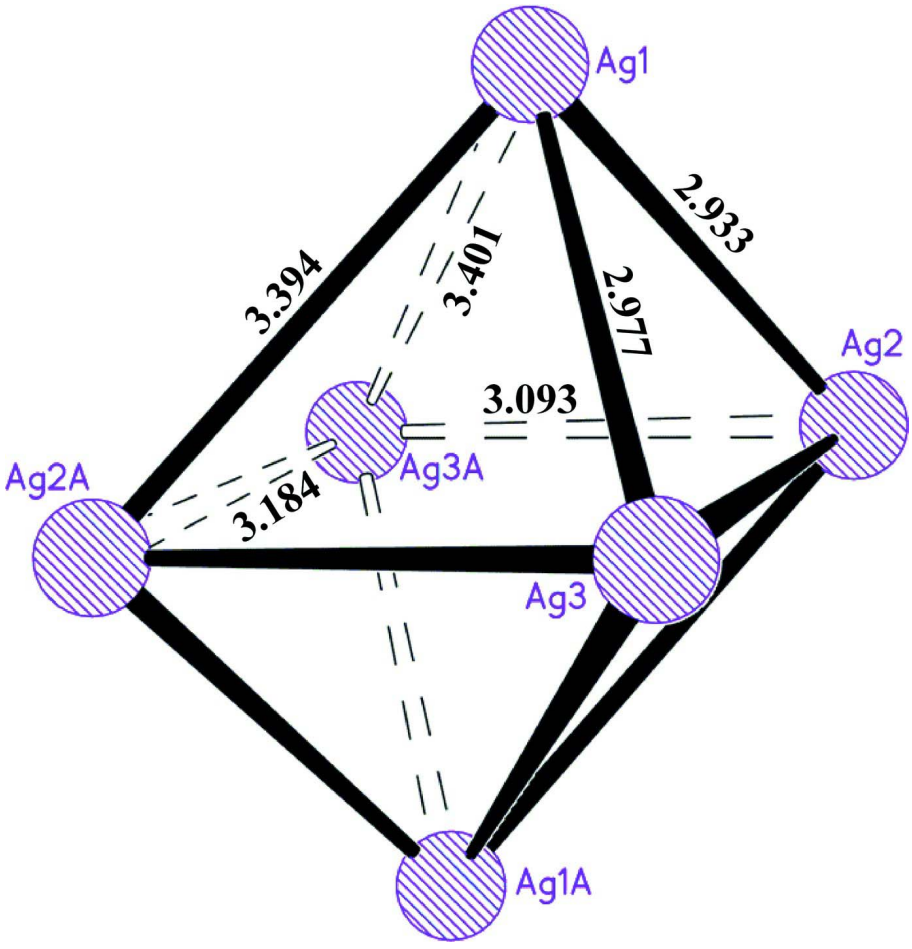


**Figure 2**

$Ag_6$ octahedron in the title compound

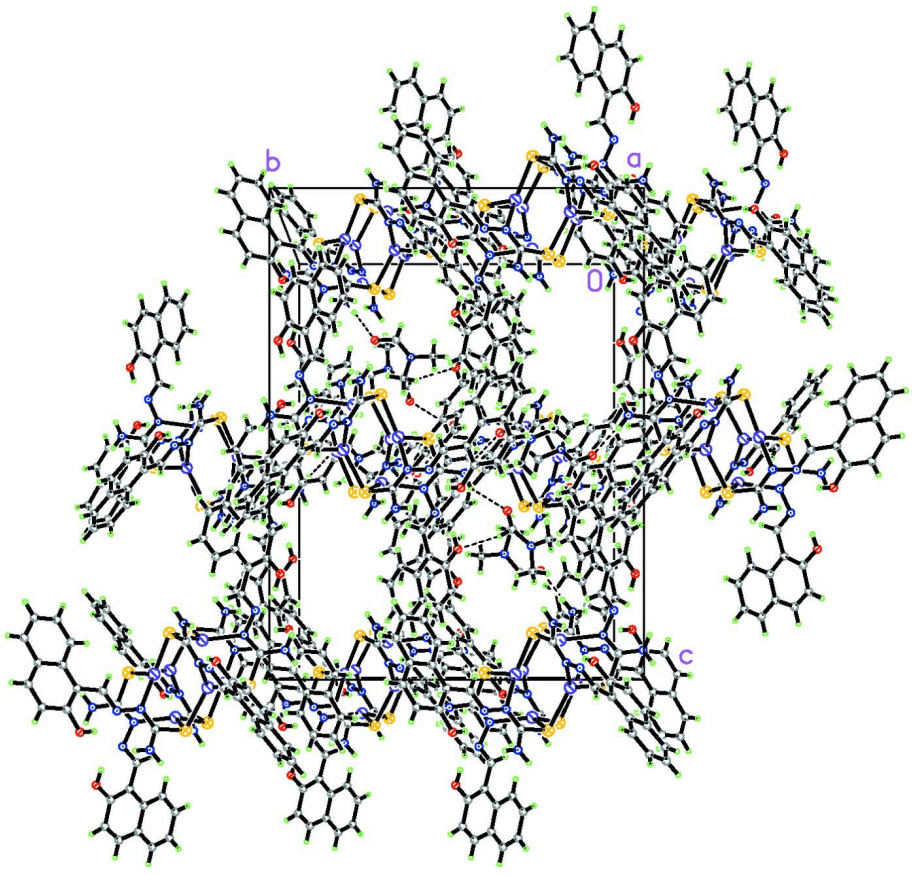


**Figure 3**

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

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*Crystal data*

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$M_r = 2405.34$
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
$a = 24.604$ (3) Å
$b = 18.877$ (3) Å
$c = 24.816$ (3) Å
$\beta = 94.763$ (3)°
$V = 11486$ (3) Å$^3$
$Z = 4$
$F(000) = 4816$
$D_x = 1.391$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6309 reflections
$\theta = 2.2$–27.2°
$\mu = 1.17$ 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
$\varphi$ and $\omega$ 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 $I > 2s(I)$

$R_{int}$ = 0.042
$\theta_{max}$ = 25.0°, $\theta_{min}$ = 1.7°
$h$ = −28→29
$k$ = −22→21
$l$ = −29→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 $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.92 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.42 e Å$^{-3}$

*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 (Å²)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ | 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 (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| 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, º)*

| | | | |
|---|---|---|---|
| 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) |

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| 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 |

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| 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 |

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| 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, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N3—H3*B*···O4 | 0.86 | 1.98 | 2.835 (8) | 175 |
| N6—H6*B*···O6$^{i}$ | 0.86 | 2.00 | 2.845 (7) | 166 |
| N9—H9*A*···O5$^{ii}$ | 0.86 | 2.31 | 3.049 (8) | 145 |
| N9—H9*B*···O7 | 0.86 | 2.02 | 2.870 (6) | 172 |
| O1—H1*B*···N1 | 0.82 | 1.86 | 2.588 (5) | 147 |
| O2—H2*B*···N4 | 0.82 | 1.85 | 2.583 (4) | 148 |
| O3—H3*C*···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.