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## Structure Reports

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## (2-Amino-5-chlorobenzenesulfonato)bis-(triphenylphosphine)silver(I)

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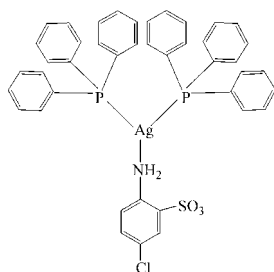
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 Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.013$  Å;  $R$  factor = 0.063;  $wR$  factor = 0.139; data-to-parameter ratio = 17.2.

The asymmetric unit of the title mononuclear compound,  $[\text{Ag}(\text{C}_6\text{H}_5\text{ClNO}_3\text{S})(\text{C}_{18}\text{H}_{15}\text{P})_2]$ , contains four independent molecules. In each of the molecules, the  $\text{Ag}^{\text{I}}$  cation is three-coordinated by two triphenylphosphine ligands, and one N atom from a 2-amino-5-chlorobenzenesulfonate anion. The molecules are linked into a one-dimensional supramolecular structure by  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds.

### Related literature

 For a related structure, see: Dong *et al.* (2007).


### Experimental

#### Crystal data

 $[\text{Ag}(\text{C}_6\text{H}_5\text{ClNO}_3\text{S})(\text{C}_{18}\text{H}_{15}\text{P})_2]$ 
 $M_r = 839.03$ 

 Triclinic,  $P\bar{1}$ 
 $a = 15.403$  (5) Å

 $b = 23.1750$  (19) Å

 $c = 23.3300$  (16) Å

 $\alpha = 100.771$  (4)°

 $\beta = 104.852$  (6)°

 $\gamma = 97.035$  (4)°

 $V = 7780$  (3) Å<sup>3</sup>
 $Z = 8$ 

 Mo  $K\alpha$  radiation

 $\mu = 0.76$  mm<sup>-1</sup>
 $T = 293$  (2) K

 $0.32 \times 0.28 \times 0.23$  mm

#### Data collection

Rigaku R-AXIS RAPID diffractometer

Absorption correction: multi-scan (ABSCOR; Higashi, 1995)

 $T_{\text{min}} = 0.788$ ,  $T_{\text{max}} = 0.841$ 

35542 measured reflections

31947 independent reflections

 19413 reflections with  $I > 2\sigma(I)$ 
 $R_{\text{int}} = 0.007$ 

#### Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.063$ 
 $wR(F^2) = 0.138$ 
 $S = 0.78$ 

31947 reflections

1861 parameters

9 restraints

H atoms treated by a mixture of independent and constrained refinement

 $\Delta\rho_{\text{max}} = 0.70$  e Å<sup>-3</sup>
 $\Delta\rho_{\text{min}} = -0.63$  e Å<sup>-3</sup>

Table 1

Selected geometric parameters (Å, °).

Ag1—N1	2.337 (6)	Ag3—N3	2.346 (5)
Ag1—P2	2.446 (2)	Ag3—P6	2.453 (2)
Ag1—P1	2.452 (2)	Ag3—P5	2.4592 (19)
Ag2—N2	2.356 (6)	Ag4—N4	2.327 (6)
Ag2—P4	2.4268 (19)	Ag4—P8	2.433 (2)
Ag2—P3	2.4288 (19)	Ag4—P7	2.4390 (19)
N1—Ag1—P2	117.59 (17)	N3—Ag3—P6	117.72 (15)
N1—Ag1—P1	121.19 (17)	N3—Ag3—P5	119.52 (15)
P2—Ag1—P1	120.18 (6)	P6—Ag3—P5	122.68 (6)
N2—Ag2—P4	112.43 (15)	N4—Ag4—P8	117.92 (16)
N2—Ag2—P3	117.99 (15)	N4—Ag4—P7	118.76 (16)
P4—Ag2—P3	129.55 (6)	P8—Ag4—P7	123.29 (6)

Table 2

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
N1—H1B $\cdots$ O2	0.82 (5)	2.21 (9)	2.879 (7)	139 (11)
N1—H1A $\cdots$ O9 <sup>i</sup>	0.90 (5)	2.08 (5)	2.976 (8)	174 (10)
N2—H2B $\cdots$ O4	0.82 (4)	2.21 (7)	2.870 (7)	139 (10)
N2—H2A $\cdots$ O11 <sup>ii</sup>	0.89 (4)	2.56 (8)	3.235 (8)	134 (9)
N2—H2A $\cdots$ O12 <sup>ii</sup>	0.89 (4)	2.05 (5)	2.916 (8)	164 (10)
N3—H3A $\cdots$ O5	0.88 (5)	2.12 (5)	2.991 (7)	175 (11)
N3—H3B $\cdots$ O7	0.86 (5)	2.18 (8)	2.900 (7)	141 (10)
N4—H4A $\cdots$ O1 <sup>iii</sup>	0.81 (5)	2.51 (9)	3.148 (8)	136 (10)
N4—H4A $\cdots$ O3 <sup>iii</sup>	0.81 (5)	2.26 (6)	3.027 (8)	159 (11)
N4—H4B $\cdots$ O10	0.85 (5)	2.13 (8)	2.877 (8)	146 (11)

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

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL-Plus* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2554).

### References

- Dong, X.-W., Wu, F.-Y. & Li, Y.-J. (2007). *Acta Cryst.* **E63**, m2885.  
 Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.  
 Rigaku (1998). *PROCESS-AUTO*. Rigaku Corporation, Tokyo, Japan.  
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.

## supporting information

*Acta Cryst.* (2008). E64, m395 [doi:10.1107/S1600536808002031]

**(2-Amino-5-chlorobenzenesulfonato)bis(triphenylphosphine)silver(I)**

Hua Wu, Li-Li Gao and Ying-Ying Liu

**S1. Comment**

The asymmetric unit of the title compound contains four independent molecules (Fig. 1). In each of the molecules, the metal atom is three-coordinated by one 2-amino-5-chlorobenzenesulfonate (*L*) anion and two triphenylphosphine ligands (Table 1). The Ag—P distances are comparable to those observed in a related structure (Dong *et al.*, 2007). Here, the coordination ability of the amino group of *L* is evidently stronger than that of sulfonate group and the latter group does not coordinate to the Ag ion.

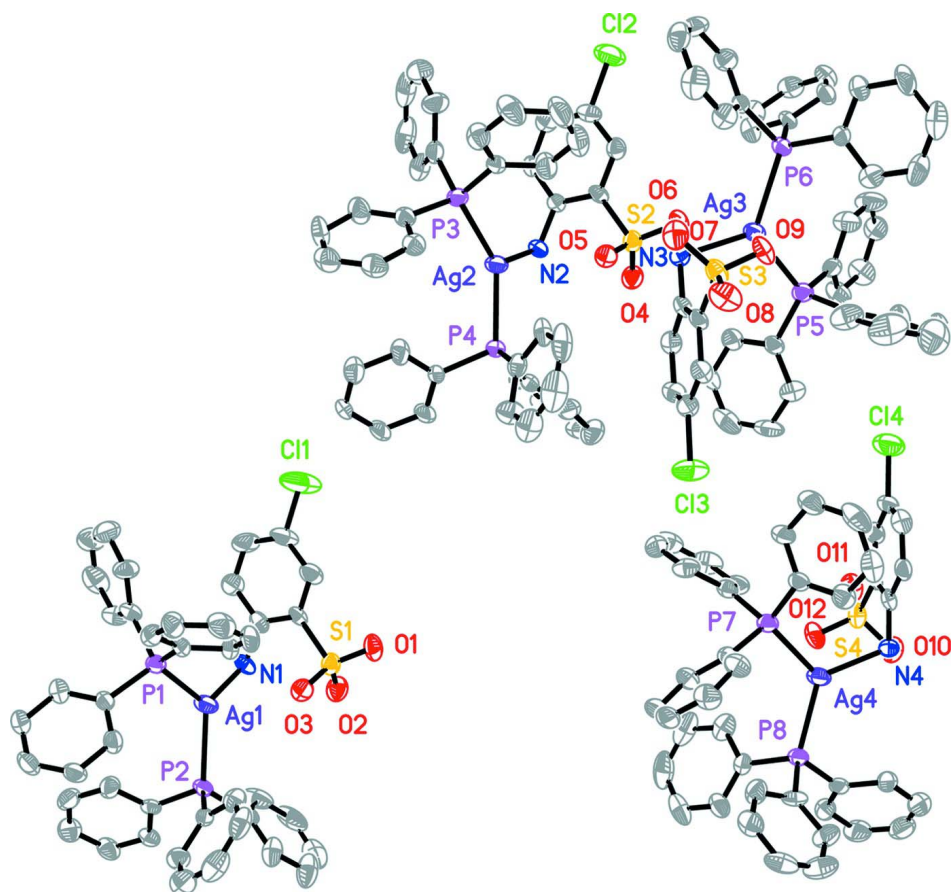
In the crystal structure of the title compound, adjacent molecules are interconnected by strong N—H···O hydrogen bonds (Table 2) to form a one-dimensional supramolecular structure (Fig. 2).

**S2. Experimental**

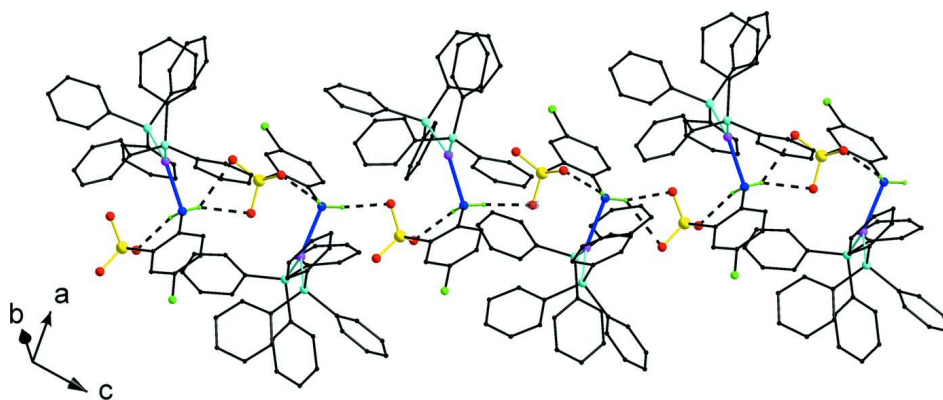
An aqueous solution (10 ml) of 2-amino-5-chlorobenzenesulfonic acid (0.104 g, 0.5 mmol) was added to solid Ag<sub>2</sub>CO<sub>3</sub> (0.069 g, 0.25 mmol) and stirred for several minutes until no further CO<sub>2</sub> was given off; triphenylphosphine (0.226 g, 1.0 mmol) in acetonitrile (10 ml) was then added and a white precipitate formed. The precipitate was dissolved by dropwise addition of an aqueous solution of NH<sub>3</sub> (14 M). Colourless blocks of the title compound were obtained by evaporation of the solution for several days at room temperature.

**S3. Refinement**

The H atoms of the amino group were located in a difference map and refined with a N—H distance restraint of 0.85 Å, and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$ . The bond distance restraint was also used in the refinement of hn2a and hn2b. C-bound H-atoms were geometrically positioned (C—H = 0.93 Å) and refined using a riding model, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

**Figure 1**

The asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 30% probability level. All C-atom labels have been omitted for clarity.

**Figure 2**

One-dimensional supramolecular structure of the title compound, formed through hydrogen-bonding (dashed lines) interactions. The H atoms not involved in hydrogen bonding interactions have been omitted.

## (2-Amino-5-chlorobenzenesulfonato)bis(triphenylphosphine)silver(I)

## Crystal data

[Ag(C<sub>6</sub>H<sub>5</sub>ClNO<sub>2</sub>S)(C<sub>18</sub>H<sub>15</sub>P)<sub>2</sub>] $M_r = 839.03$ Triclinic,  $P\bar{1}$ 

Hall symbol: -P 1

 $a = 15.403$  (5) Å $b = 23.1750$  (19) Å $c = 23.3300$  (16) Å $\alpha = 100.771$  (4)° $\beta = 104.852$  (6)° $\gamma = 97.035$  (4)° $V = 7780$  (3) Å<sup>3</sup> $Z = 8$  $F(000) = 3424$  $D_x = 1.433$  Mg m<sup>-3</sup>Mo  $K\alpha$  radiation,  $\lambda = 0.71069$  Å

Cell parameters from 9413 reflections

 $\theta = 1.4$ – $27.5$ ° $\mu = 0.76$  mm<sup>-1</sup> $T = 293$  K

Block, colourless

 $0.32 \times 0.28 \times 0.23$  mm

## Data collection

Rigaku R-AXIS RAPID

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

 $\omega$  scan

Absorption correction: multi-scan

(ABSCOR; Higashi, 1995)

 $T_{\min} = 0.788$ ,  $T_{\max} = 0.841$ 

35542 measured reflections

31947 independent reflections

19413 reflections with  $I > 2\sigma(I)$  $R_{\text{int}} = 0.007$  $\theta_{\max} = 27.5$ °,  $\theta_{\min} = 1.4$ ° $h = -19 \rightarrow 19$  $k = -29 \rightarrow 29$  $l = -30 \rightarrow 28$ 

## Refinement

Refinement on  $F^2$ 

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.063$  $wR(F^2) = 0.138$  $S = 0.78$ 

31947 reflections

1861 parameters

9 restraints

Primary atom site location: structure-invariant

direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

 $w = 1/[\sigma^2(F_o^2) + (0.0406P)^2]$ where  $P = (F_o^2 + 2F_c^2)/3$  $(\Delta/\sigma)_{\max} = 0.009$  $\Delta\rho_{\max} = 0.70$  e Å<sup>-3</sup> $\Delta\rho_{\min} = -0.63$  e Å<sup>-3</sup>

## 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 ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Ag1	0.02749 (4)	0.17954 (3)	0.88118 (3)	0.0747 (2)
Ag2	0.53367 (4)	0.16690 (2)	0.38665 (3)	0.0652 (2)
Ag3	0.47835 (4)	0.32170 (2)	0.13062 (3)	0.06427 (19)

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Ag4	0.01434 (4)	0.66717 (2)	0.37251 (3)	0.0707 (2)
C1	0.1074 (5)	0.0409 (3)	0.8513 (4)	0.057 (2)
C2	0.1397 (6)	0.0032 (3)	0.8129 (4)	0.077 (2)
H2	0.1072	-0.0080	0.7718	0.093*
C3	0.2188 (6)	-0.0193 (4)	0.8322 (5)	0.096 (3)
H3	0.2406	-0.0441	0.8050	0.115*
C4	0.2642 (7)	-0.0030 (5)	0.8945 (6)	0.103 (3)
H4	0.3160	-0.0187	0.9092	0.123*
C5	0.2352 (6)	0.0350 (5)	0.9341 (5)	0.101 (3)
H5	0.2675	0.0461	0.9752	0.121*
C6	0.1575 (6)	0.0568 (3)	0.9127 (4)	0.077 (2)
H6	0.1375	0.0830	0.9398	0.092*
C7	-0.0341 (5)	0.0544 (3)	0.7496 (3)	0.0550 (19)
C8	-0.0726 (5)	-0.0046 (3)	0.7181 (4)	0.071 (2)
H8	-0.0740	-0.0348	0.7393	0.086*
C9	-0.1085 (5)	-0.0178 (4)	0.6553 (4)	0.079 (2)
H9	-0.1341	-0.0571	0.6349	0.095*
C10	-0.1074 (6)	0.0238 (5)	0.6237 (4)	0.099 (3)
H10	-0.1298	0.0136	0.5814	0.118*
C11	-0.0731 (6)	0.0816 (5)	0.6535 (5)	0.088 (3)
H11	-0.0750	0.1112	0.6314	0.106*
C12	-0.0355 (5)	0.0972 (3)	0.7158 (4)	0.065 (2)
H12	-0.0109	0.1369	0.7351	0.078*
C13	-0.0804 (5)	0.0280 (3)	0.8532 (3)	0.0519 (19)
C14	-0.0598 (5)	-0.0123 (3)	0.8893 (3)	0.069 (2)
H14	0.0000	-0.0183	0.9024	0.083*
C15	-0.1294 (6)	-0.0444 (3)	0.9063 (4)	0.079 (3)
H15	-0.1157	-0.0728	0.9291	0.095*
C16	-0.2153 (6)	-0.0342 (4)	0.8898 (4)	0.083 (3)
H16	-0.2602	-0.0532	0.9035	0.100*
C17	-0.2367 (5)	0.0049 (3)	0.8520 (4)	0.072 (2)
H17	-0.2969	0.0100	0.8383	0.087*
C18	-0.1694 (5)	0.0365 (3)	0.8344 (3)	0.065 (2)
H18	-0.1843	0.0633	0.8099	0.078*
C19	-0.2013 (5)	0.1922 (3)	0.8681 (4)	0.0519 (19)
C20	-0.2105 (6)	0.1907 (3)	0.8080 (4)	0.071 (2)
H20	-0.1587	0.2005	0.7959	0.086*
C21	-0.2926 (9)	0.1754 (4)	0.7658 (5)	0.098 (3)
H21	-0.2965	0.1746	0.7253	0.117*
C22	-0.3709 (8)	0.1608 (4)	0.7821 (6)	0.103 (4)
H22	-0.4276	0.1522	0.7530	0.124*
C23	-0.3648 (6)	0.1592 (4)	0.8405 (5)	0.092 (3)
H23	-0.4170	0.1468	0.8513	0.111*
C24	-0.2808 (5)	0.1758 (3)	0.8845 (4)	0.070 (2)
H24	-0.2772	0.1760	0.9250	0.085*
C25	-0.0853 (6)	0.2976 (3)	0.9422 (4)	0.065 (2)
C26	-0.1587 (7)	0.3250 (4)	0.9206 (4)	0.086 (3)
H26	-0.2136	0.3013	0.8961	0.103*

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C27	-0.1522 (9)	0.3869 (4)	0.9347 (5)	0.120 (4)
H27	-0.2007	0.4046	0.9178	0.144*
C28	-0.0728 (10)	0.4211 (5)	0.9738 (6)	0.129 (5)
H28	-0.0688	0.4621	0.9862	0.155*
C29	0.0001 (8)	0.3955 (5)	0.9946 (6)	0.134 (5)
H29	0.0547	0.4198	1.0189	0.161*
C30	-0.0046 (6)	0.3331 (4)	0.9802 (5)	0.111 (4)
H30	0.0454	0.3161	0.9959	0.133*
C31	-0.0988 (4)	0.1921 (3)	0.9889 (3)	0.0488 (18)
C32	-0.1052 (5)	0.2275 (3)	1.0407 (3)	0.063 (2)
H32	-0.1076	0.2677	1.0423	0.075*
C33	-0.1081 (5)	0.2044 (4)	1.0913 (4)	0.079 (2)
H33	-0.1115	0.2288	1.1269	0.095*
C34	-0.1059 (6)	0.1454 (4)	1.0877 (4)	0.086 (3)
H34	-0.1096	0.1297	1.1211	0.103*
C35	-0.0987 (5)	0.1088 (4)	1.0379 (4)	0.081 (3)
H35	-0.0963	0.0687	1.0370	0.097*
C36	-0.0950 (5)	0.1320 (3)	0.9881 (4)	0.076 (2)
H36	-0.0899	0.1072	0.9533	0.091*
C37	0.2453 (5)	0.2269 (4)	0.7688 (4)	0.078 (3)
H37	0.2341	0.2404	0.7329	0.093*
C38	0.1997 (4)	0.2441 (3)	0.8106 (3)	0.0457 (18)
C39	0.2173 (5)	0.2261 (3)	0.8651 (4)	0.059 (2)
C40	0.2816 (5)	0.1885 (4)	0.8761 (4)	0.073 (2)
H40	0.2936	0.1750	0.9120	0.088*
C41	0.3267 (5)	0.1717 (4)	0.8337 (5)	0.092 (3)
H41	0.3705	0.1477	0.8417	0.110*
C42	0.3080 (6)	0.1895 (4)	0.7800 (4)	0.086 (3)
C43	0.4745 (5)	0.0098 (3)	0.3501 (3)	0.0536 (19)
C44	0.3819 (5)	0.0043 (3)	0.3189 (3)	0.063 (2)
H44	0.3641	0.0272	0.2906	0.075*
C45	0.3173 (5)	-0.0354 (4)	0.3305 (4)	0.077 (3)
H45	0.2559	-0.0390	0.3099	0.092*
C46	0.3429 (6)	-0.0691 (4)	0.3717 (4)	0.083 (3)
H46	0.2993	-0.0955	0.3796	0.100*
C47	0.4332 (7)	-0.0636 (4)	0.4013 (4)	0.096 (3)
H47	0.4507	-0.0864	0.4297	0.115*
C48	0.4995 (5)	-0.0247 (4)	0.3899 (4)	0.082 (3)
H48	0.5609	-0.0224	0.4097	0.098*
C49	0.6656 (5)	0.0505 (3)	0.3669 (4)	0.060 (2)
C50	0.7128 (7)	0.0741 (3)	0.4264 (5)	0.083 (3)
H50	0.6855	0.0965	0.4518	0.099*
C51	0.8018 (9)	0.0650 (4)	0.4496 (5)	0.107 (4)
H51	0.8338	0.0814	0.4902	0.128*
C52	0.8409 (8)	0.0322 (6)	0.4124 (7)	0.123 (6)
H52	0.9000	0.0260	0.4279	0.148*
C53	0.7967 (7)	0.0085 (5)	0.3542 (6)	0.105 (4)
H53	0.8248	-0.0142	0.3295	0.126*

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C54	0.7083 (6)	0.0177 (4)	0.3300 (4)	0.085 (3)
H54	0.6779	0.0017	0.2891	0.101*
C55	0.5330 (4)	0.0572 (3)	0.2574 (3)	0.0483 (18)
C56	0.5048 (5)	0.0006 (3)	0.2176 (4)	0.078 (2)
H56	0.4946	-0.0333	0.2326	0.093*
C57	0.4923 (6)	-0.0044 (4)	0.1566 (5)	0.107 (3)
H57	0.4738	-0.0418	0.1302	0.128*
C58	0.5065 (7)	0.0443 (5)	0.1345 (5)	0.115 (4)
H58	0.4993	0.0399	0.0930	0.138*
C59	0.5309 (8)	0.0990 (5)	0.1710 (5)	0.118 (4)
H59	0.5384	0.1323	0.1546	0.142*
C60	0.5446 (5)	0.1059 (3)	0.2317 (4)	0.080 (3)
H60	0.5622	0.1441	0.2567	0.096*
C61	0.3678 (4)	0.1595 (3)	0.4684 (3)	0.0481 (18)
C62	0.3515 (6)	0.1870 (3)	0.5202 (4)	0.093 (3)
H62	0.3580	0.2284	0.5297	0.112*
C63	0.3256 (6)	0.1553 (4)	0.5590 (4)	0.111 (4)
H63	0.3150	0.1754	0.5943	0.133*
C64	0.3153 (5)	0.0945 (4)	0.5465 (4)	0.077 (3)
H64	0.2982	0.0730	0.5730	0.092*
C65	0.3304 (6)	0.0664 (4)	0.4951 (4)	0.082 (3)
H65	0.3227	0.0249	0.4856	0.098*
C66	0.3573 (5)	0.0982 (3)	0.4558 (3)	0.073 (2)
H66	0.3683	0.0779	0.4207	0.087*
C67	0.2972 (5)	0.1823 (3)	0.3502 (4)	0.057 (2)
C68	0.3015 (6)	0.1682 (3)	0.2914 (4)	0.073 (2)
H68	0.3581	0.1663	0.2847	0.088*
C69	0.2246 (8)	0.1565 (4)	0.2414 (4)	0.101 (4)
H69	0.2285	0.1458	0.2018	0.121*
C70	0.1430 (8)	0.1614 (5)	0.2533 (6)	0.120 (5)
H70	0.0904	0.1543	0.2208	0.144*
C71	0.1360 (7)	0.1764 (4)	0.3112 (6)	0.104 (4)
H71	0.0795	0.1798	0.3175	0.125*
C72	0.2120 (6)	0.1865 (3)	0.3599 (4)	0.081 (3)
H72	0.2072	0.1962	0.3994	0.098*
C73	0.4179 (5)	0.2762 (3)	0.4476 (3)	0.0490 (19)
C74	0.4882 (5)	0.2995 (4)	0.4981 (4)	0.071 (2)
H74	0.5250	0.2745	0.5151	0.085*
C75	0.5071 (6)	0.3608 (4)	0.5257 (4)	0.089 (3)
H75	0.5560	0.3756	0.5606	0.107*
C76	0.4549 (8)	0.3987 (5)	0.5023 (6)	0.110 (4)
H76	0.4655	0.4390	0.5212	0.132*
C77	0.3874 (7)	0.3754 (4)	0.4506 (5)	0.099 (3)
H77	0.3520	0.4009	0.4332	0.119*
C78	0.3678 (5)	0.3157 (4)	0.4220 (4)	0.080 (3)
H78	0.3212	0.3020	0.3857	0.096*
C79	0.7131 (4)	0.2350 (3)	0.3754 (3)	0.0443 (17)
C80	0.7834 (4)	0.2030 (3)	0.3885 (3)	0.0498 (19)

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H80	0.7975	0.1909	0.4251	0.060*
C81	0.8327 (5)	0.1889 (3)	0.3476 (4)	0.068 (2)
H81	0.8804	0.1680	0.3566	0.082*
C82	0.8092 (5)	0.2066 (3)	0.2930 (4)	0.070 (2)
C83	0.7420 (5)	0.2393 (3)	0.2791 (3)	0.059 (2)
H83	0.7295	0.2523	0.2430	0.071*
C84	0.6928 (4)	0.2525 (3)	0.3208 (3)	0.0465 (18)
C85	0.4347 (5)	0.4502 (3)	0.2326 (4)	0.056 (2)
C86	0.3700 (5)	0.4869 (3)	0.2389 (4)	0.076 (2)
H86	0.3383	0.4998	0.2055	0.092*
C87	0.3530 (6)	0.5040 (4)	0.2947 (6)	0.098 (3)
H87	0.3107	0.5288	0.2984	0.118*
C88	0.3976 (7)	0.4848 (4)	0.3438 (5)	0.102 (3)
H88	0.3839	0.4949	0.3806	0.122*
C89	0.4624 (6)	0.4506 (4)	0.3389 (4)	0.077 (3)
H89	0.4951	0.4391	0.3730	0.093*
C90	0.4800 (5)	0.4329 (3)	0.2834 (4)	0.072 (2)
H90	0.5234	0.4088	0.2806	0.086*
C91	0.3815 (5)	0.4462 (3)	0.1036 (3)	0.058 (2)
C92	0.3918 (6)	0.5015 (4)	0.0889 (4)	0.096 (3)
H92	0.4419	0.5307	0.1116	0.115*
C93	0.3294 (8)	0.5133 (5)	0.0415 (5)	0.136 (5)
H93	0.3354	0.5513	0.0337	0.163*
C94	0.2585 (9)	0.4702 (7)	0.0053 (6)	0.146 (5)
H94	0.2186	0.4774	-0.0288	0.175*
C95	0.2475 (7)	0.4175 (6)	0.0199 (6)	0.135 (5)
H95	0.1976	0.3886	-0.0038	0.162*
C96	0.3072 (6)	0.4041 (4)	0.0688 (5)	0.097 (3)
H96	0.2970	0.3670	0.0780	0.116*
C97	0.5682 (5)	0.4789 (3)	0.1731 (4)	0.056 (2)
C98	0.6214 (6)	0.4649 (3)	0.1363 (4)	0.093 (3)
H98	0.6051	0.4284	0.1082	0.111*
C99	0.7002 (6)	0.5039 (4)	0.1395 (5)	0.121 (4)
H99	0.7337	0.4949	0.1121	0.145*
C100	0.7270 (5)	0.5557 (4)	0.1840 (5)	0.085 (3)
H100	0.7816	0.5807	0.1886	0.102*
C101	0.6762 (6)	0.5708 (4)	0.2208 (4)	0.087 (3)
H101	0.6934	0.6072	0.2492	0.105*
C102	0.5950 (5)	0.5309 (4)	0.2163 (4)	0.078 (2)
H102	0.5605	0.5405	0.2430	0.093*
C103	0.5231 (4)	0.3070 (3)	-0.0165 (3)	0.0504 (19)
C104	0.5561 (5)	0.2855 (3)	-0.0643 (4)	0.073 (2)
H104	0.6008	0.2618	-0.0585	0.088*
C105	0.5250 (7)	0.2979 (4)	-0.1197 (4)	0.092 (3)
H105	0.5464	0.2812	-0.1517	0.110*
C106	0.4623 (8)	0.3348 (5)	-0.1289 (5)	0.119 (4)
H106	0.4439	0.3454	-0.1661	0.142*
C107	0.4267 (7)	0.3562 (4)	-0.0818 (5)	0.100 (3)



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H107	0.3814	0.3794	-0.0880	0.121*
C108	0.4583 (5)	0.3432 (4)	-0.0262 (4)	0.082 (3)
H108	0.4359	0.3590	0.0056	0.099*
C109	0.6809 (4)	0.3247 (3)	0.0879 (3)	0.0485 (18)
C110	0.7216 (5)	0.3252 (3)	0.1491 (4)	0.069 (2)
H110	0.6878	0.3075	0.1711	0.082*
C111	0.8111 (6)	0.3515 (3)	0.1767 (4)	0.085 (3)
H111	0.8381	0.3508	0.2170	0.101*
C112	0.8611 (5)	0.3790 (3)	0.1451 (5)	0.073 (3)
H112	0.9211	0.3982	0.1643	0.088*
C113	0.8225 (6)	0.3780 (3)	0.0866 (4)	0.070 (2)
H113	0.8575	0.3942	0.0644	0.085*
C114	0.7326 (5)	0.3534 (3)	0.0587 (3)	0.062 (2)
H114	0.7062	0.3563	0.0190	0.074*
C115	0.5647 (4)	0.2099 (3)	0.0372 (3)	0.0425 (17)
C116	0.4843 (5)	0.1713 (4)	0.0175 (4)	0.070 (2)
H116	0.4302	0.1853	0.0170	0.084*
C117	0.4827 (6)	0.1114 (4)	-0.0018 (4)	0.096 (3)
H117	0.4267	0.0855	-0.0176	0.115*
C118	0.5629 (7)	0.0883 (4)	0.0017 (4)	0.083 (3)
H118	0.5613	0.0475	-0.0102	0.099*
C119	0.6426 (6)	0.1271 (4)	0.0228 (4)	0.085 (3)
H119	0.6973	0.1131	0.0258	0.102*
C120	0.6435 (5)	0.1880 (3)	0.0403 (4)	0.068 (2)
H120	0.6991	0.2142	0.0545	0.082*
C121	0.3203 (5)	0.2645 (3)	0.1752 (3)	0.0460 (18)
C122	0.2394 (5)	0.2484 (3)	0.1295 (3)	0.0488 (19)
C123	0.1588 (5)	0.2661 (3)	0.1403 (4)	0.062 (2)
H123	0.1037	0.2559	0.1096	0.074*
C124	0.1641 (5)	0.2985 (3)	0.1970 (4)	0.060 (2)
C125	0.2437 (5)	0.3161 (3)	0.2410 (4)	0.067 (2)
H125	0.2462	0.3399	0.2783	0.081*
C126	0.3230 (5)	0.2984 (3)	0.2306 (4)	0.058 (2)
H126	0.3778	0.3098	0.2615	0.070*
C127	-0.0569 (5)	0.5129 (3)	0.3545 (4)	0.0530 (19)
C128	-0.0611 (5)	0.5072 (3)	0.4121 (4)	0.069 (2)
H128	-0.0127	0.5268	0.4459	0.083*
C129	-0.1353 (6)	0.4730 (4)	0.4208 (4)	0.080 (3)
H129	-0.1372	0.4690	0.4594	0.095*
C130	-0.2070 (6)	0.4450 (3)	0.3691 (5)	0.079 (3)
H130	-0.2575	0.4220	0.3737	0.095*
C131	-0.2057 (5)	0.4502 (3)	0.3125 (4)	0.082 (3)
H131	-0.2546	0.4313	0.2788	0.098*
C132	-0.1293 (5)	0.4844 (3)	0.3058 (4)	0.074 (2)
H132	-0.1278	0.4879	0.2670	0.088*
C133	0.1367 (4)	0.5479 (3)	0.4003 (3)	0.0531 (19)
C134	0.1461 (5)	0.4905 (3)	0.4067 (4)	0.071 (2)
H134	0.1027	0.4581	0.3815	0.085*

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C135	0.2193 (6)	0.4814 (4)	0.4501 (4)	0.083 (3)
H135	0.2228	0.4431	0.4561	0.100*
C136	0.2869 (6)	0.5282 (5)	0.4844 (4)	0.099 (3)
H136	0.3388	0.5213	0.5111	0.119*
C137	0.2781 (6)	0.5846 (5)	0.4792 (4)	0.090 (3)
H137	0.3218	0.6166	0.5046	0.108*
C138	0.2043 (6)	0.5949 (3)	0.4364 (4)	0.074 (3)
H138	0.2004	0.6336	0.4319	0.089*
C139	0.0435 (5)	0.5382 (3)	0.2722 (4)	0.055 (2)
C140	0.0980 (5)	0.4981 (3)	0.2568 (4)	0.070 (2)
H140	0.1323	0.4818	0.2866	0.084*
C141	0.1017 (6)	0.4820 (4)	0.1968 (5)	0.088 (3)
H141	0.1378	0.4546	0.1867	0.106*
C142	0.0521 (7)	0.5066 (5)	0.1528 (5)	0.102 (3)
H142	0.0554	0.4964	0.1130	0.123*
C143	-0.0030 (6)	0.5466 (4)	0.1679 (5)	0.094 (3)
H143	-0.0380	0.5626	0.1380	0.113*
C144	-0.0054 (5)	0.5624 (4)	0.2268 (4)	0.074 (2)
H144	-0.0409	0.5902	0.2368	0.089*
C145	-0.0777 (4)	0.7807 (3)	0.4531 (4)	0.054 (2)
C146	-0.0865 (4)	0.8085 (3)	0.4039 (4)	0.070 (2)
H146	-0.0905	0.7865	0.3654	0.084*
C147	-0.0891 (6)	0.8697 (4)	0.4132 (5)	0.098 (3)
H147	-0.0967	0.8890	0.3812	0.117*
C148	-0.0803 (7)	0.8994 (5)	0.4703 (6)	0.102 (4)
H148	-0.0852	0.9395	0.4755	0.123*
C149	-0.0652 (6)	0.8772 (4)	0.5209 (5)	0.091 (3)
H149	-0.0558	0.9011	0.5595	0.109*
C150	-0.0645 (5)	0.8150 (3)	0.5109 (4)	0.065 (2)
H150	-0.0551	0.7970	0.5439	0.078*
C151	-0.0506 (5)	0.6838 (3)	0.5120 (3)	0.0534 (19)
C152	0.0366 (6)	0.6745 (3)	0.5367 (5)	0.080 (3)
H152	0.0772	0.6755	0.5134	0.096*
C153	0.0661 (7)	0.6641 (4)	0.5923 (6)	0.111 (4)
H153	0.1250	0.6569	0.6068	0.133*
C154	0.0070 (10)	0.6646 (4)	0.6274 (6)	0.124 (5)
H154	0.0266	0.6579	0.6664	0.149*
C155	-0.0812 (8)	0.6747 (4)	0.6062 (5)	0.107 (4)
H155	-0.1206	0.6754	0.6305	0.129*
C156	-0.1087 (6)	0.6836 (3)	0.5480 (4)	0.076 (2)
H156	-0.1680	0.6896	0.5327	0.091*
C157	-0.2003 (5)	0.6687 (3)	0.4065 (3)	0.059 (2)
C158	-0.2660 (5)	0.7011 (3)	0.3885 (4)	0.080 (3)
H158	-0.2505	0.7418	0.3913	0.096*
C159	-0.3569 (6)	0.6723 (4)	0.3656 (4)	0.098 (3)
H159	-0.4014	0.6939	0.3509	0.118*
C160	-0.3827 (6)	0.6135 (5)	0.3642 (4)	0.091 (3)
H160	-0.4441	0.5959	0.3521	0.109*

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C161	-0.3165 (6)	0.5816 (4)	0.3808 (4)	0.085 (3)
H161	-0.3324	0.5407	0.3767	0.102*
C162	-0.2251 (5)	0.6085 (3)	0.4039 (4)	0.077 (3)
H162	-0.1809	0.5863	0.4176	0.093*
C163	0.1680 (5)	0.7233 (3)	0.3206 (4)	0.053 (2)
C164	0.1622 (5)	0.6884 (3)	0.2635 (4)	0.063 (2)
H164	0.1058	0.6769	0.2341	0.076*
C165	0.2375 (7)	0.6708 (4)	0.2499 (4)	0.080 (3)
H165	0.2316	0.6459	0.2124	0.096*
C166	0.3209 (6)	0.6898 (4)	0.2911 (5)	0.077 (3)
C167	0.3300 (5)	0.7249 (4)	0.3467 (4)	0.069 (2)
H167	0.3876	0.7378	0.3745	0.083*
C168	0.2540 (5)	0.7415 (3)	0.3622 (3)	0.0494 (19)
N1	0.1697 (4)	0.2419 (3)	0.9078 (3)	0.0549 (16)
H1A	0.201 (7)	0.243 (5)	0.946 (3)	0.082*
H1B	0.157 (8)	0.275 (3)	0.908 (6)	0.082*
N2	0.6592 (4)	0.2460 (2)	0.4159 (3)	0.0513 (15)
H2A	0.687 (7)	0.245 (5)	0.454 (3)	0.077*
H2B	0.646 (7)	0.279 (3)	0.417 (5)	0.077*
N3	0.4027 (4)	0.2477 (2)	0.1658 (3)	0.0453 (15)
H3A	0.440 (6)	0.246 (5)	0.201 (3)	0.068*
H3B	0.391 (8)	0.214 (3)	0.139 (4)	0.068*
N4	0.0885 (4)	0.7379 (3)	0.3341 (3)	0.0533 (16)
H4A	0.046 (6)	0.741 (5)	0.307 (4)	0.080*
H4B	0.104 (8)	0.770 (3)	0.362 (4)	0.080*
O1	0.1189 (3)	0.3065 (2)	0.7386 (2)	0.0778 (16)
O2	0.1320 (3)	0.3368 (2)	0.8465 (3)	0.0813 (16)
O3	0.0289 (3)	0.24717 (19)	0.7861 (2)	0.0671 (15)
O4	0.6098 (3)	0.3387 (2)	0.3545 (2)	0.0715 (15)
O5	0.5195 (3)	0.24505 (19)	0.2890 (2)	0.0632 (14)
O6	0.6054 (3)	0.3125 (2)	0.2474 (2)	0.0769 (16)
O7	0.2778 (3)	0.1565 (2)	0.0668 (2)	0.0804 (16)
O8	0.1395 (3)	0.1901 (2)	0.0223 (2)	0.0889 (17)
O9	0.2870 (3)	0.2482 (2)	0.0327 (2)	0.0749 (16)
O10	0.2153 (4)	0.8336 (2)	0.4249 (2)	0.0819 (16)
O11	0.3597 (4)	0.8041 (2)	0.4666 (3)	0.0975 (19)
O12	0.2174 (3)	0.7445 (2)	0.4635 (2)	0.0782 (16)
P1	0.00610 (13)	0.07371 (8)	0.83137 (10)	0.0566 (5)
P2	-0.09104 (13)	0.21763 (8)	0.92183 (10)	0.0544 (5)
P3	0.55376 (12)	0.06892 (8)	0.33884 (9)	0.0522 (5)
P4	0.40134 (12)	0.19756 (8)	0.41339 (9)	0.0485 (5)
P5	0.46462 (13)	0.42654 (8)	0.16345 (10)	0.0564 (6)
P6	0.56177 (12)	0.28953 (8)	0.05733 (9)	0.0489 (5)
P7	0.03721 (13)	0.56412 (8)	0.34845 (10)	0.0542 (5)
P8	-0.07843 (12)	0.70087 (8)	0.43783 (10)	0.0527 (5)
S1	0.11387 (13)	0.28755 (9)	0.79372 (10)	0.0601 (6)
S2	0.59964 (12)	0.29081 (8)	0.30089 (10)	0.0551 (5)
S3	0.23400 (13)	0.20682 (9)	0.05674 (9)	0.0606 (5)

S4	0.26396 (15)	0.78513 (9)	0.43523 (10)	0.0682 (6)
Cl1	0.3668 (2)	0.16776 (18)	0.72775 (15)	0.1756 (15)
Cl2	0.87604 (17)	0.19052 (13)	0.24361 (12)	0.1175 (9)
Cl3	0.06543 (16)	0.32049 (12)	0.21181 (13)	0.1191 (9)
Cl4	0.41655 (18)	0.66937 (15)	0.27116 (14)	0.1425 (12)

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Ag1	0.0669 (4)	0.0550 (4)	0.1089 (6)	0.0008 (3)	0.0547 (4)	0.0007 (4)
Ag2	0.0653 (4)	0.0488 (4)	0.0931 (5)	0.0092 (3)	0.0488 (4)	0.0085 (3)
Ag3	0.0726 (4)	0.0519 (4)	0.0870 (5)	0.0137 (3)	0.0519 (4)	0.0193 (3)
Ag4	0.0757 (4)	0.0517 (4)	0.1023 (6)	0.0150 (3)	0.0573 (4)	0.0137 (4)
C1	0.042 (5)	0.071 (5)	0.056 (6)	0.003 (4)	0.022 (4)	0.007 (4)
C2	0.089 (7)	0.090 (6)	0.061 (6)	0.037 (5)	0.035 (5)	0.007 (5)
C3	0.086 (7)	0.088 (7)	0.123 (10)	0.037 (6)	0.039 (7)	0.019 (7)
C4	0.076 (7)	0.132 (9)	0.104 (10)	0.036 (6)	0.022 (8)	0.032 (8)
C5	0.062 (7)	0.140 (10)	0.088 (9)	-0.008 (6)	0.008 (6)	0.033 (8)
C6	0.058 (6)	0.091 (6)	0.079 (8)	0.012 (5)	0.026 (5)	0.003 (5)
C7	0.069 (5)	0.052 (5)	0.058 (6)	0.017 (4)	0.035 (4)	0.020 (4)
C8	0.085 (6)	0.069 (6)	0.072 (7)	0.030 (5)	0.032 (5)	0.023 (5)
C9	0.100 (7)	0.085 (6)	0.059 (7)	0.022 (5)	0.027 (6)	0.024 (5)
C10	0.107 (8)	0.136 (9)	0.066 (8)	0.035 (7)	0.038 (6)	0.030 (7)
C11	0.103 (7)	0.111 (8)	0.082 (8)	0.039 (6)	0.040 (6)	0.068 (7)
C12	0.080 (6)	0.048 (5)	0.087 (7)	0.019 (4)	0.045 (5)	0.030 (5)
C13	0.062 (5)	0.041 (4)	0.054 (5)	0.003 (3)	0.027 (4)	0.003 (4)
C14	0.074 (6)	0.068 (6)	0.066 (6)	0.004 (4)	0.019 (5)	0.024 (5)
C15	0.097 (7)	0.075 (6)	0.087 (7)	0.018 (5)	0.046 (6)	0.038 (5)
C16	0.088 (7)	0.083 (7)	0.096 (8)	0.002 (5)	0.057 (6)	0.026 (6)
C17	0.055 (5)	0.071 (6)	0.098 (7)	0.008 (4)	0.039 (5)	0.014 (5)
C18	0.064 (5)	0.056 (5)	0.074 (6)	0.001 (4)	0.018 (5)	0.023 (4)
C19	0.071 (5)	0.047 (4)	0.052 (6)	0.021 (4)	0.034 (5)	0.016 (4)
C20	0.086 (7)	0.054 (5)	0.069 (7)	0.015 (4)	0.018 (6)	0.005 (5)
C21	0.165 (11)	0.056 (6)	0.070 (8)	0.034 (7)	0.023 (9)	0.014 (5)
C22	0.103 (9)	0.078 (7)	0.096 (10)	0.020 (6)	-0.023 (8)	0.008 (7)
C23	0.066 (7)	0.080 (7)	0.119 (10)	0.002 (5)	0.015 (7)	0.018 (7)
C24	0.060 (6)	0.074 (6)	0.075 (7)	0.012 (4)	0.016 (5)	0.015 (5)
C25	0.070 (6)	0.067 (5)	0.058 (6)	0.000 (5)	0.039 (5)	-0.003 (4)
C26	0.140 (9)	0.054 (6)	0.057 (6)	0.010 (5)	0.022 (6)	0.007 (4)
C27	0.223 (14)	0.064 (8)	0.080 (9)	0.034 (7)	0.052 (9)	0.020 (6)
C28	0.221 (17)	0.071 (8)	0.122 (12)	0.016 (9)	0.115 (12)	0.004 (7)
C29	0.139 (11)	0.066 (8)	0.198 (14)	-0.043 (6)	0.122 (11)	-0.028 (8)
C30	0.092 (7)	0.074 (7)	0.160 (10)	-0.020 (5)	0.082 (7)	-0.032 (6)
C31	0.032 (4)	0.054 (5)	0.058 (6)	0.005 (3)	0.016 (4)	0.004 (4)
C32	0.065 (5)	0.072 (5)	0.056 (6)	0.012 (4)	0.032 (5)	0.009 (5)
C33	0.098 (7)	0.076 (6)	0.068 (7)	0.006 (5)	0.046 (5)	0.002 (5)
C34	0.095 (7)	0.105 (8)	0.065 (7)	0.025 (6)	0.025 (6)	0.027 (6)
C35	0.095 (7)	0.075 (6)	0.086 (8)	0.040 (5)	0.030 (6)	0.025 (6)

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C36	0.101 (7)	0.074 (6)	0.070 (7)	0.035 (5)	0.038 (5)	0.027 (5)
C37	0.051 (5)	0.117 (7)	0.074 (7)	0.016 (5)	0.023 (5)	0.037 (6)
C38	0.033 (4)	0.072 (5)	0.028 (5)	-0.002 (3)	0.005 (4)	0.014 (4)
C39	0.048 (5)	0.059 (5)	0.065 (6)	-0.015 (4)	0.018 (5)	0.013 (4)
C40	0.058 (6)	0.100 (7)	0.064 (7)	0.022 (5)	0.010 (5)	0.028 (5)
C41	0.051 (6)	0.138 (8)	0.093 (9)	0.047 (5)	0.014 (6)	0.032 (7)
C42	0.053 (6)	0.150 (9)	0.065 (7)	0.032 (5)	0.028 (5)	0.024 (6)
C43	0.054 (5)	0.050 (5)	0.055 (5)	0.005 (3)	0.021 (4)	0.005 (4)
C44	0.064 (5)	0.062 (5)	0.060 (6)	0.007 (4)	0.019 (5)	0.009 (4)
C45	0.053 (5)	0.085 (7)	0.089 (8)	0.001 (5)	0.024 (5)	0.012 (5)
C46	0.076 (7)	0.068 (6)	0.104 (9)	-0.012 (5)	0.040 (6)	0.008 (5)
C47	0.110 (8)	0.088 (7)	0.104 (8)	-0.003 (6)	0.038 (7)	0.059 (6)
C48	0.059 (5)	0.090 (6)	0.103 (8)	0.001 (4)	0.026 (5)	0.043 (6)
C49	0.059 (5)	0.054 (5)	0.074 (7)	0.010 (4)	0.020 (5)	0.030 (5)
C50	0.084 (7)	0.062 (6)	0.100 (9)	0.007 (5)	0.017 (6)	0.031 (6)
C51	0.118 (11)	0.060 (7)	0.108 (10)	-0.017 (6)	-0.022 (8)	0.033 (7)
C52	0.064 (8)	0.111 (11)	0.197 (18)	-0.001 (7)	0.002 (9)	0.102 (12)
C53	0.063 (7)	0.143 (10)	0.143 (12)	0.053 (7)	0.045 (7)	0.072 (9)
C54	0.065 (6)	0.097 (7)	0.099 (8)	0.034 (5)	0.028 (6)	0.023 (6)
C55	0.051 (4)	0.050 (5)	0.047 (5)	0.011 (3)	0.020 (4)	0.009 (4)
C56	0.095 (6)	0.056 (6)	0.075 (7)	-0.003 (4)	0.024 (6)	0.010 (5)
C57	0.142 (9)	0.098 (8)	0.074 (8)	-0.011 (6)	0.047 (7)	0.003 (6)
C58	0.173 (11)	0.113 (9)	0.078 (9)	0.013 (8)	0.065 (8)	0.035 (8)
C59	0.178 (11)	0.106 (9)	0.101 (10)	0.034 (8)	0.065 (9)	0.055 (8)
C60	0.109 (7)	0.063 (6)	0.072 (7)	0.005 (5)	0.034 (6)	0.020 (5)
C61	0.054 (4)	0.056 (5)	0.047 (5)	0.020 (3)	0.021 (4)	0.025 (4)
C62	0.151 (8)	0.058 (6)	0.115 (8)	0.036 (5)	0.104 (7)	0.026 (5)
C63	0.196 (10)	0.081 (7)	0.128 (9)	0.061 (7)	0.136 (9)	0.046 (6)
C64	0.094 (6)	0.084 (7)	0.094 (8)	0.034 (5)	0.067 (6)	0.053 (6)
C65	0.104 (7)	0.062 (6)	0.080 (7)	0.006 (5)	0.028 (6)	0.025 (5)
C66	0.127 (7)	0.057 (5)	0.037 (5)	0.017 (5)	0.027 (5)	0.012 (4)
C67	0.065 (6)	0.041 (4)	0.061 (6)	0.002 (3)	0.013 (5)	0.012 (4)
C68	0.101 (7)	0.059 (5)	0.062 (7)	0.002 (4)	0.021 (6)	0.028 (5)
C69	0.149 (10)	0.082 (7)	0.040 (7)	-0.012 (7)	-0.021 (8)	0.025 (5)
C70	0.115 (10)	0.093 (8)	0.096 (11)	-0.027 (7)	-0.048 (9)	0.026 (8)
C71	0.069 (7)	0.098 (8)	0.128 (11)	-0.002 (5)	-0.003 (8)	0.040 (8)
C72	0.058 (6)	0.105 (7)	0.072 (7)	0.014 (5)	0.011 (6)	0.010 (5)
C73	0.042 (4)	0.054 (5)	0.058 (6)	0.007 (4)	0.024 (4)	0.018 (4)
C74	0.070 (6)	0.067 (6)	0.087 (7)	0.019 (4)	0.036 (5)	0.024 (5)
C75	0.079 (7)	0.082 (7)	0.093 (8)	-0.008 (5)	0.039 (6)	-0.018 (6)
C76	0.117 (10)	0.072 (8)	0.167 (13)	0.018 (7)	0.097 (9)	0.006 (8)
C77	0.111 (9)	0.054 (7)	0.146 (11)	0.020 (6)	0.054 (8)	0.031 (7)
C78	0.078 (6)	0.063 (6)	0.114 (8)	0.021 (5)	0.048 (6)	0.024 (6)
C79	0.026 (4)	0.061 (4)	0.044 (5)	0.005 (3)	0.005 (4)	0.016 (4)
C80	0.050 (5)	0.053 (4)	0.050 (5)	0.006 (3)	0.012 (4)	0.025 (4)
C81	0.051 (5)	0.068 (5)	0.084 (7)	0.008 (4)	0.016 (5)	0.020 (5)
C82	0.074 (6)	0.076 (6)	0.064 (7)	0.018 (5)	0.035 (5)	0.000 (5)
C83	0.055 (5)	0.064 (5)	0.058 (6)	0.009 (4)	0.012 (4)	0.022 (4)

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C84	0.030 (4)	0.069 (5)	0.039 (5)	0.003 (3)	0.011 (4)	0.012 (4)
C85	0.051 (5)	0.052 (5)	0.074 (6)	0.005 (4)	0.035 (5)	0.018 (4)
C86	0.071 (6)	0.076 (6)	0.083 (7)	0.024 (5)	0.025 (5)	0.010 (5)
C87	0.088 (7)	0.095 (7)	0.132 (10)	0.025 (5)	0.078 (8)	0.005 (7)
C88	0.110 (9)	0.103 (8)	0.098 (10)	-0.016 (6)	0.062 (8)	0.012 (7)
C89	0.086 (7)	0.096 (7)	0.054 (6)	-0.004 (5)	0.030 (5)	0.025 (5)
C90	0.078 (6)	0.065 (5)	0.083 (7)	0.013 (4)	0.037 (6)	0.023 (5)
C91	0.045 (5)	0.061 (5)	0.065 (6)	0.002 (4)	0.013 (4)	0.012 (4)
C92	0.073 (6)	0.110 (8)	0.092 (8)	-0.008 (5)	-0.005 (6)	0.049 (6)
C93	0.119 (10)	0.156 (11)	0.106 (10)	-0.021 (8)	-0.023 (8)	0.071 (9)
C94	0.122 (12)	0.210 (17)	0.104 (11)	0.047 (12)	0.007 (9)	0.057 (12)
C95	0.060 (8)	0.164 (13)	0.143 (13)	0.016 (8)	-0.010 (8)	0.001 (10)
C96	0.060 (6)	0.084 (7)	0.131 (10)	0.006 (5)	0.019 (6)	0.001 (6)
C97	0.054 (5)	0.049 (5)	0.073 (6)	0.015 (4)	0.026 (4)	0.022 (4)
C98	0.104 (7)	0.039 (5)	0.155 (10)	0.001 (4)	0.085 (7)	0.011 (5)
C99	0.120 (8)	0.072 (7)	0.212 (13)	0.020 (6)	0.122 (9)	0.029 (8)
C100	0.057 (6)	0.082 (7)	0.130 (10)	0.005 (5)	0.039 (6)	0.044 (7)
C101	0.079 (7)	0.083 (6)	0.081 (7)	-0.014 (5)	0.016 (6)	0.000 (5)
C102	0.077 (6)	0.079 (6)	0.074 (7)	-0.009 (5)	0.035 (5)	0.005 (5)
C103	0.047 (5)	0.054 (5)	0.061 (6)	0.015 (3)	0.022 (4)	0.026 (4)
C104	0.090 (6)	0.092 (6)	0.046 (6)	0.029 (5)	0.019 (5)	0.029 (5)
C105	0.137 (9)	0.104 (7)	0.038 (6)	0.017 (6)	0.024 (6)	0.027 (5)
C106	0.137 (10)	0.116 (9)	0.102 (11)	0.014 (7)	0.008 (8)	0.065 (8)
C107	0.115 (9)	0.097 (7)	0.091 (9)	0.039 (6)	0.006 (7)	0.046 (7)
C108	0.084 (6)	0.089 (6)	0.085 (8)	0.034 (5)	0.030 (6)	0.026 (6)
C109	0.047 (4)	0.062 (5)	0.047 (5)	0.013 (3)	0.026 (4)	0.020 (4)
C110	0.076 (6)	0.071 (6)	0.063 (6)	0.003 (4)	0.024 (5)	0.024 (5)
C111	0.083 (7)	0.077 (6)	0.084 (7)	0.007 (5)	0.015 (6)	0.012 (5)
C112	0.043 (5)	0.066 (6)	0.106 (8)	-0.001 (4)	0.027 (5)	0.009 (5)
C113	0.069 (6)	0.081 (6)	0.068 (7)	0.005 (5)	0.033 (5)	0.023 (5)
C114	0.062 (5)	0.076 (5)	0.059 (6)	0.012 (4)	0.029 (5)	0.030 (4)
C115	0.040 (4)	0.052 (4)	0.039 (5)	0.008 (3)	0.013 (4)	0.017 (3)
C116	0.053 (5)	0.070 (6)	0.080 (7)	0.004 (4)	0.009 (5)	0.016 (5)
C117	0.084 (7)	0.074 (7)	0.106 (8)	-0.021 (5)	0.006 (6)	0.017 (6)
C118	0.102 (7)	0.056 (6)	0.087 (8)	0.005 (5)	0.022 (6)	0.023 (5)
C119	0.100 (7)	0.056 (6)	0.115 (8)	0.031 (5)	0.057 (6)	0.010 (5)
C120	0.055 (5)	0.064 (5)	0.093 (7)	0.009 (4)	0.031 (5)	0.021 (5)
C121	0.046 (5)	0.054 (5)	0.035 (5)	-0.004 (3)	0.011 (4)	0.011 (4)
C122	0.038 (4)	0.060 (5)	0.054 (5)	0.000 (3)	0.022 (4)	0.022 (4)
C123	0.040 (5)	0.090 (6)	0.056 (6)	0.008 (4)	0.008 (4)	0.030 (5)
C124	0.042 (5)	0.080 (6)	0.060 (6)	0.014 (4)	0.010 (5)	0.026 (5)
C125	0.068 (6)	0.065 (5)	0.073 (7)	0.007 (4)	0.034 (5)	0.009 (4)
C126	0.043 (5)	0.066 (5)	0.062 (6)	0.001 (4)	0.008 (4)	0.020 (4)
C127	0.050 (5)	0.053 (5)	0.058 (6)	0.008 (4)	0.020 (4)	0.012 (4)
C128	0.059 (5)	0.075 (6)	0.081 (7)	0.004 (4)	0.031 (5)	0.023 (5)
C129	0.071 (6)	0.082 (6)	0.104 (8)	0.014 (5)	0.052 (6)	0.029 (6)
C130	0.064 (6)	0.068 (6)	0.126 (9)	0.007 (4)	0.052 (7)	0.037 (6)
C131	0.063 (6)	0.075 (6)	0.098 (8)	-0.006 (4)	0.022 (6)	0.010 (5)

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C132	0.065 (6)	0.080 (6)	0.072 (7)	0.000 (5)	0.025 (5)	0.009 (5)
C133	0.056 (5)	0.039 (4)	0.066 (6)	0.000 (4)	0.031 (4)	0.004 (4)
C134	0.049 (5)	0.068 (6)	0.089 (7)	0.007 (4)	0.022 (5)	-0.005 (5)
C135	0.065 (6)	0.098 (7)	0.106 (8)	0.032 (6)	0.034 (6)	0.048 (6)
C136	0.061 (7)	0.153 (10)	0.086 (8)	0.023 (7)	0.029 (6)	0.021 (8)
C137	0.049 (6)	0.113 (8)	0.076 (8)	-0.007 (5)	0.004 (5)	-0.021 (6)
C138	0.065 (6)	0.057 (5)	0.110 (8)	0.004 (4)	0.049 (6)	0.014 (5)
C139	0.049 (5)	0.053 (5)	0.067 (6)	0.004 (3)	0.027 (4)	0.013 (4)
C140	0.076 (6)	0.086 (6)	0.061 (6)	0.027 (5)	0.037 (5)	0.015 (5)
C141	0.105 (8)	0.092 (7)	0.075 (8)	0.017 (5)	0.044 (7)	0.009 (6)
C142	0.132 (10)	0.103 (8)	0.064 (8)	-0.017 (7)	0.051 (7)	-0.007 (6)
C143	0.103 (8)	0.094 (8)	0.081 (9)	-0.003 (6)	0.014 (7)	0.037 (6)
C144	0.074 (6)	0.089 (6)	0.054 (6)	0.012 (5)	0.013 (5)	0.015 (5)
C145	0.039 (4)	0.055 (5)	0.077 (6)	0.009 (3)	0.027 (4)	0.022 (5)
C146	0.071 (5)	0.054 (5)	0.101 (7)	0.016 (4)	0.041 (5)	0.031 (5)
C147	0.085 (7)	0.099 (9)	0.134 (11)	0.029 (6)	0.047 (8)	0.056 (7)
C148	0.088 (7)	0.079 (8)	0.158 (13)	0.031 (6)	0.049 (9)	0.037 (8)
C149	0.100 (7)	0.076 (7)	0.096 (9)	0.024 (5)	0.044 (7)	-0.005 (6)
C150	0.078 (6)	0.046 (5)	0.073 (7)	0.010 (4)	0.026 (5)	0.010 (4)
C151	0.051 (5)	0.050 (4)	0.055 (6)	0.004 (3)	0.006 (4)	0.018 (4)
C152	0.069 (7)	0.054 (5)	0.096 (8)	-0.005 (4)	-0.003 (6)	0.013 (5)
C153	0.084 (8)	0.066 (6)	0.140 (13)	-0.007 (5)	-0.037 (8)	0.033 (7)
C154	0.143 (12)	0.076 (7)	0.125 (12)	-0.027 (8)	-0.010 (10)	0.050 (7)
C155	0.143 (10)	0.094 (7)	0.088 (9)	-0.023 (7)	0.050 (8)	0.030 (6)
C156	0.098 (7)	0.078 (6)	0.059 (7)	0.011 (5)	0.035 (6)	0.020 (5)
C157	0.048 (5)	0.070 (5)	0.056 (6)	0.018 (4)	0.023 (4)	-0.008 (4)
C158	0.063 (6)	0.057 (5)	0.113 (8)	0.014 (4)	0.017 (6)	0.009 (5)
C159	0.058 (6)	0.094 (7)	0.113 (9)	0.016 (5)	0.005 (6)	-0.021 (6)
C160	0.053 (6)	0.116 (8)	0.087 (8)	-0.010 (6)	0.031 (6)	-0.019 (6)
C161	0.063 (6)	0.079 (6)	0.107 (8)	-0.013 (5)	0.025 (6)	0.025 (6)
C162	0.060 (6)	0.070 (6)	0.100 (7)	0.006 (4)	0.011 (5)	0.036 (5)
C163	0.063 (6)	0.060 (5)	0.038 (5)	0.006 (4)	0.017 (5)	0.021 (4)
C164	0.054 (5)	0.070 (5)	0.077 (7)	0.005 (4)	0.021 (5)	0.042 (5)
C165	0.089 (7)	0.086 (6)	0.076 (7)	0.018 (5)	0.032 (6)	0.034 (5)
C166	0.061 (6)	0.122 (8)	0.077 (8)	0.040 (5)	0.039 (6)	0.048 (6)
C167	0.051 (5)	0.105 (7)	0.062 (7)	0.016 (5)	0.016 (5)	0.041 (6)
C168	0.052 (5)	0.069 (5)	0.031 (5)	0.009 (4)	0.010 (4)	0.023 (4)
N1	0.048 (4)	0.085 (4)	0.029 (4)	0.000 (3)	0.014 (3)	0.012 (3)
N2	0.051 (4)	0.058 (4)	0.051 (4)	0.009 (3)	0.025 (3)	0.013 (3)
N3	0.033 (3)	0.054 (4)	0.047 (4)	0.007 (3)	0.008 (3)	0.013 (3)
N4	0.041 (4)	0.062 (4)	0.062 (5)	0.013 (3)	0.019 (3)	0.018 (3)
O1	0.077 (4)	0.093 (4)	0.067 (4)	0.007 (3)	0.011 (3)	0.046 (3)
O2	0.101 (4)	0.055 (3)	0.085 (5)	0.011 (3)	0.026 (4)	0.013 (3)
O3	0.047 (3)	0.062 (3)	0.084 (4)	0.002 (2)	0.008 (3)	0.016 (3)
O4	0.086 (4)	0.058 (3)	0.071 (4)	0.014 (3)	0.022 (3)	0.015 (3)
O5	0.038 (3)	0.069 (3)	0.082 (4)	0.004 (2)	0.014 (3)	0.024 (3)
O6	0.060 (3)	0.125 (5)	0.058 (4)	0.025 (3)	0.011 (3)	0.055 (4)
O7	0.101 (4)	0.061 (4)	0.067 (4)	0.001 (3)	0.015 (3)	0.006 (3)

O8	0.049 (3)	0.132 (5)	0.065 (4)	-0.003 (3)	0.000 (3)	0.007 (4)
O9	0.076 (4)	0.098 (4)	0.060 (4)	0.000 (3)	0.028 (3)	0.036 (3)
O10	0.103 (4)	0.067 (4)	0.070 (4)	0.020 (3)	0.015 (3)	0.015 (3)
O11	0.078 (4)	0.115 (5)	0.080 (5)	-0.003 (3)	-0.010 (4)	0.034 (4)
O12	0.113 (4)	0.075 (4)	0.047 (4)	0.004 (3)	0.029 (3)	0.016 (3)
P1	0.0596 (13)	0.0475 (12)	0.0681 (16)	0.0085 (9)	0.0321 (12)	0.0079 (10)
P2	0.0540 (12)	0.0494 (12)	0.0648 (15)	0.0042 (9)	0.0336 (11)	0.0058 (10)
P3	0.0484 (12)	0.0475 (12)	0.0643 (15)	0.0092 (9)	0.0249 (11)	0.0090 (10)
P4	0.0478 (12)	0.0505 (12)	0.0540 (14)	0.0135 (9)	0.0228 (10)	0.0137 (10)
P5	0.0526 (13)	0.0482 (12)	0.0751 (17)	0.0102 (9)	0.0292 (12)	0.0148 (11)
P6	0.0486 (12)	0.0564 (12)	0.0481 (14)	0.0113 (9)	0.0215 (10)	0.0156 (10)
P7	0.0567 (13)	0.0432 (12)	0.0682 (16)	0.0082 (9)	0.0318 (12)	0.0075 (10)
P8	0.0498 (12)	0.0509 (12)	0.0625 (15)	0.0109 (9)	0.0268 (11)	0.0090 (10)
S1	0.0531 (12)	0.0568 (13)	0.0667 (16)	0.0024 (9)	0.0087 (11)	0.0217 (11)
S2	0.0484 (12)	0.0628 (13)	0.0566 (15)	0.0100 (9)	0.0107 (10)	0.0256 (11)
S3	0.0528 (13)	0.0792 (15)	0.0437 (14)	-0.0044 (10)	0.0095 (11)	0.0159 (11)
S4	0.0786 (16)	0.0677 (14)	0.0566 (16)	0.0080 (11)	0.0101 (13)	0.0265 (12)
Cl1	0.138 (3)	0.292 (4)	0.132 (3)	0.098 (3)	0.083 (2)	0.034 (3)
Cl2	0.115 (2)	0.164 (2)	0.102 (2)	0.0525 (18)	0.0689 (18)	0.0308 (19)
Cl3	0.0755 (16)	0.152 (2)	0.142 (3)	0.0472 (15)	0.0512 (17)	0.0188 (19)
Cl4	0.107 (2)	0.232 (3)	0.134 (3)	0.084 (2)	0.070 (2)	0.069 (3)

*Geometric parameters (Å, °)*

Ag1—N1	2.337 (6)	C86—H86	0.93
Ag1—P2	2.446 (2)	C87—C88	1.359 (11)
Ag1—P1	2.452 (2)	C87—H87	0.93
Ag2—N2	2.356 (6)	C88—C89	1.361 (11)
Ag2—P4	2.4268 (19)	C88—H88	0.93
Ag2—P3	2.4288 (19)	C89—C90	1.390 (10)
Ag3—N3	2.346 (5)	C89—H89	0.93
Ag3—P6	2.453 (2)	C90—H90	0.93
Ag3—P5	2.4592 (19)	C91—C96	1.370 (10)
Ag4—N4	2.327 (6)	C91—C92	1.387 (9)
Ag4—P8	2.433 (2)	C91—P5	1.807 (7)
Ag4—P7	2.4390 (19)	C92—C93	1.362 (11)
C1—C2	1.363 (9)	C92—H92	0.93
C1—C6	1.396 (10)	C93—C94	1.359 (14)
C1—P1	1.811 (7)	C93—H93	0.93
C2—C3	1.386 (10)	C94—C95	1.331 (13)
C2—H2	0.93	C94—H94	0.93
C3—C4	1.398 (12)	C95—C96	1.381 (13)
C3—H3	0.93	C95—H95	0.93
C4—C5	1.354 (12)	C96—H96	0.93
C4—H4	0.93	C97—C98	1.356 (9)
C5—C6	1.369 (10)	C97—C102	1.360 (10)
C5—H5	0.93	C97—P5	1.819 (7)
C6—H6	0.93	C98—C99	1.398 (10)



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C7—C12	1.378 (8)	C98—H98	0.93
C7—C8	1.402 (9)	C99—C100	1.373 (12)
C7—P1	1.797 (7)	C99—H99	0.93
C8—C9	1.386 (10)	C100—C101	1.331 (10)
C8—H8	0.93	C100—H100	0.93
C9—C10	1.322 (10)	C101—C102	1.430 (9)
C9—H9	0.93	C101—H101	0.93
C10—C11	1.359 (11)	C102—H102	0.93
C10—H10	0.93	C103—C104	1.377 (9)
C11—C12	1.378 (11)	C103—C108	1.383 (9)
C11—H11	0.93	C103—P6	1.810 (7)
C12—H12	0.93	C104—C105	1.356 (9)
C13—C18	1.379 (8)	C104—H104	0.93
C13—C14	1.384 (8)	C105—C106	1.369 (11)
C13—P1	1.832 (6)	C105—H105	0.93
C14—C15	1.412 (9)	C106—C107	1.389 (12)
C14—H14	0.93	C106—H106	0.93
C15—C16	1.343 (9)	C107—C108	1.367 (11)
C15—H15	0.93	C107—H107	0.93
C16—C17	1.391 (9)	C108—H108	0.93
C16—H16	0.93	C109—C114	1.365 (8)
C17—C18	1.387 (8)	C109—C110	1.401 (9)
C17—H17	0.93	C109—P6	1.812 (7)
C18—H18	0.93	C110—C111	1.370 (10)
C19—C20	1.365 (10)	C110—H110	0.93
C19—C24	1.405 (9)	C111—C112	1.374 (10)
C19—P2	1.786 (8)	C111—H111	0.93
C20—C21	1.348 (11)	C112—C113	1.337 (10)
C20—H20	0.93	C112—H112	0.93
C21—C22	1.375 (12)	C113—C114	1.368 (9)
C21—H21	0.93	C113—H113	0.93
C22—C23	1.351 (12)	C114—H114	0.93
C22—H22	0.93	C115—C116	1.353 (8)
C23—C24	1.387 (10)	C115—C120	1.363 (8)
C23—H23	0.93	C115—P6	1.826 (6)
C24—H24	0.93	C116—C117	1.371 (10)
C25—C30	1.385 (11)	C116—H116	0.93
C25—C26	1.392 (10)	C117—C118	1.394 (10)
C25—P2	1.810 (8)	C117—H117	0.93
C26—C27	1.397 (11)	C118—C119	1.346 (10)
C26—H26	0.93	C118—H118	0.93
C27—C28	1.370 (14)	C119—C120	1.390 (9)
C27—H27	0.93	C119—H119	0.93
C28—C29	1.355 (14)	C120—H120	0.93
C28—H28	0.93	C121—C126	1.369 (9)
C29—C30	1.412 (11)	C121—C122	1.373 (9)
C29—H29	0.93	C121—N3	1.428 (8)
C30—H30	0.93	C122—C123	1.421 (8)

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C31—C32	1.361 (9)	C122—S3	1.764 (7)
C31—C36	1.399 (9)	C123—C124	1.371 (10)
C31—P2	1.800 (7)	C123—H123	0.93
C32—C33	1.394 (9)	C124—C125	1.342 (9)
C32—H32	0.93	C124—C13	1.756 (7)
C33—C34	1.360 (10)	C125—C126	1.397 (9)
C33—H33	0.93	C125—H125	0.93
C34—C35	1.342 (10)	C126—H126	0.93
C34—H34	0.93	C127—C132	1.364 (9)
C35—C36	1.380 (9)	C127—C128	1.393 (9)
C35—H35	0.93	C127—P7	1.810 (7)
C36—H36	0.93	C128—C129	1.390 (9)
C37—C38	1.370 (9)	C128—H128	0.93
C37—C42	1.384 (10)	C129—C130	1.393 (11)
C37—H37	0.93	C129—H129	0.93
C38—C39	1.385 (9)	C130—C131	1.352 (10)
C38—S1	1.767 (7)	C130—H130	0.93
C39—N1	1.402 (9)	C131—C132	1.397 (9)
C39—C40	1.404 (9)	C131—H131	0.93
C40—C41	1.374 (10)	C132—H132	0.93
C40—H40	0.93	C133—C138	1.382 (9)
C41—C42	1.365 (10)	C133—C134	1.386 (9)
C41—H41	0.93	C133—P7	1.820 (7)
C42—C11	1.733 (8)	C134—C135	1.378 (10)
C43—C48	1.350 (9)	C134—H134	0.93
C43—C44	1.403 (9)	C135—C136	1.369 (11)
C43—P3	1.823 (7)	C135—H135	0.93
C44—C45	1.385 (9)	C136—C137	1.355 (11)
C44—H44	0.93	C136—H136	0.93
C45—C46	1.363 (10)	C137—C138	1.386 (10)
C45—H45	0.93	C137—H137	0.93
C46—C47	1.363 (10)	C138—H138	0.93
C46—H46	0.93	C139—C140	1.383 (9)
C47—C48	1.390 (9)	C139—C144	1.385 (9)
C47—H47	0.93	C139—P7	1.800 (8)
C48—H48	0.93	C140—C141	1.397 (10)
C49—C50	1.363 (11)	C140—H140	0.93
C49—C54	1.386 (10)	C141—C142	1.373 (11)
C49—P3	1.812 (7)	C141—H141	0.93
C50—C51	1.395 (12)	C142—C143	1.389 (11)
C50—H50	0.93	C142—H142	0.93
C51—C52	1.354 (14)	C143—C144	1.367 (11)
C51—H51	0.93	C143—H143	0.93
C52—C53	1.328 (14)	C144—H144	0.93
C52—H52	0.93	C145—C150	1.382 (10)
C53—C54	1.392 (10)	C145—C146	1.404 (9)
C53—H53	0.93	C145—P8	1.815 (7)
C54—H54	0.93	C146—C147	1.401 (10)

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C55—C60	1.386 (9)	C146—H146	0.93
C55—C56	1.405 (9)	C147—C148	1.344 (13)
C55—P3	1.806 (7)	C147—H147	0.93
C56—C57	1.366 (10)	C148—C149	1.352 (12)
C56—H56	0.93	C148—H148	0.93
C57—C58	1.343 (11)	C149—C150	1.419 (10)
C57—H57	0.93	C149—H149	0.93
C58—C59	1.338 (12)	C150—H150	0.93
C58—H58	0.93	C151—C156	1.376 (9)
C59—C60	1.353 (11)	C151—C152	1.380 (9)
C59—H59	0.93	C151—P8	1.802 (7)
C60—H60	0.93	C152—C153	1.337 (12)
C61—C62	1.354 (9)	C152—H152	0.93
C61—C66	1.377 (8)	C153—C154	1.372 (14)
C61—P4	1.829 (6)	C153—H153	0.93
C62—C63	1.371 (9)	C154—C155	1.387 (13)
C62—H62	0.93	C154—H154	0.93
C63—C64	1.364 (10)	C155—C156	1.377 (11)
C63—H63	0.93	C155—H155	0.93
C64—C65	1.344 (10)	C156—H156	0.93
C64—H64	0.93	C157—C158	1.360 (9)
C65—C66	1.388 (9)	C157—C162	1.385 (9)
C65—H65	0.93	C157—P8	1.835 (7)
C66—H66	0.93	C158—C159	1.395 (10)
C67—C68	1.369 (10)	C158—H158	0.93
C67—C72	1.400 (9)	C159—C160	1.363 (10)
C67—P4	1.823 (8)	C159—H159	0.93
C68—C69	1.390 (10)	C160—C161	1.353 (10)
C68—H68	0.93	C160—H160	0.93
C69—C70	1.368 (13)	C161—C162	1.390 (9)
C69—H69	0.93	C161—H161	0.93
C70—C71	1.366 (14)	C162—H162	0.93
C70—H70	0.93	C163—C168	1.388 (9)
C71—C72	1.367 (11)	C163—C164	1.397 (10)
C71—H71	0.93	C163—N4	1.405 (9)
C72—H72	0.93	C164—C165	1.368 (9)
C73—C74	1.349 (9)	C164—H164	0.93
C73—C78	1.390 (9)	C165—C166	1.356 (11)
C73—P4	1.805 (7)	C165—H165	0.93
C74—C75	1.406 (10)	C166—C167	1.358 (11)
C74—H74	0.93	C166—Cl4	1.747 (8)
C75—C76	1.357 (11)	C167—C168	1.389 (9)
C75—H75	0.93	C167—H167	0.93
C76—C77	1.343 (12)	C168—S4	1.769 (7)
C76—H76	0.93	N1—H1A	0.90 (5)
C77—C78	1.377 (11)	N1—H1B	0.82 (5)
C77—H77	0.93	N2—H2A	0.89 (4)
C78—H78	0.93	N2—H2B	0.82 (4)

C79—C84	1.380 (8)	N3—H3A	0.88 (5)
C79—C80	1.388 (8)	N3—H3B	0.86 (5)
C79—N2	1.419 (8)	N4—H4A	0.81 (5)
C80—C81	1.380 (9)	N4—H4B	0.85 (5)
C80—H80	0.93	O1—S1	1.452 (5)
C81—C82	1.384 (10)	O2—S1	1.455 (5)
C81—H81	0.93	O3—S1	1.462 (4)
C82—C83	1.365 (9)	O4—S2	1.470 (5)
C82—C12	1.752 (8)	O5—S2	1.456 (4)
C83—C84	1.393 (9)	O6—S2	1.448 (4)
C83—H83	0.93	O7—S3	1.444 (5)
C84—S2	1.786 (6)	O8—S3	1.435 (5)
C85—C90	1.367 (9)	O9—S3	1.464 (4)
C85—C86	1.405 (9)	O10—S4	1.448 (5)
C85—P5	1.798 (7)	O11—S4	1.438 (5)
C86—C87	1.387 (11)	O12—S4	1.464 (5)
N1—Ag1—P2	117.59 (17)	C100—C99—C98	118.6 (9)
N1—Ag1—P1	121.19 (17)	C100—C99—H99	120.7
P2—Ag1—P1	120.18 (6)	C98—C99—H99	120.7
N2—Ag2—P4	112.43 (15)	C101—C100—C99	121.1 (8)
N2—Ag2—P3	117.99 (15)	C101—C100—H100	119.5
P4—Ag2—P3	129.55 (6)	C99—C100—H100	119.5
N3—Ag3—P6	117.72 (15)	C100—C101—C102	119.6 (8)
N3—Ag3—P5	119.52 (15)	C100—C101—H101	120.2
P6—Ag3—P5	122.68 (6)	C102—C101—H101	120.2
N4—Ag4—P8	117.92 (16)	C97—C102—C101	120.0 (8)
N4—Ag4—P7	118.76 (16)	C97—C102—H102	120.0
P8—Ag4—P7	123.29 (6)	C101—C102—H102	120.0
C2—C1—C6	117.3 (7)	C104—C103—C108	117.8 (7)
C2—C1—P1	127.0 (7)	C104—C103—P6	122.3 (5)
C6—C1—P1	115.7 (6)	C108—C103—P6	119.9 (6)
C1—C2—C3	123.0 (9)	C105—C104—C103	121.6 (8)
C1—C2—H2	118.5	C105—C104—H104	119.2
C3—C2—H2	118.5	C103—C104—H104	119.2
C2—C3—C4	116.8 (9)	C104—C105—C106	120.6 (9)
C2—C3—H3	121.6	C104—C105—H105	119.7
C4—C3—H3	121.6	C106—C105—H105	119.7
C5—C4—C3	122.1 (10)	C105—C106—C107	118.9 (10)
C5—C4—H4	118.9	C105—C106—H106	120.6
C3—C4—H4	118.9	C107—C106—H106	120.6
C4—C5—C6	118.9 (10)	C108—C107—C106	119.9 (10)
C4—C5—H5	120.6	C108—C107—H107	120.0
C6—C5—H5	120.6	C106—C107—H107	120.0
C5—C6—C1	121.9 (9)	C107—C108—C103	121.1 (9)
C5—C6—H6	119.1	C107—C108—H108	119.4
C1—C6—H6	119.1	C103—C108—H108	119.4
C12—C7—C8	117.3 (7)	C114—C109—C110	117.3 (7)

C12—C7—P1	121.7 (6)	C114—C109—P6	126.7 (6)
C8—C7—P1	120.8 (6)	C110—C109—P6	115.9 (5)
C9—C8—C7	119.8 (7)	C111—C110—C109	120.3 (7)
C9—C8—H8	120.1	C111—C110—H110	119.9
C7—C8—H8	120.1	C109—C110—H110	119.9
C10—C9—C8	121.9 (9)	C110—C111—C112	120.4 (8)
C10—C9—H9	119.1	C110—C111—H111	119.8
C8—C9—H9	119.1	C112—C111—H111	119.8
C9—C10—C11	119.3 (10)	C113—C112—C111	119.3 (8)
C9—C10—H10	120.4	C113—C112—H112	120.4
C11—C10—H10	120.4	C111—C112—H112	120.4
C10—C11—C12	121.3 (8)	C112—C113—C114	121.2 (7)
C10—C11—H11	119.3	C112—C113—H113	119.4
C12—C11—H11	119.3	C114—C113—H113	119.4
C11—C12—C7	120.4 (8)	C109—C114—C113	121.3 (7)
C11—C12—H12	119.8	C109—C114—H114	119.3
C7—C12—H12	119.8	C113—C114—H114	119.3
C18—C13—C14	119.1 (6)	C116—C115—C120	118.9 (7)
C18—C13—P1	117.7 (5)	C116—C115—P6	117.9 (6)
C14—C13—P1	123.2 (6)	C120—C115—P6	123.2 (5)
C13—C14—C15	120.2 (7)	C115—C116—C117	120.0 (7)
C13—C14—H14	119.9	C115—C116—H116	120.0
C15—C14—H14	119.9	C117—C116—H116	120.0
C16—C15—C14	120.3 (7)	C116—C117—C118	121.6 (8)
C16—C15—H15	119.9	C116—C117—H117	119.2
C14—C15—H15	119.9	C118—C117—H117	119.2
C15—C16—C17	119.5 (7)	C119—C118—C117	117.7 (8)
C15—C16—H16	120.2	C119—C118—H118	121.1
C17—C16—H16	120.2	C117—C118—H118	121.1
C18—C17—C16	120.8 (7)	C118—C119—C120	120.4 (8)
C18—C17—H17	119.6	C118—C119—H119	119.8
C16—C17—H17	119.6	C120—C119—H119	119.8
C13—C18—C17	119.9 (7)	C115—C120—C119	121.4 (7)
C13—C18—H18	120.1	C115—C120—H120	119.3
C17—C18—H18	120.1	C119—C120—H120	119.3
C20—C19—C24	117.5 (8)	C126—C121—C122	119.7 (7)
C20—C19—P2	119.0 (6)	C126—C121—N3	119.0 (7)
C24—C19—P2	123.4 (6)	C122—C121—N3	121.3 (7)
C21—C20—C19	121.8 (9)	C121—C122—C123	119.8 (7)
C21—C20—H20	119.1	C121—C122—S3	121.0 (6)
C19—C20—H20	119.1	C123—C122—S3	119.1 (6)
C20—C21—C22	120.8 (10)	C124—C123—C122	118.5 (7)
C20—C21—H21	119.6	C124—C123—H123	120.7
C22—C21—H21	119.6	C122—C123—H123	120.7
C23—C22—C21	119.5 (10)	C125—C124—C123	121.6 (7)
C23—C22—H22	120.2	C125—C124—C13	118.8 (7)
C21—C22—H22	120.2	C123—C124—C13	119.5 (6)
C22—C23—C24	120.1 (10)	C124—C125—C126	119.9 (8)

C22—C23—H23	119.9	C124—C125—H125	120.0
C24—C23—H23	119.9	C126—C125—H125	120.0
C23—C24—C19	120.1 (8)	C121—C126—C125	120.3 (7)
C23—C24—H24	119.9	C121—C126—H126	119.8
C19—C24—H24	119.9	C125—C126—H126	119.8
C30—C25—C26	118.6 (8)	C132—C127—C128	117.9 (7)
C30—C25—P2	118.9 (7)	C132—C127—P7	123.0 (6)
C26—C25—P2	122.5 (6)	C128—C127—P7	118.7 (6)
C25—C26—C27	122.0 (10)	C129—C128—C127	122.0 (8)
C25—C26—H26	119.0	C129—C128—H128	119.0
C27—C26—H26	119.0	C127—C128—H128	119.0
C28—C27—C26	118.5 (12)	C128—C129—C130	117.2 (8)
C28—C27—H27	120.8	C128—C129—H129	121.4
C26—C27—H27	120.8	C130—C129—H129	121.4
C29—C28—C27	120.5 (12)	C131—C130—C129	122.4 (8)
C29—C28—H28	119.7	C131—C130—H130	118.8
C27—C28—H28	119.7	C129—C130—H130	118.8
C28—C29—C30	121.7 (12)	C130—C131—C132	118.7 (8)
C28—C29—H29	119.1	C130—C131—H131	120.7
C30—C29—H29	119.1	C132—C131—H131	120.7
C25—C30—C29	118.6 (10)	C127—C132—C131	121.9 (8)
C25—C30—H30	120.7	C127—C132—H132	119.1
C29—C30—H30	120.7	C131—C132—H132	119.1
C32—C31—C36	118.1 (7)	C138—C133—C134	118.5 (7)
C32—C31—P2	124.6 (6)	C138—C133—P7	118.7 (6)
C36—C31—P2	117.2 (6)	C134—C133—P7	122.7 (6)
C31—C32—C33	120.8 (7)	C135—C134—C133	120.2 (7)
C31—C32—H32	119.6	C135—C134—H134	119.9
C33—C32—H32	119.6	C133—C134—H134	119.9
C34—C33—C32	118.6 (8)	C136—C135—C134	120.5 (8)
C34—C33—H33	120.7	C136—C135—H135	119.8
C32—C33—H33	120.7	C134—C135—H135	119.8
C35—C34—C33	122.8 (9)	C137—C136—C135	119.7 (9)
C35—C34—H34	118.6	C137—C136—H136	120.1
C33—C34—H34	118.6	C135—C136—H136	120.1
C34—C35—C36	118.4 (8)	C136—C137—C138	120.6 (9)
C34—C35—H35	120.8	C136—C137—H137	119.7
C36—C35—H35	120.8	C138—C137—H137	119.7
C35—C36—C31	121.2 (8)	C133—C138—C137	120.2 (7)
C35—C36—H36	119.4	C133—C138—H138	119.9
C31—C36—H36	119.4	C137—C138—H138	119.9
C38—C37—C42	120.0 (8)	C140—C139—C144	118.1 (8)
C38—C37—H37	120.0	C140—C139—P7	124.1 (6)
C42—C37—H37	120.0	C144—C139—P7	117.7 (6)
C37—C38—C39	121.0 (7)	C139—C140—C141	120.5 (8)
C37—C38—S1	119.8 (6)	C139—C140—H140	119.7
C39—C38—S1	119.1 (6)	C141—C140—H140	119.7
C38—C39—N1	122.0 (7)	C142—C141—C140	119.9 (9)

C38—C39—C40	118.4 (8)	C142—C141—H141	120.0
N1—C39—C40	119.6 (7)	C140—C141—H141	120.0
C41—C40—C39	119.8 (8)	C141—C142—C143	119.9 (9)
C41—C40—H40	120.1	C141—C142—H142	120.1
C39—C40—H40	120.1	C143—C142—H142	120.1
C42—C41—C40	121.0 (8)	C144—C143—C142	119.5 (9)
C42—C41—H41	119.5	C144—C143—H143	120.3
C40—C41—H41	119.5	C142—C143—H143	120.3
C41—C42—C37	119.7 (8)	C143—C144—C139	122.0 (9)
C41—C42—Cl1	119.7 (8)	C143—C144—H144	119.0
C37—C42—Cl1	120.5 (8)	C139—C144—H144	119.0
C48—C43—C44	119.5 (6)	C150—C145—C146	119.3 (7)
C48—C43—P3	123.4 (6)	C150—C145—P8	123.0 (6)
C44—C43—P3	116.8 (6)	C146—C145—P8	117.6 (6)
C45—C44—C43	119.6 (7)	C147—C146—C145	119.6 (9)
C45—C44—H44	120.2	C147—C146—H146	120.2
C43—C44—H44	120.2	C145—C146—H146	120.2
C46—C45—C44	120.6 (8)	C148—C147—C146	117.3 (10)
C46—C45—H45	119.7	C148—C147—H147	121.4
C44—C45—H45	119.7	C146—C147—H147	121.4
C45—C46—C47	119.2 (8)	C147—C148—C149	127.1 (10)
C45—C46—H46	120.4	C147—C148—H148	116.5
C47—C46—H46	120.4	C149—C148—H148	116.5
C46—C47—C48	121.4 (8)	C148—C149—C150	115.2 (9)
C46—C47—H47	119.3	C148—C149—H149	122.4
C48—C47—H47	119.3	C150—C149—H149	122.4
C43—C48—C47	119.8 (8)	C145—C150—C149	121.3 (8)
C43—C48—H48	120.1	C145—C150—H150	119.4
C47—C48—H48	120.1	C149—C150—H150	119.4
C50—C49—C54	118.4 (8)	C156—C151—C152	116.9 (8)
C50—C49—P3	118.0 (7)	C156—C151—P8	124.3 (6)
C54—C49—P3	123.4 (7)	C152—C151—P8	118.6 (7)
C49—C50—C51	120.7 (10)	C153—C152—C151	123.9 (10)
C49—C50—H50	119.6	C153—C152—H152	118.0
C51—C50—H50	119.6	C151—C152—H152	118.0
C52—C51—C50	119.2 (12)	C152—C153—C154	117.9 (11)
C52—C51—H51	120.4	C152—C153—H153	121.0
C50—C51—H51	120.4	C154—C153—H153	121.0
C53—C52—C51	121.6 (13)	C153—C154—C155	121.6 (12)
C53—C52—H52	119.2	C153—C154—H154	119.2
C51—C52—H52	119.2	C155—C154—H154	119.2
C52—C53—C54	120.0 (12)	C156—C155—C154	117.9 (10)
C52—C53—H53	120.0	C156—C155—H155	121.1
C54—C53—H53	120.0	C154—C155—H155	121.1
C49—C54—C53	120.1 (9)	C151—C156—C155	121.7 (9)
C49—C54—H54	120.0	C151—C156—H156	119.1
C53—C54—H54	120.0	C155—C156—H156	119.1
C60—C55—C56	117.1 (7)	C158—C157—C162	119.6 (7)

C60—C55—P3	119.6 (6)	C158—C157—P8	123.5 (6)
C56—C55—P3	123.3 (6)	C162—C157—P8	116.8 (6)
C57—C56—C55	119.5 (7)	C157—C158—C159	119.0 (8)
C57—C56—H56	120.3	C157—C158—H158	120.5
C55—C56—H56	120.3	C159—C158—H158	120.5
C58—C57—C56	120.7 (9)	C160—C159—C158	122.1 (8)
C58—C57—H57	119.7	C160—C159—H159	118.9
C56—C57—H57	119.7	C158—C159—H159	118.9
C59—C58—C57	121.3 (10)	C161—C160—C159	118.0 (8)
C59—C58—H58	119.4	C161—C160—H160	121.0
C57—C58—H58	119.4	C159—C160—H160	121.0
C58—C59—C60	119.9 (9)	C160—C161—C162	121.4 (8)
C58—C59—H59	120.0	C160—C161—H161	119.3
C60—C59—H59	120.0	C162—C161—H161	119.3
C59—C60—C55	121.4 (8)	C157—C162—C161	119.6 (7)
C59—C60—H60	119.3	C157—C162—H162	120.2
C55—C60—H60	119.3	C161—C162—H162	120.2
C62—C61—C66	117.7 (6)	C168—C163—C164	117.4 (7)
C62—C61—P4	125.0 (6)	C168—C163—N4	122.6 (7)
C66—C61—P4	117.3 (6)	C164—C163—N4	120.0 (7)
C61—C62—C63	121.6 (7)	C165—C164—C163	121.5 (8)
C61—C62—H62	119.2	C165—C164—H164	119.2
C63—C62—H62	119.2	C163—C164—H164	119.2
C64—C63—C62	120.8 (8)	C166—C165—C164	119.9 (9)
C64—C63—H63	119.6	C166—C165—H165	120.1
C62—C63—H63	119.6	C164—C165—H165	120.1
C65—C64—C63	118.5 (7)	C165—C166—C167	120.5 (8)
C65—C64—H64	120.8	C165—C166—C14	118.9 (9)
C63—C64—H64	120.8	C167—C166—C14	120.6 (8)
C64—C65—C66	121.2 (8)	C166—C167—C168	120.5 (8)
C64—C65—H65	119.4	C166—C167—H167	119.7
C66—C65—H65	119.4	C168—C167—H167	119.7
C61—C66—C65	120.3 (7)	C163—C168—C167	120.1 (7)
C61—C66—H66	119.8	C163—C168—S4	118.7 (6)
C65—C66—H66	119.8	C167—C168—S4	121.2 (6)
C68—C67—C72	118.3 (8)	C39—N1—Ag1	111.1 (4)
C68—C67—P4	120.1 (7)	C39—N1—H1A	114 (7)
C72—C67—P4	121.5 (7)	Ag1—N1—H1A	111 (7)
C67—C68—C69	122.7 (9)	C39—N1—H1B	111 (9)
C67—C68—H68	118.6	Ag1—N1—H1B	104 (9)
C69—C68—H68	118.6	H1A—N1—H1B	105 (10)
C70—C69—C68	116.8 (11)	C79—N2—Ag2	108.2 (4)
C70—C69—H69	121.6	C79—N2—H2A	114 (7)
C68—C69—H69	121.6	Ag2—N2—H2A	104 (7)
C71—C70—C69	122.4 (11)	C79—N2—H2B	110 (8)
C71—C70—H70	118.8	Ag2—N2—H2B	115 (8)
C69—C70—H70	118.8	H2A—N2—H2B	106 (6)
C70—C71—C72	120.1 (11)	C121—N3—Ag3	109.6 (4)



C70—C71—H71	119.9	C121—N3—H3A	109 (8)
C72—C71—H71	119.9	Ag3—N3—H3A	106 (7)
C71—C72—C67	119.7 (9)	C121—N3—H3B	110 (8)
C71—C72—H72	120.2	Ag3—N3—H3B	109 (8)
C67—C72—H72	120.2	H3A—N3—H3B	112 (9)
C74—C73—C78	117.1 (7)	C163—N4—Ag4	114.2 (4)
C74—C73—P4	118.5 (6)	C163—N4—H4A	119 (9)
C78—C73—P4	124.1 (7)	Ag4—N4—H4A	100 (8)
C73—C74—C75	121.5 (8)	C163—N4—H4B	108 (8)
C73—C74—H74	119.3	Ag4—N4—H4B	106 (8)
C75—C74—H74	119.3	H4A—N4—H4B	110 (10)
C76—C75—C74	120.9 (10)	C7—P1—C1	105.7 (3)
C76—C75—H75	119.5	C7—P1—C13	102.8 (3)
C74—C75—H75	119.5	C1—P1—C13	104.6 (3)
C77—C76—C75	117.1 (11)	C7—P1—Ag1	117.0 (2)
C77—C76—H76	121.5	C1—P1—Ag1	113.9 (3)
C75—C76—H76	121.5	C13—P1—Ag1	111.6 (2)
C76—C77—C78	123.4 (10)	C19—P2—C31	105.6 (3)
C76—C77—H77	118.3	C19—P2—C25	103.0 (4)
C78—C77—H77	118.3	C31—P2—C25	104.9 (3)
C77—C78—C73	119.8 (9)	C19—P2—Ag1	111.2 (2)
C77—C78—H78	120.1	C31—P2—Ag1	112.3 (2)
C73—C78—H78	120.1	C25—P2—Ag1	118.7 (2)
C84—C79—C80	119.2 (7)	C55—P3—C49	105.3 (4)
C84—C79—N2	120.5 (6)	C55—P3—C43	105.5 (3)
C80—C79—N2	120.2 (6)	C49—P3—C43	104.8 (3)
C81—C80—C79	120.6 (7)	C55—P3—Ag2	113.6 (2)
C81—C80—H80	119.7	C49—P3—Ag2	115.5 (3)
C79—C80—H80	119.7	C43—P3—Ag2	111.3 (2)
C80—C81—C82	118.4 (7)	C73—P4—C67	105.6 (3)
C80—C81—H81	120.8	C73—P4—C61	105.0 (3)
C82—C81—H81	120.8	C67—P4—C61	103.4 (3)
C83—C82—C81	122.7 (8)	C73—P4—Ag2	113.7 (2)
C83—C82—Cl2	120.0 (7)	C67—P4—Ag2	115.0 (3)
C81—C82—Cl2	117.1 (7)	C61—P4—Ag2	113.1 (2)
C82—C83—C84	117.7 (7)	C85—P5—C91	106.7 (4)
C82—C83—H83	121.1	C85—P5—C97	103.6 (4)
C84—C83—H83	121.1	C91—P5—C97	103.3 (3)
C79—C84—C83	121.3 (6)	C85—P5—Ag3	119.6 (2)
C79—C84—S2	120.5 (5)	C91—P5—Ag3	109.0 (3)
C83—C84—S2	118.2 (5)	C97—P5—Ag3	113.2 (2)
C90—C85—C86	117.4 (7)	C103—P6—C109	105.9 (3)
C90—C85—P5	117.9 (6)	C103—P6—C115	102.4 (3)
C86—C85—P5	124.6 (7)	C109—P6—C115	104.2 (3)
C87—C86—C85	120.5 (8)	C103—P6—Ag3	116.1 (2)
C87—C86—H86	119.8	C109—P6—Ag3	109.7 (2)
C85—C86—H86	119.8	C115—P6—Ag3	117.3 (2)
C88—C87—C86	120.6 (9)	C139—P7—C127	104.5 (3)

C88—C87—H87	119.7	C139—P7—C133	107.4 (3)
C86—C87—H87	119.7	C127—P7—C133	103.7 (3)
C87—C88—C89	119.6 (10)	C139—P7—Ag4	114.8 (2)
C87—C88—H88	120.2	C127—P7—Ag4	111.1 (2)
C89—C88—H88	120.2	C133—P7—Ag4	114.4 (2)
C88—C89—C90	120.4 (9)	C151—P8—C145	104.5 (4)
C88—C89—H89	119.8	C151—P8—C157	102.7 (3)
C90—C89—H89	119.8	C145—P8—C157	103.2 (3)
C85—C90—C89	121.4 (8)	C151—P8—Ag4	116.1 (3)
C85—C90—H90	119.3	C145—P8—Ag4	114.7 (2)
C89—C90—H90	119.3	C157—P8—Ag4	114.1 (2)
C96—C91—C92	118.0 (8)	O1—S1—O2	113.5 (3)
C96—C91—P5	119.1 (7)	O1—S1—O3	113.4 (3)
C92—C91—P5	122.9 (6)	O2—S1—O3	110.9 (3)
C93—C92—C91	120.8 (9)	O1—S1—C38	107.1 (3)
C93—C92—H92	119.6	O2—S1—C38	106.8 (3)
C91—C92—H92	119.6	O3—S1—C38	104.4 (3)
C94—C93—C92	120.7 (11)	O6—S2—O5	112.9 (3)
C94—C93—H93	119.6	O6—S2—O4	113.5 (3)
C92—C93—H93	119.6	O5—S2—O4	112.4 (3)
C95—C94—C93	118.5 (13)	O6—S2—C84	107.6 (3)
C95—C94—H94	120.7	O5—S2—C84	103.6 (3)
C93—C94—H94	120.7	O4—S2—C84	106.0 (3)
C94—C95—C96	122.7 (12)	O8—S3—O7	113.4 (3)
C94—C95—H95	118.6	O8—S3—O9	113.5 (3)
C96—C95—H95	118.6	O7—S3—O9	111.6 (3)
C91—C96—C95	119.1 (9)	O8—S3—C122	107.6 (3)
C91—C96—H96	120.5	O7—S3—C122	106.1 (3)
C95—C96—H96	120.5	O9—S3—C122	103.7 (3)
C98—C97—C102	118.9 (7)	O11—S4—O10	114.2 (3)
C98—C97—P5	118.4 (6)	O11—S4—O12	113.0 (3)
C102—C97—P5	122.7 (6)	O10—S4—O12	111.2 (3)
C97—C98—C99	121.6 (8)	O11—S4—C168	107.7 (4)
C97—C98—H98	119.2	O10—S4—C168	106.0 (3)
C99—C98—H98	119.2	O12—S4—C168	104.1 (3)
C6—C1—C2—C3	-0.1 (12)	C164—C163—C168—C167	-0.3 (10)
P1—C1—C2—C3	179.2 (6)	N4—C163—C168—C167	178.9 (6)
C1—C2—C3—C4	1.9 (13)	C164—C163—C168—S4	-179.4 (5)
C2—C3—C4—C5	-2.8 (15)	N4—C163—C168—S4	-0.2 (9)
C3—C4—C5—C6	1.8 (16)	C166—C167—C168—C163	-1.1 (11)
C4—C5—C6—C1	0.2 (14)	C166—C167—C168—S4	177.9 (6)
C2—C1—C6—C5	-1.0 (12)	C38—C39—N1—Ag1	80.8 (7)
P1—C1—C6—C5	179.6 (6)	C40—C39—N1—Ag1	-95.9 (7)
C12—C7—C8—C9	1.0 (10)	P2—Ag1—N1—C39	-157.0 (4)
P1—C7—C8—C9	175.8 (6)	P1—Ag1—N1—C39	34.7 (5)
C7—C8—C9—C10	0.3 (12)	C84—C79—N2—Ag2	85.6 (6)
C8—C9—C10—C11	-2.4 (13)	C80—C79—N2—Ag2	-90.2 (6)

C9—C10—C11—C12	3.2 (14)	P4—Ag2—N2—C79	-151.6 (4)
C10—C11—C12—C7	-1.8 (13)	P3—Ag2—N2—C79	30.3 (5)
C8—C7—C12—C11	-0.3 (10)	C126—C121—N3—Ag3	-88.6 (6)
P1—C7—C12—C11	-175.1 (6)	C122—C121—N3—Ag3	90.0 (6)
C18—C13—C14—C15	0.3 (11)	P6—Ag3—N3—C121	-145.2 (4)
P1—C13—C14—C15	177.5 (6)	P5—Ag3—N3—C121	31.5 (5)
C13—C14—C15—C16	-2.9 (13)	C168—C163—N4—Ag4	-92.1 (7)
C14—C15—C16—C17	4.8 (14)	C164—C163—N4—Ag4	87.1 (7)
C15—C16—C17—C18	-4.2 (13)	P8—Ag4—N4—C163	153.6 (5)
C14—C13—C18—C17	0.3 (11)	P7—Ag4—N4—C163	-24.3 (6)
P1—C13—C18—C17	-177.1 (6)	C12—C7—P1—C1	-115.3 (6)
C16—C17—C18—C13	1.7 (12)	C8—C7—P1—C1	70.1 (6)
C24—C19—C20—C21	1.5 (11)	C12—C7—P1—C13	135.3 (6)
P2—C19—C20—C21	-175.9 (6)	C8—C7—P1—C13	-39.3 (6)
C19—C20—C21—C22	0.3 (13)	C12—C7—P1—Ag1	12.8 (6)
C20—C21—C22—C23	-3.2 (14)	C8—C7—P1—Ag1	-161.8 (5)
C21—C22—C23—C24	4.2 (14)	C2—C1—P1—C7	-7.4 (8)
C22—C23—C24—C19	-2.5 (13)	C6—C1—P1—C7	171.9 (5)
C20—C19—C24—C23	-0.4 (10)	C2—C1—P1—C13	100.7 (7)
P2—C19—C24—C23	176.9 (6)	C6—C1—P1—C13	-80.0 (6)
C30—C25—C26—C27	2.0 (13)	C2—C1—P1—Ag1	-137.2 (6)
P2—C25—C26—C27	-177.3 (6)	C6—C1—P1—Ag1	42.1 (6)
C25—C26—C27—C28	-4.0 (15)	C18—C13—P1—C7	-59.5 (6)
C26—C27—C28—C29	5.0 (18)	C14—C13—P1—C7	123.2 (6)
C27—C28—C29—C30	-4.3 (19)	C18—C13—P1—C1	-169.7 (6)
C26—C25—C30—C29	-1.0 (13)	C14—C13—P1—C1	13.0 (7)
P2—C25—C30—C29	178.3 (7)	C18—C13—P1—Ag1	66.6 (6)
C28—C29—C30—C25	2.1 (16)	C14—C13—P1—Ag1	-110.7 (6)
C36—C31—C32—C33	-0.2 (11)	N1—Ag1—P1—C7	-94.2 (3)
P2—C31—C32—C33	-178.0 (5)	P2—Ag1—P1—C7	97.7 (3)
C31—C32—C33—C34	-1.0 (12)	N1—Ag1—P1—C1	29.7 (3)
C32—C33—C34—C35	1.8 (13)	P2—Ag1—P1—C1	-138.4 (3)
C33—C34—C35—C36	-1.2 (14)	N1—Ag1—P1—C13	147.9 (3)
C34—C35—C36—C31	-0.1 (13)	P2—Ag1—P1—C13	-20.2 (3)
C32—C31—C36—C35	0.8 (11)	C20—C19—P2—C31	-162.8 (5)
P2—C31—C36—C35	178.7 (6)	C24—C19—P2—C31	20.0 (7)
C42—C37—C38—C39	2.0 (12)	C20—C19—P2—C25	87.4 (6)
C42—C37—C38—S1	-175.5 (6)	C24—C19—P2—C25	-89.8 (6)
C37—C38—C39—N1	-178.3 (6)	C20—C19—P2—Ag1	-40.7 (6)
S1—C38—C39—N1	-0.7 (9)	C24—C19—P2—Ag1	142.0 (5)
C37—C38—C39—C40	-1.5 (10)	C32—C31—P2—C19	-104.4 (6)
S1—C38—C39—C40	176.0 (5)	C36—C31—P2—C19	77.9 (6)
C38—C39—C40—C41	1.5 (11)	C32—C31—P2—C25	4.0 (7)
N1—C39—C40—C41	178.3 (7)	C36—C31—P2—C25	-173.8 (6)
C39—C40—C41—C42	-2.0 (14)	C32—C31—P2—Ag1	134.3 (6)
C40—C41—C42—C37	2.4 (14)	C36—C31—P2—Ag1	-43.5 (6)
C40—C41—C42—C11	179.6 (7)	C30—C25—P2—C19	-174.8 (7)
C38—C37—C42—C41	-2.4 (13)	C26—C25—P2—C19	4.5 (8)

C38—C37—C42—C11	-179.6 (6)	C30—C25—P2—C31	74.9 (7)
C48—C43—C44—C45	1.6 (12)	C26—C25—P2—C31	-105.8 (7)
P3—C43—C44—C45	-173.1 (6)	C30—C25—P2—Ag1	-51.5 (8)
C43—C44—C45—C46	-0.2 (12)	C26—C25—P2—Ag1	127.8 (6)
C44—C45—C46—C47	-0.4 (14)	N1—Ag1—P2—C19	144.6 (3)
C45—C46—C47—C48	-0.4 (15)	P1—Ag1—P2—C19	-46.9 (3)
C44—C43—C48—C47	-2.4 (13)	N1—Ag1—P2—C31	-97.3 (3)
P3—C43—C48—C47	172.0 (7)	P1—Ag1—P2—C31	71.2 (3)
C46—C47—C48—C43	1.8 (15)	N1—Ag1—P2—C25	25.5 (4)
C54—C49—C50—C51	-0.3 (11)	P1—Ag1—P2—C25	-166.0 (3)
P3—C49—C50—C51	-175.5 (6)	C60—C55—P3—C49	-101.4 (6)
C49—C50—C51—C52	-0.3 (13)	C56—C55—P3—C49	79.0 (6)
C50—C51—C52—C53	0.3 (17)	C60—C55—P3—C43	148.0 (6)
C51—C52—C53—C54	0.5 (17)	C56—C55—P3—C43	-31.6 (7)
C50—C49—C54—C53	1.1 (11)	C60—C55—P3—Ag2	25.9 (6)
P3—C49—C54—C53	176.0 (6)	C56—C55—P3—Ag2	-153.7 (5)
C52—C53—C54—C49	-1.2 (14)	C50—C49—P3—C55	157.5 (6)
C60—C55—C56—C57	1.6 (12)	C54—C49—P3—C55	-17.4 (7)
P3—C55—C56—C57	-178.7 (7)	C50—C49—P3—C43	-91.5 (6)
C55—C56—C57—C58	-0.2 (15)	C54—C49—P3—C43	93.6 (7)
C56—C57—C58—C59	-1.7 (17)	C50—C49—P3—Ag2	31.4 (6)
C57—C58—C59—C60	2.2 (18)	C54—C49—P3—Ag2	-143.5 (6)
C58—C59—C60—C55	-0.7 (16)	C48—C43—P3—C55	131.8 (7)
C56—C55—C60—C59	-1.2 (12)	C44—C43—P3—C55	-53.7 (6)
P3—C55—C60—C59	179.2 (8)	C48—C43—P3—C49	20.9 (8)
C66—C61—C62—C63	0.1 (14)	C44—C43—P3—C49	-164.6 (6)
P4—C61—C62—C63	179.3 (7)	C48—C43—P3—Ag2	-104.6 (7)
C61—C62—C63—C64	-0.1 (15)	C44—C43—P3—Ag2	69.9 (6)
C62—C63—C64—C65	-0.5 (15)	N2—Ag2—P3—C55	-86.6 (3)
C63—C64—C65—C66	1.0 (14)	P4—Ag2—P3—C55	95.7 (2)
C62—C61—C66—C65	0.4 (12)	N2—Ag2—P3—C49	35.2 (3)
P4—C61—C66—C65	-178.9 (6)	P4—Ag2—P3—C49	-142.5 (3)
C64—C65—C66—C61	-1.0 (13)	N2—Ag2—P3—C43	154.6 (3)
C72—C67—C68—C69	-1.7 (11)	P4—Ag2—P3—C43	-23.1 (3)
P4—C67—C68—C69	-179.5 (6)	C74—C73—P4—C67	176.5 (6)
C67—C68—C69—C70	1.9 (12)	C78—C73—P4—C67	-9.8 (7)
C68—C69—C70—C71	-0.6 (15)	C74—C73—P4—C61	67.6 (6)
C69—C70—C71—C72	-0.8 (16)	C78—C73—P4—C61	-118.7 (6)
C70—C71—C72—C67	1.0 (14)	C74—C73—P4—Ag2	-56.5 (6)
C68—C67—C72—C71	0.2 (11)	C78—C73—P4—Ag2	117.2 (6)
P4—C67—C72—C71	178.0 (6)	C68—C67—P4—C73	111.4 (6)
C78—C73—C74—C75	3.4 (11)	C72—C67—P4—C73	-66.3 (6)
P4—C73—C74—C75	177.5 (6)	C68—C67—P4—C61	-138.5 (6)
C73—C74—C75—C76	-0.1 (13)	C72—C67—P4—C61	43.7 (6)
C74—C75—C76—C77	-2.6 (14)	C68—C67—P4—Ag2	-14.8 (6)
C75—C76—C77—C78	1.8 (15)	C72—C67—P4—Ag2	167.5 (5)
C76—C77—C78—C73	1.6 (14)	C62—C61—P4—C73	5.6 (8)
C74—C73—C78—C77	-4.1 (11)	C66—C61—P4—C73	-175.2 (6)

P4—C73—C78—C77	-177.9 (6)	C62—C61—P4—C67	-104.9 (8)
C84—C79—C80—C81	0.1 (10)	C66—C61—P4—C67	74.3 (6)
N2—C79—C80—C81	176.0 (6)	C62—C61—P4—Ag2	130.1 (7)
C79—C80—C81—C82	-1.0 (11)	C66—C61—P4—Ag2	-50.7 (6)
C80—C81—C82—C83	2.6 (12)	N2—Ag2—P4—C73	3.0 (3)
C80—C81—C82—C12	177.6 (5)	P3—Ag2—P4—C73	-179.2 (3)
C81—C82—C83—C84	-3.2 (12)	N2—Ag2—P4—C67	124.9 (3)
C12—C82—C83—C84	-178.0 (5)	P3—Ag2—P4—C67	-57.3 (2)
C80—C79—C84—C83	-0.7 (10)	N2—Ag2—P4—C61	-116.6 (3)
N2—C79—C84—C83	-176.6 (6)	P3—Ag2—P4—C61	61.2 (3)
C80—C79—C84—S2	177.2 (5)	C90—C85—P5—C91	171.1 (6)
N2—C79—C84—S2	1.3 (9)	C86—C85—P5—C91	-11.0 (7)
C82—C83—C84—C79	2.2 (10)	C90—C85—P5—C97	-80.3 (6)
C82—C83—C84—S2	-175.8 (5)	C86—C85—P5—C97	97.7 (6)
C90—C85—C86—C87	-0.6 (11)	C90—C85—P5—Ag3	46.9 (6)
P5—C85—C86—C87	-178.5 (6)	C86—C85—P5—Ag3	-135.1 (5)
C85—C86—C87—C88	-1.0 (14)	C96—C91—P5—C85	-95.5 (7)
C86—C87—C88—C89	2.9 (15)	C92—C91—P5—C85	88.0 (7)
C87—C88—C89—C90	-3.1 (14)	C96—C91—P5—C97	155.7 (7)
C86—C85—C90—C89	0.3 (11)	C92—C91—P5—C97	-20.8 (8)
P5—C85—C90—C89	178.4 (6)	C96—C91—P5—Ag3	35.0 (7)
C88—C89—C90—C85	1.6 (12)	C92—C91—P5—Ag3	-141.5 (7)
C96—C91—C92—C93	0.3 (14)	C98—C97—P5—C85	163.6 (6)
P5—C91—C92—C93	176.9 (8)	C102—C97—P5—C85	-15.2 (7)
C91—C92—C93—C94	-3.8 (18)	C98—C97—P5—C91	-85.3 (7)
C92—C93—C94—C95	5 (2)	C102—C97—P5—C91	96.0 (7)
C93—C94—C95—C96	-3 (2)	C98—C97—P5—Ag3	32.5 (7)
C92—C91—C96—C95	1.9 (14)	C102—C97—P5—Ag3	-146.2 (6)
P5—C91—C96—C95	-174.8 (8)	N3—Ag3—P5—C85	22.7 (3)
C94—C95—C96—C91	-0.8 (19)	P6—Ag3—P5—C85	-160.8 (3)
C102—C97—C98—C99	-3.6 (13)	N3—Ag3—P5—C91	-100.4 (3)
P5—C97—C98—C99	177.7 (7)	P6—Ag3—P5—C91	76.1 (3)
C97—C98—C99—C100	4.6 (15)	N3—Ag3—P5—C97	145.2 (3)
C98—C99—C100—C101	-4.6 (15)	P6—Ag3—P5—C97	-38.3 (3)
C99—C100—C101—C102	3.7 (14)	C104—C103—P6—C109	66.0 (7)
C98—C97—C102—C101	2.5 (12)	C108—C103—P6—C109	-113.9 (6)
P5—C97—C102—C101	-178.7 (6)	C104—C103—P6—C115	-42.9 (7)
C100—C101—C102—C97	-2.6 (13)	C108—C103—P6—C115	137.2 (6)
C108—C103—C104—C105	-1.5 (12)	C104—C103—P6—Ag3	-172.0 (5)
P6—C103—C104—C105	178.6 (6)	C108—C103—P6—Ag3	8.1 (7)
C103—C104—C105—C106	3.0 (14)	C114—C109—P6—C103	-5.6 (7)
C104—C105—C106—C107	-4.1 (16)	C110—C109—P6—C103	170.2 (5)
C105—C106—C107—C108	3.9 (17)	C114—C109—P6—C115	102.0 (7)
C106—C107—C108—C103	-2.5 (15)	C110—C109—P6—C115	-82.1 (6)
C104—C103—C108—C107	1.3 (12)	C114—C109—P6—Ag3	-131.7 (6)
P6—C103—C108—C107	-178.8 (7)	C110—C109—P6—Ag3	44.2 (6)
C114—C109—C110—C111	-2.7 (11)	C116—C115—P6—C103	-75.2 (6)
P6—C109—C110—C111	-179.0 (6)	C120—C115—P6—C103	103.9 (6)

C109—C110—C111—C112	1.6 (12)	C116—C115—P6—C109	174.6 (6)
C110—C111—C112—C113	-2.4 (13)	C120—C115—P6—C109	-6.3 (7)
C111—C112—C113—C114	4.3 (12)	C116—C115—P6—Ag3	53.2 (6)
C110—C109—C114—C113	4.6 (11)	C120—C115—P6—Ag3	-127.7 (6)
P6—C109—C114—C113	-179.6 (6)	N3—Ag3—P6—C103	118.6 (3)
C112—C113—C114—C109	-5.5 (12)	P5—Ag3—P6—C103	-58.0 (3)
C120—C115—C116—C117	-3.2 (12)	N3—Ag3—P6—C109	-121.5 (3)
P6—C115—C116—C117	175.9 (6)	P5—Ag3—P6—C109	62.0 (2)
C115—C116—C117—C118	3.9 (13)	N3—Ag3—P6—C115	-2.9 (3)
C116—C117—C118—C119	-2.2 (14)	P5—Ag3—P6—C115	-179.5 (2)
C117—C118—C119—C120	-0.1 (13)	C140—C139—P7—C127	-92.2 (7)
C116—C115—C120—C119	1.0 (11)	C144—C139—P7—C127	91.5 (6)
P6—C115—C120—C119	-178.1 (6)	C140—C139—P7—C133	17.4 (7)
C118—C119—C120—C115	0.6 (13)	C144—C139—P7—C133	-158.8 (6)
C126—C121—C122—C123	-1.1 (10)	C140—C139—P7—Ag4	145.9 (6)
N3—C121—C122—C123	-179.8 (5)	C144—C139—P7—Ag4	-30.4 (6)
C126—C121—C122—S3	177.9 (5)	C132—C127—P7—C139	-29.1 (7)
N3—C121—C122—S3	-0.7 (8)	C128—C127—P7—C139	158.2 (6)
C121—C122—C123—C124	-0.8 (10)	C132—C127—P7—C133	-141.4 (6)
S3—C122—C123—C124	-179.9 (5)	C128—C127—P7—C133	45.9 (6)
C122—C123—C124—C125	3.3 (11)	C132—C127—P7—Ag4	95.3 (6)
C122—C123—C124—C13	-179.5 (4)	C128—C127—P7—Ag4	-77.5 (6)
C123—C124—C125—C126	-3.7 (11)	C138—C133—P7—C139	110.2 (6)
C13—C124—C125—C126	179.1 (5)	C134—C133—P7—C139	-72.1 (7)
C122—C121—C126—C125	0.7 (10)	C138—C133—P7—C127	-139.6 (6)
N3—C121—C126—C125	179.4 (5)	C134—C133—P7—C127	38.1 (7)
C124—C125—C126—C121	1.7 (10)	C138—C133—P7—Ag4	-18.4 (7)
C132—C127—C128—C129	0.9 (11)	C134—C133—P7—Ag4	159.2 (5)
P7—C127—C128—C129	174.0 (6)	N4—Ag4—P7—C139	-38.3 (3)
C127—C128—C129—C130	-0.9 (12)	P8—Ag4—P7—C139	143.9 (3)
C128—C129—C130—C131	0.1 (13)	N4—Ag4—P7—C127	-156.5 (3)
C129—C130—C131—C132	0.5 (13)	P8—Ag4—P7—C127	25.7 (3)
C128—C127—C132—C131	-0.2 (12)	N4—Ag4—P7—C133	86.6 (3)
P7—C127—C132—C131	-173.0 (6)	P8—Ag4—P7—C133	-91.3 (2)
C130—C131—C132—C127	-0.5 (13)	C156—C151—P8—C145	71.8 (7)
C138—C133—C134—C135	2.9 (11)	C152—C151—P8—C145	-103.3 (6)
P7—C133—C134—C135	-174.8 (6)	C156—C151—P8—C157	-35.7 (7)
C133—C134—C135—C136	-4.7 (13)	C152—C151—P8—C157	149.2 (6)
C134—C135—C136—C137	5.6 (14)	C156—C151—P8—Ag4	-160.8 (6)
C135—C136—C137—C138	-4.7 (15)	C152—C151—P8—Ag4	24.0 (6)
C134—C133—C138—C137	-2.1 (12)	C150—C145—P8—C151	-4.3 (7)
P7—C133—C138—C137	175.7 (6)	C146—C145—P8—C151	172.5 (5)
C136—C137—C138—C133	3.0 (13)	C150—C145—P8—C157	102.8 (6)
C144—C139—C140—C141	-1.2 (11)	C146—C145—P8—C157	-80.4 (6)
P7—C139—C140—C141	-177.5 (6)	C150—C145—P8—Ag4	-132.5 (5)
C139—C140—C141—C142	0.9 (13)	C146—C145—P8—Ag4	44.2 (6)
C140—C141—C142—C143	-1.1 (14)	C158—C157—P8—C151	121.1 (7)
C141—C142—C143—C144	1.7 (14)	C162—C157—P8—C151	-56.3 (7)

C142—C143—C144—C139	-2.0 (13)	C158—C157—P8—C145	12.6 (8)
C140—C139—C144—C143	1.8 (12)	C162—C157—P8—C145	-164.8 (6)
P7—C139—C144—C143	178.3 (6)	C158—C157—P8—Ag4	-112.4 (7)
C150—C145—C146—C147	-5.1 (11)	C162—C157—P8—Ag4	70.2 (7)
P8—C145—C146—C147	178.0 (6)	N4—Ag4—P8—C151	-124.4 (3)
C145—C146—C147—C148	1.9 (13)	P7—Ag4—P8—C151	53.5 (3)
C146—C147—C148—C149	3.0 (17)	N4—Ag4—P8—C145	-2.2 (3)
C147—C148—C149—C150	-4.3 (16)	P7—Ag4—P8—C145	175.6 (3)
C146—C145—C150—C149	3.8 (11)	N4—Ag4—P8—C157	116.5 (3)
P8—C145—C150—C149	-179.5 (5)	P7—Ag4—P8—C157	-65.7 (3)
C148—C149—C150—C145	0.7 (12)	C37—C38—S1—O1	-10.1 (7)
C156—C151—C152—C153	1.5 (12)	C39—C38—S1—O1	172.4 (5)
P8—C151—C152—C153	177.0 (7)	C37—C38—S1—O2	-132.0 (6)
C151—C152—C153—C154	-2.0 (14)	C39—C38—S1—O2	50.4 (6)
C152—C153—C154—C155	0.7 (16)	C37—C38—S1—O3	110.4 (6)
C153—C154—C155—C156	0.9 (15)	C39—C38—S1—O3	-67.2 (6)
C152—C151—C156—C155	0.2 (11)	C79—C84—S2—O6	170.0 (5)
P8—C151—C156—C155	-175.0 (6)	C83—C84—S2—O6	-12.0 (6)
C154—C155—C156—C151	-1.3 (13)	C79—C84—S2—O5	-70.3 (6)
C162—C157—C158—C159	-2.3 (13)	C83—C84—S2—O5	107.7 (5)
P8—C157—C158—C159	-179.6 (7)	C79—C84—S2—O4	48.2 (6)
C157—C158—C159—C160	4.0 (15)	C83—C84—S2—O4	-133.8 (5)
C158—C159—C160—C161	-5.7 (15)	C121—C122—S3—O8	172.1 (5)
C159—C160—C161—C162	5.7 (15)	C123—C122—S3—O8	-8.9 (6)
C158—C157—C162—C161	2.4 (13)	C121—C122—S3—O7	50.3 (6)
P8—C157—C162—C161	179.8 (7)	C123—C122—S3—O7	-130.6 (5)
C160—C161—C162—C157	-4.2 (14)	C121—C122—S3—O9	-67.4 (6)
C168—C163—C164—C165	2.6 (10)	C123—C122—S3—O9	111.6 (5)
N4—C163—C164—C165	-176.7 (6)	C163—C168—S4—O11	-173.1 (5)
C163—C164—C165—C166	-3.4 (11)	C167—C168—S4—O11	7.9 (6)
C164—C165—C166—C167	1.8 (12)	C163—C168—S4—O10	-50.5 (6)
C164—C165—C166—C14	-177.1 (5)	C167—C168—S4—O10	130.4 (6)
C165—C166—C167—C168	0.4 (13)	C163—C168—S4—O12	66.8 (6)
C14—C166—C167—C168	179.3 (5)	C167—C168—S4—O12	-112.2 (6)

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ )

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
N1—H1B $\cdots$ O2	0.82 (5)	2.21 (9)	2.879 (7)	139 (11)
N1—H1A $\cdots$ O9 <sup>i</sup>	0.90 (5)	2.08 (5)	2.976 (8)	174 (10)
N2—H2B $\cdots$ O4	0.82 (4)	2.21 (7)	2.870 (7)	139 (10)
N2—H2A $\cdots$ O11 <sup>ii</sup>	0.89 (4)	2.56 (8)	3.235 (8)	134 (9)
N2—H2A $\cdots$ O12 <sup>ii</sup>	0.89 (4)	2.05 (5)	2.916 (8)	164 (10)
N3—H3A $\cdots$ O5	0.88 (5)	2.12 (5)	2.991 (7)	175 (11)
N3—H3B $\cdots$ O7	0.86 (5)	2.18 (8)	2.900 (7)	141 (10)
N4—H4A $\cdots$ O1 <sup>iii</sup>	0.81 (5)	2.51 (9)	3.148 (8)	136 (10)

N4—H4A···O3 <sup>iii</sup>	0.81 (5)	2.26 (6)	3.027 (8)	159 (11)
N4—H4B···O10	0.85 (5)	2.13 (8)	2.877 (8)	146 (11)

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