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

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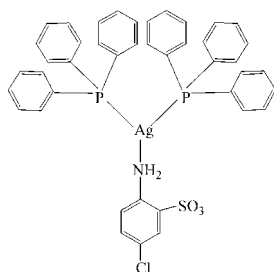
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 Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.013$ Å; R factor = 0.063; wR factor = 0.139; data-to-parameter ratio = 17.2.

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 Ag^{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) Å³
 $Z = 8$

 Mo $K\alpha$ radiation

 $\mu = 0.76$ mm⁻¹
 $T = 293$ (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⁻³
 $\Delta\rho_{\text{min}} = -0.63$ e Å⁻³

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, °).

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|-----------------------------------|----------|-------------|-------------|---------------|
| N1—H1B \cdots O2 | 0.82 (5) | 2.21 (9) | 2.879 (7) | 139 (11) |
| N1—H1A \cdots O9 ⁱ | 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 ⁱⁱ | 0.89 (4) | 2.56 (8) | 3.235 (8) | 134 (9) |
| N2—H2A \cdots O12 ⁱⁱ | 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 ⁱⁱⁱ | 0.81 (5) | 2.51 (9) | 3.148 (8) | 136 (10) |
| N4—H4A \cdots O3 ⁱⁱⁱ | 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.
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supplementary materials

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

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

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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).

Experimental

An aqueous solution (10 ml) of 2-amino-5-chlorobenzenesulfonic acid (0.104 g, 0.5 mmol) was added to solid Ag₂CO₃ (0.069 g, 0.25 mmol) and stirred for several minutes until no further CO₂ 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 NH₃ (14 *M*). Colourless blocks of the title compound were obtained by evaporation of the solution for several days at room temperature.

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 $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Figures

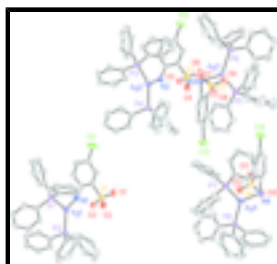


Fig. 1. The asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 30% probability level. All C-atom labels have been omitted for clarity.

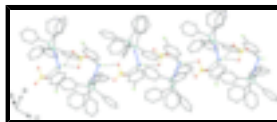


Fig. 2. One-dimensional supramolecular structure of the title compound, formed through hydrogen-bonding (dashed lines) interactions. The H atoms not involved in hydrogen bonding interactions have been omitted.

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

Crystal data

| | |
|--|---|
| [Ag(C ₆ H ₅ ClNO ₃ S)(C ₁₈ H ₁₅ P) ₂] | $Z = 8$ |
| $M_r = 839.03$ | $F_{000} = 3424$ |
| Triclinic, $P\bar{1}$ | $D_x = 1.433 \text{ Mg m}^{-3}$ |
| Hall symbol: -P 1 | Mo $K\alpha$ radiation |
| $a = 15.403 (5) \text{ \AA}$ | $\lambda = 0.71069 \text{ \AA}$ |
| $b = 23.1750 (19) \text{ \AA}$ | Cell parameters from 9413 reflections |
| $c = 23.3300 (16) \text{ \AA}$ | $\theta = 1.4\text{--}27.5^\circ$ |
| $\alpha = 100.771 (4)^\circ$ | $\mu = 0.76 \text{ mm}^{-1}$ |
| $\beta = 104.852 (6)^\circ$ | $T = 293 (2) \text{ K}$ |
| $\gamma = 97.035 (4)^\circ$ | Block, colourless |
| $V = 7780 (3) \text{ \AA}^3$ | $0.32 \times 0.28 \times 0.23 \text{ mm}$ |

Data collection

| | |
|---|---|
| Rigaku R-Axis RAPID diffractometer | 31947 independent reflections |
| Radiation source: fine-focus sealed tube | 19413 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{\text{int}} = 0.007$ |
| $T = 293(2) \text{ K}$ | $\theta_{\text{max}} = 27.5^\circ$ |
| ω scan | $\theta_{\text{min}} = 1.4^\circ$ |
| Absorption correction: multi-scan (ABSCOR; Higashi, 1995) | $h = -19 \rightarrow 19$ |
| $T_{\text{min}} = 0.788, T_{\text{max}} = 0.841$ | $k = -29 \rightarrow 29$ |
| 35542 measured reflections | $l = -30 \rightarrow 28$ |

Refinement

| | |
|--|--|
| Refinement on F^2 | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.063$ | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2) = 0.138$ | $w = 1/[\sigma^2(F_o^2) + (0.0406P)^2]$ |
| $S = 0.78$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| 31947 reflections | $(\Delta/\sigma)_{\text{max}} = 0.009$ |
| 1861 parameters | $\Delta\rho_{\text{max}} = 0.70 \text{ e \AA}^{-3}$ |
| 9 restraints | $\Delta\rho_{\text{min}} = -0.63 \text{ e \AA}^{-3}$ |
| Primary atom site location: structure-invariant direct methods | Extinction correction: none |

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 $F^2 > 2\sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

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

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|-------------|-------------|-------------|----------------------------------|
| 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) |
| 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* |

supplementary materials

| | | | | |
|-----|--------------|------------|------------|-------------|
| 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* |
| 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* |
| 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) |

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

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|------|------------|------------|-------------|-------------|
| 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) |
| 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* |

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|------|-------------|------------|------------|-------------|
| 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* |
| 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* |

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|------|-------------|--------------|------------|-------------|
| 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* |
| 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) |

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| 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 (\AA^2)

| | 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) |

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| 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) |
| 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) |

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| 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) |
| 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) |

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| 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) |
| 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) |

supplementary materials

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

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|---------|------------|-----------|------------|
| 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) |
| 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—Cl3 | 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—Cl1 | 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) |

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|---------|------------|-----------|------------|
| 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) |
| 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—C14 | 1.747 (8) |
| C75—C76 | 1.357 (11) | C167—C168 | 1.389 (9) |
| C75—H75 | 0.93 | C167—H167 | 0.93 |

supplementary materials

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| 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) |

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

supplementary materials

| | | | |
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| 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 |

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|-------------|------------|----------------|------------|
| 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—C11 | 119.7 (8) | C143—C144—H144 | 119.0 |
| C37—C42—C11 | 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) |

supplementary materials

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| 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) |

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| 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) |

supplementary materials

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| 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) |

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| 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) |

supplementary materials

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| 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) |

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| 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) |

supplementary materials

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| 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 (\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 ⁱ | 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 ⁱⁱ | 0.89 (4) | 2.56 (8) | 3.235 (8) | 134 (9) |
| N2—H2A \cdots O12 ⁱⁱ | 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 ⁱⁱⁱ | 0.81 (5) | 2.51 (9) | 3.148 (8) | 136 (10) |
| N4—H4A \cdots O3 ⁱⁱⁱ | 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) $-x, -y+1, -z+1$.

Fig. 1

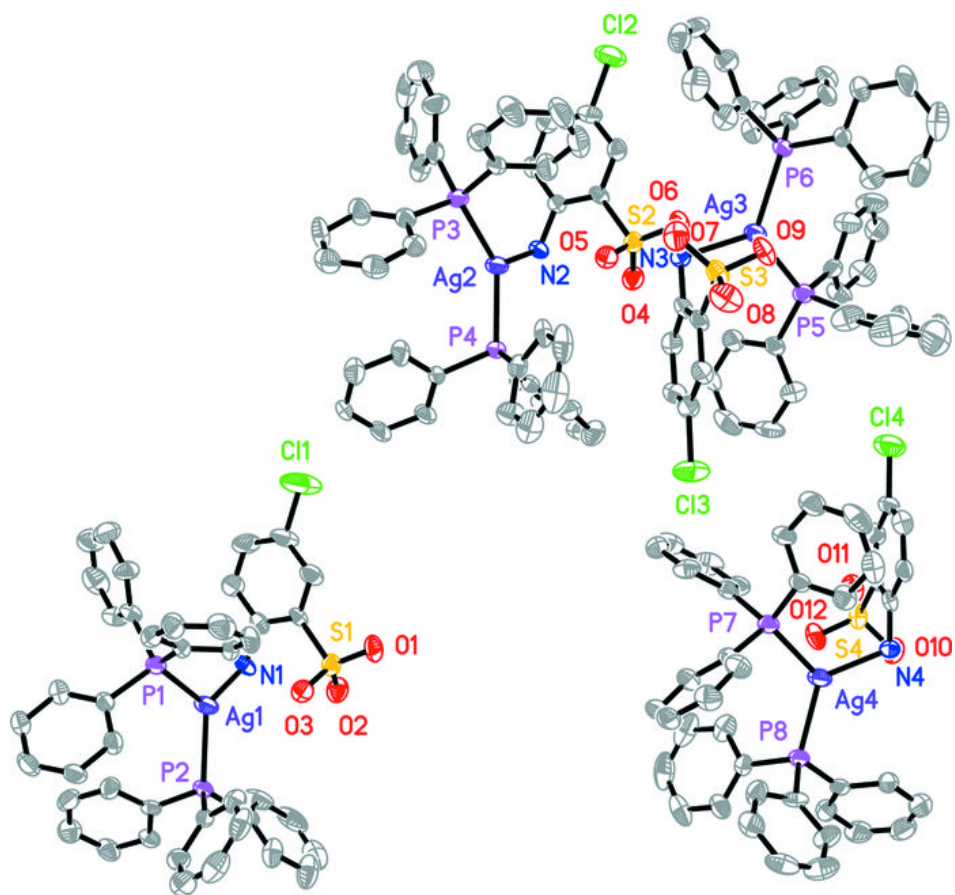


Fig. 2

