Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis[μ-bis(diphenylphosphino)methane-κ^2P:P']bis[(4-toluenesulfonato-κO)-silver(I)] monohydrate

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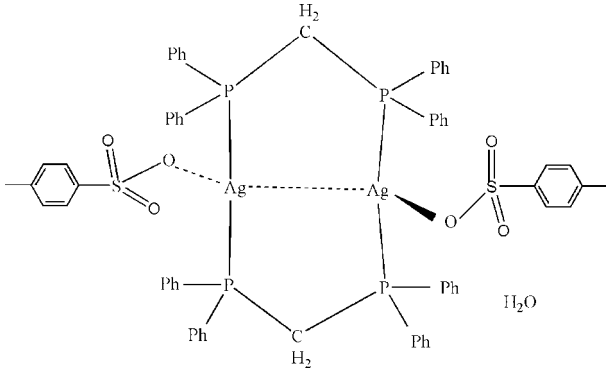
Received 29 October 2007; accepted 17 December 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.007 Å; H-atom completeness 97%; disorder in solvent or counterion; R factor = 0.041; wR factor = 0.131; data-to-parameter ratio = 18.6.

The title complex, $[Ag_2(C_7H_7O_3S)_2(C_{25}H_{22}P_2)_2]\cdot H_2O$, was obtained by the reaction of silver toluenesulfonate with diphenylphosphinomethane (dppm) in acetonitrile. There are two unique half-molecules of the complex in the asymmetric unit, together with one water molecule, which is disordered over two positions with site occupancy factors of 0.6 and 0.4. In each centrosymmetric neutral dimeric molecule, two Ag atoms are bridged by a pair of dppm ligands to give an eight-membered $Ag_2P_4C_2$ ring with a distorted $AgOP_2$ trigonal–planar environment. The Ag—Ag distances of 2.9215 (9) and 3.027 (1) Å indicate a direct bonding interaction.

Related literature

For similar structures, see: Chen *et al.* (2004); Effendy *et al.* (2005); Fournier, Decken & Harvey (2004); Fournier, Lebrun *et al.* (2004); Hong *et al.* (1997); Youm *et al.* (2000).



Experimental

Crystal data

$[Ag_2(C_7H_7O_3S)_2(C_{25}H_{22}P_2)_2]\cdot H_2O$
M_r = 1344.86
Triclinic, $P\overline{1}$
a = 11.239 (2) Å
b = 11.802 (2) Å
c = 23.363 (5) Å
α = 103.86 (3)°
β = 93.79 (3)°
γ = 91.95 (3)°
V = 2998.1 (10) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.88 mm^{-1}
T = 293 (2) K
0.36 × 0.31 × 0.28 mm

Data collection

Rigaku Weissenberg IP diffractometer
Absorption correction: none
27870 measured reflections
13424 independent reflections
11383 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.131
S = 1.05
13424 reflections
721 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.71 e Å^{-3}
$\Delta\rho_{min}$ = −1.86 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ag1—P2	2.4067 (11)	Ag2—P4	2.4033 (11)
Ag1—P1	2.4255 (11)	Ag2—P3	2.4181 (12)
Ag1—O6	2.491 (3)	Ag2—O3	2.500 (3)
P2—Ag1—P1	164.99 (3)	P4—Ag2—P3	158.11 (3)
P2—Ag1—O6	112.29 (10)	P4—Ag2—O3	111.55 (9)
P1—Ag1—O6	82.57 (10)	P3—Ag2—O3	90.29 (9)

Data collection: *CrystalClear* (Rigaku, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Sheldrick, 1993); software used to prepare material for publication: *SHELXL97*.

The authors are grateful for financial support from the innovation fund of Fujian Province (2003J044).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CF2162).

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 doi:10.1107/S1600536807067311

supporting information

Acta Cryst. (2008). E**64**, m269 [doi:10.1107/S1600536807067311]

Bis[μ-bis(diphenylphosphino)methane-$\kappa^2P:P'$]bis[(4-toluenesulfonato-κO)silver(I)] monohydrate

Zhen Ma, Jianhua Sun, Baoqing Liu, Miao Hu and Yanpeng Xing

S1. Comment

There has been, in recent years, considerable interest in the study of compounds of dppm (Effendy *et al.*, 2005; Fournier, Decken & Harvey, 2004; Forunier, Lebrun *et al.*, 2004), since this diphosphine is a very convenient ligand to coordinate to silver ions, to form complexes with interesting structures. These compounds have attracted considerable interest because they can be used as building blocks for reactions with other chemical groups to construct complexes which often display interesting properties (Chen *et al.*, 2004; Youm *et al.*, 2000).

The molecules of the title complex (1) (Fig. 1) are centrosymmetric, with the two toluenesulfonate ions coordinated to two silver atoms lying *trans* to each other. The structure contains two crystallographically independent complex molecules.

The structure consists of a neutral dimeric molecule with two silver atoms bridged by a pair of dppm ligands to give an eight-membered $Ag_2P_4C_2$ ring, similar to the structures of $[Ag(dppm)(O_2CCF_3)]_2$, $[Ag(dppm)(O_2CCH_2Ph)]_2$ and $[Ag(dppm)(O_2CCH_2Ph)]_2$. There are several reported examples, which show similar distorted triangle structures (Effendy *et al.*, 2005; Fournier, Decken & Harvey, 2004; Forunier, Lebrun *et al.*, 2004; Hong *et al.*, 1997). Each silver ion is coordinated by two phosphorus atoms from two dppm molecules and one oxygen atom from one toluenesulfonate ligand. Therefore, each silver atom is in a highly distorted $AgOP_2$ trigonal-planar coordination environment. There is a metal-metal contact between the two silver ions in each molecule of the title complex. The distances between the two silver atoms are 2.9215 (9) Å and 3.027 (1) Å in the two molecules.

One water molecule is contained in the asymmetric unit and it is disordered over two alternative sites. This water originates from the moisture contained in the solvents, acetonitrile and diethyl ether, which were used in the synthesis. There are no hydrogen bonds between the water molecules and oxygen atoms of the toluenesulfonate ligands.

S2. Experimental

The title compound was obtained by the reaction of silver toluenesulfonate ($AgSO_3C_6H_4CH_3$) and diphenylphosphino-methane (dppm) in acetonitrile. In a 50 cm^3 flask fitted with a funnel, silver toluenesulfonate (1.0 g, 3.6 mmol) was dissolved in 20 cm^3 of acetonitrile. To this solution was added dropwise an equimolar quantity of diphenylphosphino-methane (dppm) (1.4 g, 3.6 mmol) dissolved in 20 cm^3 of acetonitrile, over a period of half an hour with stirring. The mixture was then stirred for 24 h. The solution was concentrated and the white solid formed by adding a large quantity of diethyl ether was filtered off and washed with diethyl ether (2 × 10 cm^3) (yield 81%). All processes were undertaken under dinitrogen gas. Slow evaporation of an acetonitrile solution of the title complex led to the formation of colorless crystals, which were suitable for X-ray characterization.

S3. Refinement

All H atoms were positioned geometrically and refined using a riding model with C—H = 0.93–0.97 Å and with U_{iso}(H) = 1.2U_{eq}(C). The occupancy factors of the disordered water molecule were initially refined and then fixed. H atoms were not included for this molecule.

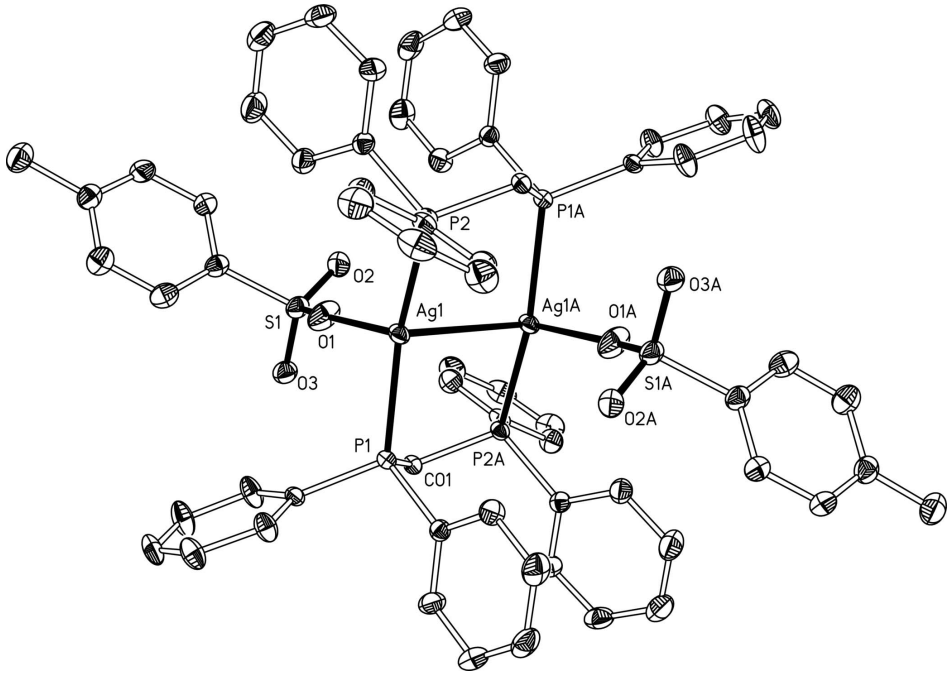

Figure 1

The structure of one molecule of the title complex, showing the atom labeling scheme and 20% probability displacement ellipsoids. H atoms have been omitted for clarity.

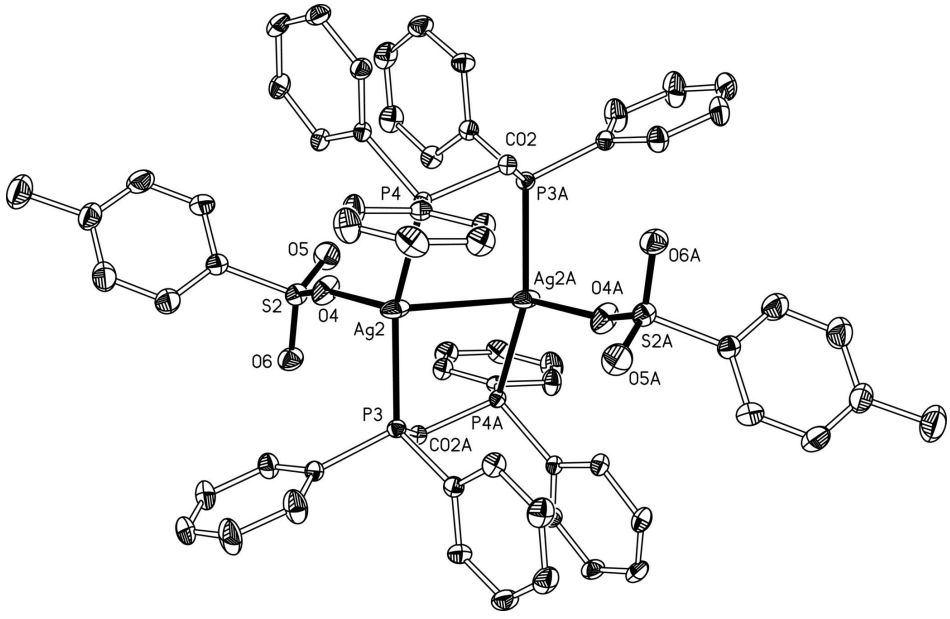

Figure 2

The structure of the other independent molecule of the title complex, showing the atom labeling scheme and 20% probability displacement ellipsoids. H atoms have been omitted for clarity.

Bis[μ-bis(diphenylphosphino)methane-κ^2P:P']bis[(4-toluenesulfonato-\ κO)silver(I)] monohydrate

Crystal data

$[Ag_2(C_7H_7O_3S)_2(C_{25}H_{22}P_2)_2]\cdot H_2O$
M_r = 1344.86
Triclinic, $P\overline{1}$
a = 11.239 (2) Å
b = 11.802 (2) Å
c = 23.363 (5) Å
α = 103.86 (3)°
β = 93.79 (3)°
γ = 91.95 (3)°
V = 2998.1 (10) Å^3
Z = 2
$F(000)$ = 1372
D_x = 1.490 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 27870 reflections
θ = 0.9–27.5°
μ = 0.88 mm^{-1}
T = 293 K
Prism, colorless
0.36 × 0.31 × 0.28 mm

Data collection

Rigaku Weissenberg IP diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
27870 measured reflections
13424 independent reflections
11383 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 27.5°, θ_{min} = 0.9°
h = −14→14
k = 0→15
l = −30→29

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.131
S = 1.05
13424 reflections
721 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

$w = 1/[\sigma^2(F_o^2) + (0.0589P)^2 + 6.0201P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.71$ e Å^{-3}
$\Delta\rho_{min} = -1.86$ 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	0.11622 (2)	0.48402 (2)	0.475474 (11)	0.03703 (8)	
Ag2	0.52075 (3)	−0.12811 (4)	−0.005498 (15)	0.05974 (11)	
S1	0.17891 (10)	0.82300 (8)	0.53039 (5)	0.0482 (2)	
S2	0.32006 (9)	−0.14579 (10)	0.12284 (4)	0.0468 (2)	
P1	0.20944 (7)	0.48870 (7)	0.57271 (4)	0.02923 (16)	
P2	0.02266 (7)	0.42514 (8)	0.37653 (4)	0.03273 (18)	
P3	0.33812 (8)	−0.17322 (7)	−0.06908 (4)	0.03266 (17)	
P4	0.72861 (7)	−0.07571 (7)	0.02262 (4)	0.03080 (17)	
O1	0.2033 (3)	−0.1768 (3)	0.09323 (16)	0.0647 (9)	
O2	0.3227 (4)	−0.0401 (3)	0.16896 (17)	0.0817 (11)	
O3	0.4092 (3)	−0.1455 (4)	0.08136 (16)	0.0742 (11)	
O4	0.2356 (3)	0.8514 (3)	0.58977 (13)	0.0560 (7)	
O5	0.0663 (3)	0.8772 (3)	0.52626 (17)	0.0671 (9)	
O6	0.1714 (4)	0.6974 (3)	0.50571 (16)	0.0792 (12)	
O7	0.5206 (6)	−0.4429 (5)	−0.0011 (4)	0.088 (2)	0.60
O7′	0.5506 (10)	−0.3613 (10)	−0.0078 (6)	0.089 (3)	0.40
C2	0.3684 (3)	0.5306 (3)	0.58370 (14)	0.0331 (7)	
C6	0.7859 (3)	−0.1123 (3)	0.08989 (15)	0.0333 (7)	
C7	0.0743 (3)	0.2859 (3)	0.33560 (15)	0.0378 (7)	
C8	0.3349 (3)	−0.1564 (3)	−0.14428 (15)	0.0376 (7)	
C9	0.2753 (3)	−0.3222 (3)	−0.07880 (17)	0.0393 (7)	
C12	0.0512 (3)	0.5273 (3)	0.33133 (16)	0.0383 (7)	
C13	0.8185 (3)	−0.1551 (3)	−0.03427 (15)	0.0357 (7)	
C14	0.1999 (3)	0.3577 (3)	0.60008 (16)	0.0367 (7)	
C15	0.2273 (4)	−0.1704 (4)	−0.17894 (17)	0.0478 (9)	
H15A	0.1569	−0.1888	−0.1636	0.057*	
C17	0.8550 (4)	−0.1080 (4)	−0.07943 (17)	0.0467 (9)	
H17A	0.8406	−0.0307	−0.0791	0.056*	
C19	0.7052 (3)	−0.1347 (3)	0.12909 (16)	0.0400 (8)	
H19A	0.6235	−0.1371	0.1193	0.048*	

C20	0.7485 (4)	−0.1536 (4)	0.18303 (18)	0.0496 (9)
H20A	0.6952	−0.1674	0.2097	0.060*
C21	0.3563 (4)	−0.2598 (4)	0.15795 (17)	0.0463 (9)
C22	0.2751 (4)	0.8784 (3)	0.48523 (18)	0.0473 (9)
C23	0.4493 (3)	0.4454 (4)	0.5664 (2)	0.0512 (10)
H23A	0.4219	0.3681	0.5512	0.061*
C24	0.1552 (4)	0.2805 (4)	0.29251 (19)	0.0538 (10)
H24A	0.1796	0.3479	0.2816	0.065*
C26	0.9490 (4)	−0.1326 (4)	0.15803 (19)	0.0517 (10)
H26A	1.0306	−0.1331	0.1676	0.062*
C27	0.9081 (3)	−0.1125 (3)	0.10436 (17)	0.0417 (8)
H27A	0.9622	−0.0992	0.0779	0.050*
C29	0.8692 (4)	−0.1519 (4)	0.19723 (18)	0.0534 (10)
H29A	0.8971	−0.1639	0.2336	0.064*
C30	0.4389 (4)	−0.1289 (4)	−0.16758 (18)	0.0478 (9)
H30A	0.5112	−0.1184	−0.1447	0.057*
C31	0.2081 (4)	−0.3538 (4)	−0.0374 (2)	0.0537 (10)
H31A	0.1895	−0.2975	−0.0044	0.064*
C32	0.0403 (4)	0.1840 (4)	0.3511 (2)	0.0542 (10)
H32A	−0.0120	0.1870	0.3806	0.065*
C33	0.0006 (4)	0.5106 (4)	0.27401 (18)	0.0517 (10)
H33A	−0.0534	0.4476	0.2583	0.062*
C38	0.4246 (4)	0.9528 (4)	0.4089 (2)	0.0553 (10)
C39	0.1301 (4)	0.6226 (4)	0.3540 (2)	0.0530 (10)
H39A	0.1643	0.6357	0.3925	0.064*
C40	0.8402 (4)	−0.2709 (4)	−0.0359 (2)	0.0565 (11)
H40A	0.8163	−0.3039	−0.0059	0.068*
C41	0.1347 (4)	0.2598 (3)	0.5671 (2)	0.0506 (9)
H41A	0.0956	0.2610	0.5309	0.061*
C42	0.9330 (5)	−0.2888 (4)	−0.1265 (2)	0.0646 (13)
H42A	0.9712	−0.3339	−0.1576	0.078*
C43	0.3292 (6)	−0.3750 (5)	0.1302 (2)	0.0782 (16)
H43A	0.2921	−0.3946	0.0921	0.094*
C45	0.4113 (3)	0.6444 (4)	0.6055 (2)	0.0571 (12)
H45A	0.3586	0.7035	0.6163	0.069*
C46	0.2370 (4)	0.9589 (5)	0.4548 (2)	0.0614 (12)
H46A	0.1614	0.9881	0.4592	0.074*
C48	0.0302 (5)	0.5871 (5)	0.2401 (2)	0.0638 (12)
H48A	−0.0040	0.5750	0.2016	0.077*
C49	0.3296 (5)	−0.1306 (4)	−0.25938 (19)	0.0649 (13)
H49A	0.3280	−0.1222	−0.2980	0.078*
C50	0.9128 (4)	−0.1759 (4)	−0.12514 (19)	0.0577 (11)
H50A	0.9380	−0.1435	−0.1551	0.069*
C51	0.2566 (4)	0.3543 (4)	0.6541 (2)	0.0566 (11)
H51A	0.2993	0.4203	0.6772	0.068*
C53	0.4351 (5)	−0.1169 (5)	−0.2258 (2)	0.0630 (12)
H53A	0.5052	−0.0994	−0.2416	0.076*
C54	0.8970 (5)	−0.3371 (4)	−0.0820 (3)	0.0697 (14)

H54A	0.9111	−0.4147	−0.0830	0.084*
C55	0.2253 (5)	−0.1568 (4)	−0.23639 (19)	0.0595 (11)
H55A	0.1533	−0.1655	−0.2594	0.071*
C56	0.1858 (5)	0.1565 (4)	0.6406 (3)	0.0690 (14)
H56A	0.1819	0.0885	0.6539	0.083*
C57	0.1992 (5)	0.1740 (5)	0.2660 (2)	0.0671 (14)
H57A	0.2545	0.1707	0.2379	0.081*
C58	0.6119 (4)	0.5862 (5)	0.5946 (2)	0.0620 (12)
H58A	0.6935	0.6051	0.5992	0.074*
C59	0.5332 (4)	0.6708 (4)	0.6112 (3)	0.0713 (15)
H59A	0.5618	0.7477	0.6266	0.086*
C60	0.1949 (6)	−0.5531 (4)	−0.0928 (3)	0.0740 (15)
H60A	0.1672	−0.6303	−0.0979	0.089*
C61	0.2631 (7)	−0.5224 (4)	−0.1333 (3)	0.092 (2)
H61A	0.2832	−0.5794	−0.1657	0.110*
C62	0.1624 (5)	0.0729 (5)	0.2808 (2)	0.0672 (14)
H62A	0.1913	0.0016	0.2621	0.081*
C64	0.3126 (5)	0.9959 (5)	0.4174 (2)	0.0660 (13)
H64A	0.2872	1.0514	0.3975	0.079*
C66	0.3889 (5)	0.8387 (4)	0.4794 (2)	0.0590 (11)
H66A	0.4163	0.7873	0.5014	0.071*
C67	0.5707 (4)	0.4744 (5)	0.5714 (2)	0.0624 (12)
H67A	0.6242	0.4168	0.5589	0.075*
C68	0.1278 (5)	0.1597 (4)	0.5881 (3)	0.0678 (13)
H68A	0.0830	0.0941	0.5661	0.081*
C70	0.1094 (5)	0.6806 (5)	0.2626 (3)	0.0705 (14)
H70A	0.1296	0.7313	0.2394	0.085*
C73	0.1676 (5)	−0.4697 (4)	−0.0447 (3)	0.0663 (13)
H73A	0.1219	−0.4903	−0.0167	0.080*
C78	0.4108 (5)	−0.2348 (5)	0.2141 (2)	0.0680 (13)
H78A	0.4303	−0.1574	0.2337	0.082*
C81	0.4107 (5)	−0.4374 (5)	0.2148 (3)	0.0704 (14)
C83	0.0827 (5)	0.0782 (4)	0.3233 (3)	0.0674 (13)
H83A	0.0573	0.0102	0.3335	0.081*
C84	0.1582 (5)	0.6988 (5)	0.3191 (3)	0.0723 (14)
H84A	0.2110	0.7628	0.3346	0.087*
C85	0.4626 (5)	0.8747 (4)	0.4412 (2)	0.0632 (12)
H85A	0.5385	0.8461	0.4372	0.076*
C87	0.3025 (6)	−0.4082 (4)	−0.1268 (2)	0.0752 (16)
H87A	0.3481	−0.3887	−0.1551	0.090*
C88	0.2498 (5)	0.2531 (5)	0.6737 (3)	0.0716 (14)
H88A	0.2891	0.2506	0.7096	0.086*
C90	0.4370 (6)	−0.3222 (6)	0.2419 (3)	0.0800 (17)
H90A	0.4736	−0.3025	0.2801	0.096*
C96	0.1402 (3)	0.5998 (3)	0.62743 (14)	0.0318 (6)
H96A	0.1589	0.6763	0.6209	0.038*
H96B	0.1735	0.5990	0.6667	0.038*
C97	0.7757 (3)	0.0787 (3)	0.03314 (15)	0.0337 (7)

H97A	0.7883	0.0948	−0.0049	0.040*
H97B	0.8507	0.0954	0.0573	0.040*
C98	0.5038 (5)	0.9900 (5)	0.3662 (2)	0.0739 (15)
H98A	0.5768	0.9500	0.3656	0.111*
H98B	0.5214	1.0728	0.3786	0.111*
H98C	0.4636	0.9709	0.3273	0.111*
C99	0.4362 (7)	−0.5352 (7)	0.2452 (4)	0.107 (2)
H99A	0.4112	−0.6090	0.2187	0.161*
H99B	0.3933	−0.5244	0.2801	0.161*
H99C	0.5203	−0.5340	0.2559	0.161*
C101	0.3570 (7)	−0.4622 (5)	0.1587 (3)	0.0879 (19)
H10A	0.3385	−0.5398	0.1391	0.105*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.02949 (13)	0.05165 (17)	0.02728 (12)	0.00223 (10)	−0.00020 (9)	0.00493 (10)
Ag2	0.03214 (16)	0.1020 (3)	0.04636 (18)	−0.00563 (16)	−0.00490 (12)	0.02374 (18)
S1	0.0611 (6)	0.0363 (5)	0.0468 (5)	−0.0101 (4)	−0.0032 (4)	0.0132 (4)
S2	0.0446 (5)	0.0581 (6)	0.0402 (5)	0.0047 (4)	0.0103 (4)	0.0144 (4)
P1	0.0275 (4)	0.0300 (4)	0.0289 (4)	0.0025 (3)	−0.0004 (3)	0.0051 (3)
P2	0.0282 (4)	0.0415 (5)	0.0263 (4)	0.0019 (3)	0.0013 (3)	0.0040 (3)
P3	0.0328 (4)	0.0324 (4)	0.0320 (4)	0.0027 (3)	0.0011 (3)	0.0065 (3)
P4	0.0304 (4)	0.0321 (4)	0.0316 (4)	0.0038 (3)	0.0027 (3)	0.0107 (3)
O1	0.0455 (17)	0.080 (2)	0.073 (2)	0.0070 (15)	0.0001 (15)	0.0274 (18)
O2	0.116 (3)	0.062 (2)	0.061 (2)	0.013 (2)	0.005 (2)	0.0021 (17)
O3	0.0556 (19)	0.117 (3)	0.068 (2)	0.0161 (19)	0.0280 (17)	0.050 (2)
O4	0.0642 (19)	0.0592 (18)	0.0449 (15)	−0.0055 (14)	−0.0003 (14)	0.0153 (13)
O5	0.0529 (18)	0.073 (2)	0.084 (2)	−0.0070 (16)	−0.0007 (17)	0.0381 (19)
O6	0.130 (3)	0.0410 (17)	0.064 (2)	−0.0213 (19)	0.004 (2)	0.0114 (15)
O7	0.067 (4)	0.050 (3)	0.160 (7)	0.009 (3)	−0.008 (4)	0.053 (4)
O7′	0.082 (7)	0.069 (7)	0.118 (9)	0.015 (5)	−0.014 (6)	0.030 (6)
C2	0.0264 (15)	0.0412 (18)	0.0313 (15)	0.0033 (12)	0.0000 (12)	0.0085 (13)
C6	0.0345 (16)	0.0326 (16)	0.0344 (16)	0.0028 (12)	0.0027 (13)	0.0113 (13)
C7	0.0299 (16)	0.048 (2)	0.0319 (16)	0.0082 (14)	−0.0004 (13)	0.0017 (14)
C8	0.0439 (19)	0.0366 (18)	0.0310 (16)	0.0032 (14)	0.0050 (14)	0.0050 (13)
C9	0.0424 (19)	0.0316 (17)	0.0433 (19)	0.0044 (14)	−0.0026 (15)	0.0089 (14)
C12	0.0389 (18)	0.0421 (19)	0.0348 (17)	0.0054 (14)	0.0071 (14)	0.0094 (14)
C13	0.0320 (16)	0.0399 (18)	0.0337 (16)	0.0027 (13)	0.0000 (13)	0.0066 (14)
C14	0.0344 (17)	0.0363 (17)	0.0409 (18)	0.0047 (13)	0.0044 (14)	0.0112 (14)
C15	0.048 (2)	0.054 (2)	0.0384 (19)	−0.0008 (17)	−0.0033 (16)	0.0061 (17)
C17	0.054 (2)	0.046 (2)	0.042 (2)	0.0077 (17)	0.0102 (17)	0.0110 (16)
C19	0.0395 (18)	0.0420 (19)	0.0430 (19)	0.0068 (14)	0.0072 (15)	0.0174 (15)
C20	0.058 (2)	0.057 (2)	0.041 (2)	0.0102 (19)	0.0128 (18)	0.0231 (18)
C21	0.045 (2)	0.058 (2)	0.0385 (19)	0.0019 (17)	0.0085 (15)	0.0154 (17)
C22	0.062 (2)	0.0354 (19)	0.045 (2)	−0.0049 (17)	−0.0005 (18)	0.0123 (16)
C23	0.0357 (19)	0.043 (2)	0.069 (3)	0.0072 (15)	0.0046 (18)	0.0010 (19)
C24	0.048 (2)	0.065 (3)	0.047 (2)	0.0126 (19)	0.0138 (18)	0.0066 (19)

C26	0.041 (2)	0.062 (3)	0.052 (2)	0.0079 (18)	−0.0085 (17)	0.018 (2)
C27	0.0354 (18)	0.049 (2)	0.0443 (19)	0.0025 (15)	0.0019 (15)	0.0177 (16)
C29	0.066 (3)	0.059 (3)	0.038 (2)	0.013 (2)	−0.0041 (18)	0.0182 (18)
C30	0.048 (2)	0.052 (2)	0.044 (2)	0.0070 (17)	0.0105 (17)	0.0117 (17)
C31	0.065 (3)	0.039 (2)	0.058 (2)	0.0033 (18)	0.011 (2)	0.0123 (18)
C32	0.046 (2)	0.057 (3)	0.061 (3)	0.0145 (18)	0.0103 (19)	0.015 (2)
C33	0.054 (2)	0.061 (3)	0.039 (2)	0.0014 (19)	0.0009 (17)	0.0129 (18)
C38	0.066 (3)	0.048 (2)	0.050 (2)	−0.011 (2)	0.002 (2)	0.0095 (18)
C39	0.054 (2)	0.055 (2)	0.049 (2)	−0.0085 (19)	0.0034 (18)	0.0128 (19)
C40	0.075 (3)	0.039 (2)	0.059 (3)	0.0149 (19)	0.021 (2)	0.0144 (18)
C41	0.054 (2)	0.037 (2)	0.057 (2)	−0.0024 (17)	−0.0037 (19)	0.0087 (17)
C42	0.067 (3)	0.061 (3)	0.055 (3)	0.003 (2)	0.020 (2)	−0.011 (2)
C43	0.111 (5)	0.067 (3)	0.053 (3)	−0.006 (3)	−0.012 (3)	0.015 (2)
C45	0.0327 (19)	0.040 (2)	0.088 (3)	0.0046 (15)	0.0014 (19)	−0.006 (2)
C46	0.053 (3)	0.071 (3)	0.069 (3)	−0.001 (2)	0.001 (2)	0.037 (2)
C48	0.073 (3)	0.081 (3)	0.044 (2)	0.015 (3)	0.008 (2)	0.027 (2)
C49	0.101 (4)	0.060 (3)	0.033 (2)	0.009 (3)	0.008 (2)	0.0095 (19)
C50	0.064 (3)	0.069 (3)	0.040 (2)	0.005 (2)	0.0167 (19)	0.008 (2)
C51	0.068 (3)	0.056 (3)	0.049 (2)	−0.005 (2)	−0.008 (2)	0.024 (2)
C53	0.075 (3)	0.070 (3)	0.047 (2)	0.009 (2)	0.022 (2)	0.016 (2)
C54	0.087 (4)	0.041 (2)	0.079 (3)	0.014 (2)	0.022 (3)	0.006 (2)
C55	0.074 (3)	0.061 (3)	0.038 (2)	0.003 (2)	−0.012 (2)	0.0054 (19)
C56	0.075 (3)	0.055 (3)	0.092 (4)	0.012 (2)	0.024 (3)	0.042 (3)
C57	0.065 (3)	0.086 (4)	0.048 (2)	0.030 (3)	0.017 (2)	0.002 (2)
C58	0.0260 (18)	0.084 (3)	0.069 (3)	0.0000 (19)	0.0031 (18)	0.005 (2)
C59	0.040 (2)	0.053 (3)	0.106 (4)	−0.0103 (19)	0.001 (2)	−0.007 (3)
C60	0.104 (4)	0.032 (2)	0.084 (4)	−0.005 (2)	−0.009 (3)	0.015 (2)
C61	0.161 (7)	0.030 (2)	0.078 (4)	0.000 (3)	0.026 (4)	0.000 (2)
C62	0.065 (3)	0.067 (3)	0.059 (3)	0.029 (2)	−0.005 (2)	−0.006 (2)
C64	0.069 (3)	0.070 (3)	0.070 (3)	−0.010 (2)	−0.007 (2)	0.041 (3)
C66	0.075 (3)	0.046 (2)	0.060 (3)	0.009 (2)	0.009 (2)	0.019 (2)
C67	0.034 (2)	0.070 (3)	0.077 (3)	0.0134 (19)	0.008 (2)	0.003 (2)
C68	0.075 (3)	0.036 (2)	0.092 (4)	−0.004 (2)	0.010 (3)	0.014 (2)
C70	0.077 (3)	0.071 (3)	0.076 (3)	0.011 (3)	0.022 (3)	0.038 (3)
C73	0.077 (3)	0.047 (3)	0.082 (3)	−0.003 (2)	0.012 (3)	0.028 (2)
C78	0.072 (3)	0.074 (3)	0.055 (3)	−0.008 (3)	−0.014 (2)	0.017 (2)
C81	0.068 (3)	0.078 (4)	0.077 (3)	0.006 (3)	0.008 (3)	0.041 (3)
C83	0.061 (3)	0.054 (3)	0.086 (4)	0.017 (2)	0.004 (3)	0.014 (2)
C84	0.077 (3)	0.066 (3)	0.078 (4)	−0.014 (3)	0.013 (3)	0.026 (3)
C85	0.074 (3)	0.048 (2)	0.070 (3)	0.010 (2)	0.016 (2)	0.015 (2)
C87	0.115 (5)	0.044 (2)	0.066 (3)	0.005 (3)	0.035 (3)	0.005 (2)
C88	0.083 (4)	0.075 (3)	0.070 (3)	0.001 (3)	−0.001 (3)	0.046 (3)
C90	0.083 (4)	0.105 (5)	0.058 (3)	−0.005 (3)	−0.012 (3)	0.038 (3)
C96	0.0271 (15)	0.0364 (17)	0.0297 (15)	0.0019 (12)	0.0007 (12)	0.0042 (12)
C97	0.0359 (17)	0.0314 (16)	0.0344 (16)	0.0023 (12)	0.0045 (13)	0.0088 (13)
C98	0.085 (4)	0.072 (3)	0.064 (3)	−0.018 (3)	0.011 (3)	0.016 (3)
C99	0.115 (6)	0.107 (5)	0.122 (6)	0.010 (4)	0.008 (5)	0.073 (5)
C101	0.122 (5)	0.060 (3)	0.083 (4)	−0.006 (3)	−0.004 (4)	0.024 (3)

Geometric parameters (Å, º)

Ag1—P2	2.4067 (11)	C38—C85	1.385 (7)
Ag1—P1	2.4255 (11)	C38—C98	1.510 (7)
Ag1—O6	2.491 (3)	C39—C84	1.392 (7)
Ag1—Ag1^{i}	2.9215 (9)	C39—H39A	0.930
Ag2—P4	2.4033 (11)	C40—C54	1.378 (6)
Ag2—P3	2.4181 (12)	C40—H40A	0.930
Ag2—O3	2.500 (3)	C41—C68	1.384 (6)
Ag2—Ag2^{ii}	3.0278 (11)	C41—H41A	0.930
S1—O5	1.445 (4)	C42—C50	1.353 (7)
S1—O4	1.446 (3)	C42—C54	1.376 (8)
S1—O6	1.454 (3)	C42—H42A	0.930
S1—C22	1.773 (4)	C43—C101	1.387 (8)
S2—O1	1.436 (3)	C43—H43A	0.930
S2—O2	1.438 (4)	C45—C59	1.386 (6)
S2—O3	1.439 (3)	C45—H45A	0.930
S2—C21	1.781 (4)	C46—C64	1.390 (7)
P1—C14	1.812 (4)	C46—H46A	0.930
P1—C2	1.823 (3)	C48—C70	1.371 (8)
P1—C96	1.832 (3)	C48—H48A	0.930
P2—C12	1.817 (4)	C49—C53	1.360 (7)
P2—C7	1.827 (4)	C49—C55	1.378 (8)
P2—C96^{i}	1.837 (3)	C49—H49A	0.930
P3—C8	1.813 (4)	C50—H50A	0.930
P3—C9	1.828 (4)	C51—C88	1.379 (6)
P3—C97^{ii}	1.837 (3)	C51—H51A	0.930
P4—C6	1.811 (3)	C53—H53A	0.930
P4—C13	1.820 (4)	C54—H54A	0.930
P4—C97	1.835 (3)	C55—H55A	0.930
O7—O7′	1.060 (12)	C56—C68	1.360 (8)
O7—O7^{iii}	1.423 (12)	C56—C88	1.365 (8)
C2—C45	1.375 (5)	C56—H56A	0.930
C2—C23	1.384 (5)	C57—C62	1.376 (8)
C6—C19	1.393 (5)	C57—H57A	0.930
C6—C27	1.393 (5)	C58—C67	1.354 (7)
C7—C32	1.385 (6)	C58—C59	1.359 (7)
C7—C24	1.393 (5)	C58—H58A	0.930
C8—C30	1.383 (5)	C59—H59A	0.930
C8—C15	1.392 (5)	C60—C61	1.360 (9)
C9—C31	1.377 (6)	C60—C73	1.365 (8)
C9—C87	1.379 (6)	C60—H60A	0.930
C12—C39	1.385 (5)	C61—C87	1.374 (7)
C12—C33	1.386 (5)	C61—H61A	0.930
C13—C17	1.383 (5)	C62—C83	1.374 (8)
C13—C40	1.388 (5)	C62—H62A	0.930
C14—C41	1.381 (5)	C64—H64A	0.930
C14—C51	1.386 (5)	C66—C85	1.386 (7)

C15—C55	1.388 (6)	C66—H66A	0.930
C15—H15A	0.930	C67—H67A	0.930
C17—C50	1.387 (6)	C68—H68A	0.930
C17—H17A	0.930	C70—C84	1.361 (8)
C19—C20	1.391 (5)	C70—H70A	0.930
C19—H19A	0.930	C73—H73A	0.930
C20—C29	1.374 (6)	C78—C90	1.375 (8)
C20—H20A	0.930	C78—H78A	0.930
C21—C78	1.370 (6)	C81—C101	1.367 (8)
C21—C43	1.373 (7)	C81—C90	1.369 (8)
C22—C46	1.380 (6)	C81—C99	1.518 (8)
C22—C66	1.381 (7)	C83—H83A	0.930
C23—C67	1.386 (6)	C84—H84A	0.930
C23—H23A	0.930	C85—H85A	0.930
C24—C57	1.384 (6)	C87—H87A	0.930
C24—H24A	0.930	C88—H88A	0.930
C26—C29	1.374 (6)	C90—H90A	0.930
C26—C27	1.383 (5)	C96—P2^{i}	1.837 (3)
C26—H26A	0.930	C96—H96A	0.970
C27—H27A	0.930	C96—H96B	0.970
C29—H29A	0.930	C97—P3^{ii}	1.837 (3)
C30—C53	1.399 (6)	C97—H97A	0.970
C30—H30A	0.930	C97—H97B	0.970
C31—C73	1.394 (6)	C98—H98A	0.960
C31—H31A	0.930	C98—H98B	0.960
C32—C83	1.379 (6)	C98—H98C	0.960
C32—H32A	0.930	C99—H99A	0.960
C33—C48	1.382 (6)	C99—H99B	0.960
C33—H33A	0.930	C99—H99C	0.960
C38—C64	1.382 (7)	C101—H10A	0.930

P2—Ag1—P1	164.99 (3)	C13—C40—H40A	119.9
P2—Ag1—O6	112.29 (10)	C14—C41—C68	119.7 (4)
P1—Ag1—O6	82.57 (10)	C14—C41—H41A	120.1
P2—Ag1—Ag1^{i}	91.08 (3)	C68—C41—H41A	120.1
P1—Ag1—Ag1^{i}	90.23 (3)	C50—C42—C54	120.0 (4)
O6—Ag1—Ag1^{i}	92.55 (11)	C50—C42—H42A	120.0
P4—Ag2—P3	158.11 (3)	C54—C42—H42A	120.0
P4—Ag2—O3	111.55 (9)	C21—C43—C101	120.3 (5)
P3—Ag2—O3	90.29 (9)	C21—C43—H43A	119.8
P4—Ag2—Ag2^{ii}	88.54 (4)	C101—C43—H43A	119.8
P3—Ag2—Ag2^{ii}	87.92 (4)	C2—C45—C59	119.8 (4)
O3—Ag2—Ag2^{ii}	95.78 (10)	C2—C45—H45A	120.1
O5—S1—O4	112.8 (2)	C59—C45—H45A	120.1
O5—S1—O6	113.6 (2)	C22—C46—C64	119.3 (5)
O4—S1—O6	110.8 (2)	C22—C46—H46A	120.3
O5—S1—C22	107.0 (2)	C64—C46—H46A	120.3
O4—S1—C22	107.45 (19)	C70—C48—C33	120.7 (5)

O6—S1—C22	104.5 (2)	C70—C48—H48A	119.7
O1—S2—O2	112.5 (2)	C33—C48—H48A	119.7
O1—S2—O3	111.5 (2)	C53—C49—C55	120.2 (4)
O2—S2—O3	113.8 (3)	C53—C49—H49A	119.9
O1—S2—C21	106.5 (2)	C55—C49—H49A	119.9
O2—S2—C21	106.5 (2)	C42—C50—C17	120.7 (4)
O3—S2—C21	105.5 (2)	C42—C50—H50A	119.7
C14—P1—C2	103.14 (16)	C17—C50—H50A	119.7
C14—P1—C96	104.78 (16)	C88—C51—C14	119.9 (4)
C2—P1—C96	104.75 (15)	C88—C51—H51A	120.1
C14—P1—Ag1	118.76 (12)	C14—C51—H51A	120.1
C2—P1—Ag1	115.51 (11)	C49—C53—C30	120.6 (5)
C96—P1—Ag1	108.56 (11)	C49—C53—H53A	119.7
C12—P2—C7	105.20 (17)	C30—C53—H53A	119.7
C12—P2—C96^{i}	106.36 (16)	C42—C54—C40	120.3 (5)
C7—P2—C96^{i}	103.85 (16)	C42—C54—H54A	119.8
C12—P2—Ag1	114.08 (12)	C40—C54—H54A	119.8
C7—P2—Ag1	112.04 (12)	C49—C55—C15	120.2 (4)
C96^{i}—P2—Ag1	114.38 (11)	C49—C55—H55A	119.9
C8—P3—C9	102.78 (17)	C15—C55—H55A	119.9
C8—P3—C97^{ii}	105.92 (16)	C68—C56—C88	120.1 (4)
C9—P3—C97^{ii}	104.90 (16)	C68—C56—H56A	119.9
C8—P3—Ag2	120.08 (13)	C88—C56—H56A	119.9
C9—P3—Ag2	114.48 (12)	C62—C57—C24	121.1 (5)
C97^{ii}—P3—Ag2	107.44 (11)	C62—C57—H57A	119.5
C6—P4—C13	104.61 (16)	C24—C57—H57A	119.5
C6—P4—C97	104.25 (16)	C67—C58—C59	119.6 (4)
C13—P4—C97	105.29 (16)	C67—C58—H58A	120.2
C6—P4—Ag2	115.22 (11)	C59—C58—H58A	120.2
C13—P4—Ag2	109.60 (11)	C58—C59—C45	121.1 (4)
C97—P4—Ag2	116.76 (12)	C58—C59—H59A	119.4
S2—O3—Ag2	165.2 (2)	C45—C59—H59A	119.4
S1—O6—Ag1	167.0 (3)	C61—C60—C73	119.4 (4)
O7′—O7—O7^{iii}	173.8 (14)	C61—C60—H60A	120.3
C45—C2—C23	118.5 (3)	C73—C60—H60A	120.3
C45—C2—P1	122.7 (3)	C60—C61—C87	120.7 (5)
C23—C2—P1	118.7 (3)	C60—C61—H61A	119.6
C19—C6—C27	119.8 (3)	C87—C61—H61A	119.6
C19—C6—P4	118.7 (3)	C83—C62—C57	119.4 (5)
C27—C6—P4	121.4 (3)	C83—C62—H62A	120.3
C32—C7—C24	118.8 (4)	C57—C62—H62A	120.3
C32—C7—P2	119.4 (3)	C38—C64—C46	121.9 (4)
C24—C7—P2	121.6 (3)	C38—C64—H64A	119.1
C30—C8—C15	119.4 (4)	C46—C64—H64A	119.1
C30—C8—P3	120.4 (3)	C22—C66—C85	120.5 (4)
C15—C8—P3	120.2 (3)	C22—C66—H66A	119.7
C31—C9—C87	118.2 (4)	C85—C66—H66A	119.7
C31—C9—P3	122.1 (3)	C58—C67—C23	120.3 (4)

C87—C9—P3	119.6 (3)	C58—C67—H67A	119.9
C39—C12—C33	118.8 (4)	C23—C67—H67A	119.9
C39—C12—P2	118.9 (3)	C56—C68—C41	120.6 (5)
C33—C12—P2	122.3 (3)	C56—C68—H68A	119.7
C17—C13—C40	118.9 (4)	C41—C68—H68A	119.7
C17—C13—P4	122.0 (3)	C84—C70—C48	119.5 (5)
C40—C13—P4	118.7 (3)	C84—C70—H70A	120.2
C41—C14—C51	119.3 (4)	C48—C70—H70A	120.2
C41—C14—P1	119.9 (3)	C60—C73—C31	120.3 (5)
C51—C14—P1	120.8 (3)	C60—C73—H73A	119.8
C55—C15—C8	119.9 (4)	C31—C73—H73A	119.8
C55—C15—H15A	120.0	C21—C78—C90	121.2 (5)
C8—C15—H15A	120.0	C21—C78—H78A	119.4
C13—C17—C50	120.0 (4)	C90—C78—H78A	119.4
C13—C17—H17A	120.0	C101—C81—C90	117.2 (5)
C50—C17—H17A	120.0	C101—C81—C99	120.2 (6)
C20—C19—C6	119.2 (4)	C90—C81—C99	122.6 (6)
C20—C19—H19A	120.4	C62—C83—C32	120.1 (5)
C6—C19—H19A	120.4	C62—C83—H83A	119.9
C29—C20—C19	120.6 (4)	C32—C83—H83A	119.9
C29—C20—H20A	119.7	C70—C84—C39	120.8 (5)
C19—C20—H20A	119.7	C70—C84—H84A	119.6
C78—C21—C43	117.9 (5)	C39—C84—H84A	119.6
C78—C21—S2	120.8 (4)	C38—C85—C66	120.8 (5)
C43—C21—S2	121.3 (4)	C38—C85—H85A	119.6
C46—C22—C66	119.5 (4)	C66—C85—H85A	119.6
C46—C22—S1	120.9 (4)	C61—C87—C9	120.9 (5)
C66—C22—S1	119.6 (3)	C61—C87—H87A	119.5
C2—C23—C67	120.6 (4)	C9—C87—H87A	119.5
C2—C23—H23A	119.7	C56—C88—C51	120.4 (5)
C67—C23—H23A	119.7	C56—C88—H88A	119.8
C57—C24—C7	119.5 (5)	C51—C88—H88A	119.8
C57—C24—H24A	120.2	C81—C90—C78	121.6 (5)
C7—C24—H24A	120.2	C81—C90—H90A	119.2
C29—C26—C27	120.1 (4)	C78—C90—H90A	119.2
C29—C26—H26A	119.9	P1—C96—P2^{i}	112.06 (17)
C27—C26—H26A	119.9	P1—C96—H96A	109.2
C26—C27—C6	120.0 (4)	P2^{i}—C96—H96A	109.2
C26—C27—H27A	120.0	P1—C96—H96B	109.2
C6—C27—H27A	120.0	P2^{i}—C96—H96B	109.2
C20—C29—C26	120.4 (4)	H96A—C96—H96B	107.9
C20—C29—H29A	119.8	P4—C97—P3^{ii}	110.50 (18)
C26—C29—H29A	119.8	P4—C97—H97A	109.6
C8—C30—C53	119.7 (4)	P3^{ii}—C97—H97A	109.6
C8—C30—H30A	120.2	P4—C97—H97B	109.6
C53—C30—H30A	120.2	P3^{ii}—C97—H97B	109.6
C9—C31—C73	120.4 (4)	H97A—C97—H97B	108.1
C9—C31—H31A	119.8	C38—C98—H98A	109.5

C73—C31—H31A	119.8	C38—C98—H98B	109.5
C83—C32—C7	121.0 (4)	H98A—C98—H98B	109.5
C83—C32—H32A	119.5	C38—C98—H98C	109.5
C7—C32—H32A	119.5	H98A—C98—H98C	109.5
C48—C33—C12	120.3 (4)	H98B—C98—H98C	109.5
C48—C33—H33A	119.9	C81—C99—H99A	109.5
C12—C33—H33A	119.9	C81—C99—H99B	109.5
C64—C38—C85	117.9 (4)	H99A—C99—H99B	109.5
C64—C38—C98	121.3 (5)	C81—C99—H99C	109.5
C85—C38—C98	120.8 (5)	H99A—C99—H99C	109.5
C12—C39—C84	119.9 (4)	H99B—C99—H99C	109.5
C12—C39—H39A	120.0	C81—C101—C43	121.9 (6)
C84—C39—H39A	120.0	C81—C101—H10A	119.1
C54—C40—C13	120.1 (4)	C43—C101—H10A	119.1
C54—C40—H40A	119.9		

P2—Ag1—P1—C14	−14.84 (19)	P4—C13—C17—C50	−173.4 (3)
O6—Ag1—P1—C14	172.73 (17)	C27—C6—C19—C20	2.0 (6)
Ag1^{i}—Ag1—P1—C14	80.19 (13)	P4—C6—C19—C20	−174.9 (3)
P2—Ag1—P1—C2	108.48 (17)	C6—C19—C20—C29	−1.0 (6)
O6—Ag1—P1—C2	−63.95 (17)	O1—S2—C21—C78	−138.1 (4)
Ag1^{i}—Ag1—P1—C2	−156.49 (13)	O2—S2—C21—C78	−17.9 (5)
P2—Ag1—P1—C96	−134.27 (15)	O3—S2—C21—C78	103.3 (4)
O6—Ag1—P1—C96	53.30 (16)	O1—S2—C21—C43	40.9 (5)
Ag1^{i}—Ag1—P1—C96	−39.24 (12)	O2—S2—C21—C43	161.1 (5)
P1—Ag1—P2—C12	−152.08 (15)	O3—S2—C21—C43	−77.6 (5)
O6—Ag1—P2—C12	19.80 (18)	O5—S1—C22—C46	0.5 (4)
Ag1^{i}—Ag1—P2—C12	113.00 (13)	O4—S1—C22—C46	−120.9 (4)
P1—Ag1—P2—C7	−32.69 (19)	O6—S1—C22—C46	121.3 (4)
O6—Ag1—P2—C7	139.19 (18)	O5—S1—C22—C66	−178.1 (4)
Ag1^{i}—Ag1—P2—C7	−127.61 (13)	O4—S1—C22—C66	60.5 (4)
P1—Ag1—P2—C96^{i}	85.16 (17)	O6—S1—C22—C66	−57.3 (4)
O6—Ag1—P2—C96^{i}	−102.97 (17)	C45—C2—C23—C67	0.6 (7)
Ag1^{i}—Ag1—P2—C96^{i}	−9.77 (12)	P1—C2—C23—C67	177.0 (4)
P4—Ag2—P3—C8	−6.50 (18)	C32—C7—C24—C57	0.3 (6)
O3—Ag2—P3—C8	170.12 (17)	P2—C7—C24—C57	174.8 (3)
Ag2^{ii}—Ag2—P3—C8	74.34 (14)	C29—C26—C27—C6	−0.2 (6)
P4—Ag2—P3—C9	116.50 (16)	C19—C6—C27—C26	−1.4 (6)
O3—Ag2—P3—C9	−66.88 (17)	P4—C6—C27—C26	175.4 (3)
Ag2^{ii}—Ag2—P3—C9	−162.66 (14)	C19—C20—C29—C26	−0.6 (7)
P4—Ag2—P3—C97^{ii}	−127.45 (14)	C27—C26—C29—C20	1.2 (7)
O3—Ag2—P3—C97^{ii}	49.17 (15)	C15—C8—C30—C53	−0.8 (6)
Ag2^{ii}—Ag2—P3—C97^{ii}	−46.60 (12)	P3—C8—C30—C53	179.6 (3)
P3—Ag2—P4—C6	−160.23 (14)	C87—C9—C31—C73	−0.8 (7)
O3—Ag2—P4—C6	23.41 (17)	P3—C9—C31—C73	−176.2 (4)
Ag2^{ii}—Ag2—P4—C6	119.05 (13)	C24—C7—C32—C83	−1.8 (6)
P3—Ag2—P4—C13	−42.60 (16)	P2—C7—C32—C83	−176.4 (4)
O3—Ag2—P4—C13	141.04 (16)	C39—C12—C33—C48	0.9 (6)

Ag2^{ii}—Ag2—P4—C13	−123.32 (13)	P2—C12—C33—C48	−176.3 (4)
P3—Ag2—P4—C97	76.94 (16)	C33—C12—C39—C84	−0.7 (7)
O3—Ag2—P4—C97	−99.42 (16)	P2—C12—C39—C84	176.7 (4)
Ag2^{ii}—Ag2—P4—C97	−3.79 (12)	C17—C13—C40—C54	0.0 (7)
O1—S2—O3—Ag2	33.0 (12)	P4—C13—C40—C54	173.1 (4)
O2—S2—O3—Ag2	−95.4 (11)	C51—C14—C41—C68	−0.6 (7)
C21—S2—O3—Ag2	148.2 (11)	P1—C14—C41—C68	179.9 (4)
P4—Ag2—O3—S2	149.2 (11)	C78—C21—C43—C101	−0.1 (9)
P3—Ag2—O3—S2	−29.5 (11)	S2—C21—C43—C101	−179.2 (5)
Ag2^{ii}—Ag2—O3—S2	58.5 (11)	C23—C2—C45—C59	−1.9 (7)
O5—S1—O6—Ag1	−43.5 (12)	P1—C2—C45—C59	−178.2 (4)
O4—S1—O6—Ag1	84.8 (12)	C66—C22—C46—C64	1.9 (7)
C22—S1—O6—Ag1	−159.8 (11)	S1—C22—C46—C64	−176.7 (4)
P2—Ag1—O6—S1	100.6 (11)	C12—C33—C48—C70	−0.2 (8)
P1—Ag1—O6—S1	−81.5 (11)	C54—C42—C50—C17	−0.6 (8)
Ag1^{i}—Ag1—O6—S1	8.4 (12)	C13—C17—C50—C42	0.8 (7)
C14—P1—C2—C45	−137.3 (4)	C41—C14—C51—C88	1.5 (7)
C96—P1—C2—C45	−27.9 (4)	P1—C14—C51—C88	−178.9 (4)
Ag1—P1—C2—C45	91.4 (4)	C55—C49—C53—C30	−0.2 (8)
C14—P1—C2—C23	46.4 (3)	C8—C30—C53—C49	0.8 (7)
C96—P1—C2—C23	155.8 (3)	C50—C42—C54—C40	0.1 (9)
Ag1—P1—C2—C23	−84.9 (3)	C13—C40—C54—C42	0.2 (8)
C13—P4—C6—C19	−138.7 (3)	C53—C49—C55—C15	−0.5 (7)
C97—P4—C6—C19	111.0 (3)	C8—C15—C55—C49	0.6 (7)
Ag2—P4—C6—C19	−18.3 (3)	C7—C24—C57—C62	1.3 (7)
C13—P4—C6—C27	44.5 (3)	C67—C58—C59—C45	0.8 (9)
C97—P4—C6—C27	−65.8 (3)	C2—C45—C59—C58	1.2 (9)
Ag2—P4—C6—C27	164.9 (3)	C73—C60—C61—C87	−1.3 (11)
C12—P2—C7—C32	−165.1 (3)	C24—C57—C62—C83	−1.4 (8)
C96^{i}—P2—C7—C32	−53.5 (3)	C85—C38—C64—C46	−3.1 (8)
Ag1—P2—C7—C32	70.5 (3)	C98—C38—C64—C46	177.4 (5)
C12—P2—C7—C24	20.4 (4)	C22—C46—C64—C38	1.3 (8)
C96^{i}—P2—C7—C24	132.0 (3)	C46—C22—C66—C85	−3.1 (7)
Ag1—P2—C7—C24	−104.0 (3)	S1—C22—C66—C85	175.5 (4)
C9—P3—C8—C30	−122.1 (3)	C59—C58—C67—C23	−2.1 (9)
C97^{ii}—P3—C8—C30	128.1 (3)	C2—C23—C67—C58	1.5 (8)
Ag2—P3—C8—C30	6.4 (4)	C88—C56—C68—C41	1.2 (8)
C9—P3—C8—C15	58.3 (3)	C14—C41—C68—C56	−0.8 (8)
C97^{ii}—P3—C8—C15	−51.6 (3)	C33—C48—C70—C84	−0.7 (8)
Ag2—P3—C8—C15	−173.2 (3)	C61—C60—C73—C31	0.7 (9)
C8—P3—C9—C31	−147.3 (3)	C9—C31—C73—C60	0.4 (8)
C97^{ii}—P3—C9—C31	−36.7 (4)	C43—C21—C78—C90	−0.3 (8)
Ag2—P3—C9—C31	80.8 (4)	S2—C21—C78—C90	178.8 (5)
C8—P3—C9—C87	37.4 (4)	C57—C62—C83—C32	−0.1 (8)
C97^{ii}—P3—C9—C87	148.0 (4)	C7—C32—C83—C62	1.7 (7)
Ag2—P3—C9—C87	−94.5 (4)	C48—C70—C84—C39	1.0 (9)
C7—P2—C12—C39	−117.6 (3)	C12—C39—C84—C70	−0.3 (8)
C96^{i}—P2—C12—C39	132.6 (3)	C64—C38—C85—C66	1.9 (7)

Ag1—P2—C12—C39	5.6 (4)	C98—C38—C85—C66	−178.7 (5)
C7—P2—C12—C33	59.6 (4)	C22—C66—C85—C38	1.2 (8)
C96^{i}—P2—C12—C33	−50.1 (4)	C60—C61—C87—C9	0.8 (11)
Ag1—P2—C12—C33	−177.2 (3)	C31—C9—C87—C61	0.3 (9)
C6—P4—C13—C17	−142.1 (3)	P3—C9—C87—C61	175.7 (5)
C97—P4—C13—C17	−32.5 (4)	C68—C56—C88—C51	−0.3 (9)
Ag2—P4—C13—C17	93.8 (3)	C14—C51—C88—C56	−1.1 (8)
C6—P4—C13—C40	45.0 (4)	C101—C81—C90—C78	−0.1 (10)
C97—P4—C13—C40	154.5 (3)	C99—C81—C90—C78	−178.5 (6)
Ag2—P4—C13—C40	−79.1 (3)	C21—C78—C90—C81	0.4 (9)
C2—P1—C14—C41	−132.8 (3)	C14—P1—C96—P2^{i}	−72.4 (2)
C96—P1—C14—C41	117.8 (3)	C2—P1—C96—P2^{i}	179.37 (17)
Ag1—P1—C14—C41	−3.6 (4)	Ag1—P1—C96—P2^{i}	55.44 (19)
C2—P1—C14—C51	47.6 (4)	C6—P4—C97—P3^{ii}	−89.6 (2)
C96—P1—C14—C51	−61.8 (4)	C13—P4—C97—P3^{ii}	160.60 (17)
Ag1—P1—C14—C51	176.8 (3)	Ag2—P4—C97—P3^{ii}	38.8 (2)
C30—C8—C15—C55	0.1 (6)	C90—C81—C101—C43	−0.4 (10)
P3—C8—C15—C55	179.7 (3)	C99—C81—C101—C43	178.2 (7)
C40—C13—C17—C50	−0.5 (6)	C21—C43—C101—C81	0.5 (11)

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