

# (Thiocyanato- $\kappa$ S)tris(triphenylphosphane- $\kappa$ P)-silver(I)

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Received 12 August 2017

Accepted 15 August 2017

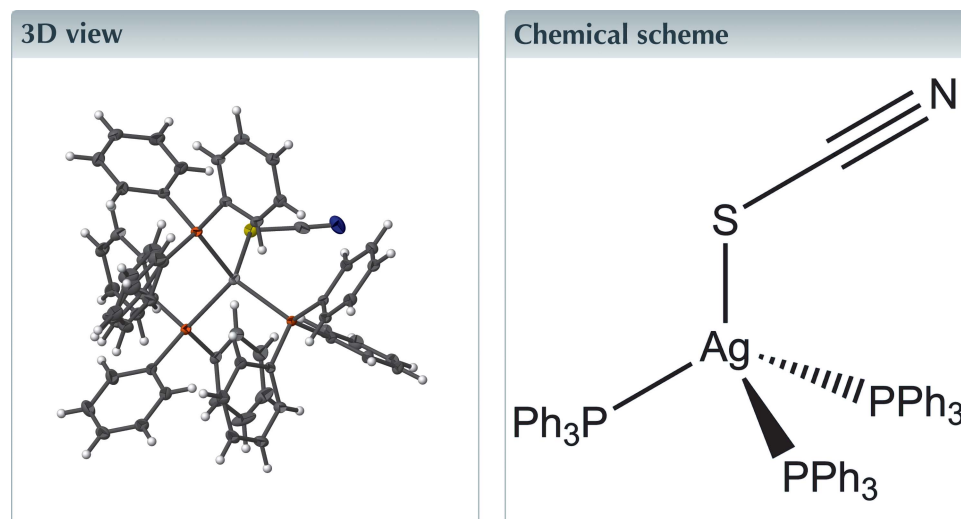
Edited by E. R. T. Tiekink, Sunway University, Malaysia

Keywords: crystal structure; hydrogen bonding; silver(I); thiocyanate.

CCDC reference: 1569028

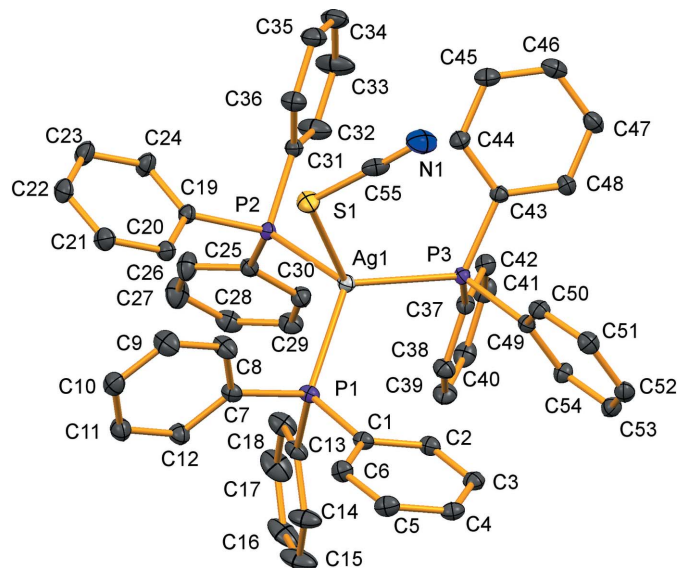
Structural data: full structural data are available from [iucrdata.iucr.org](http://iucrdata.iucr.org)

In the mononuclear title complex,  $[\text{Ag}(\text{SCN})(\text{C}_{18}\text{H}_{15}\text{P})_3]$ , the  $\text{Ag}^{\text{I}}$  center is in a slightly distorted tetrahedral coordination geometry formed by one S atom from a terminal thiocyanate ligand and three P atoms from three triphenylphosphane ligands. In the crystal, weak  $\text{C}-\text{H}\cdots\text{N}$  hydrogen bonds connect molecules into a two-dimensional network parallel to  $(10\bar{1})$ . One of the phenyl rings is disordered over two positions which were refined with an occupancy ratio of 0.715 (16):0.285 (16).



## Structure description

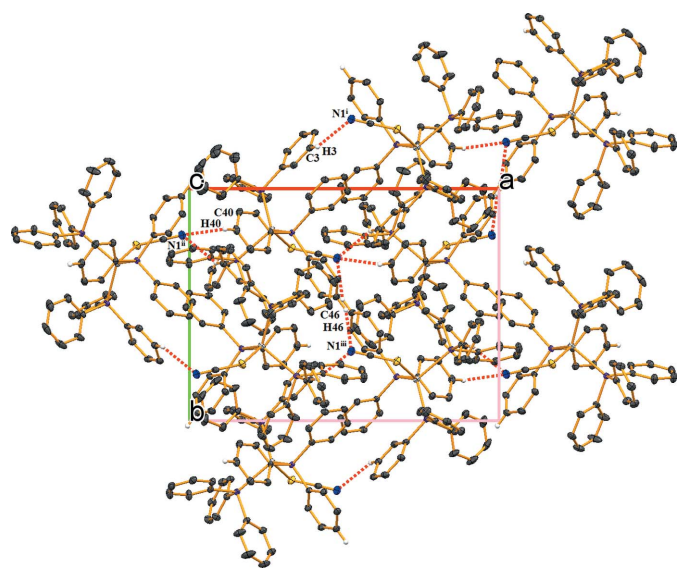
Silver(I) complexes with phosphorus and sulfur donor ligands have been of increasing interest because of the variety of their biological properties such as antibacterial, anti-inflammatory (Papanikolaou *et al.*, 2015) and antitumor (Liu *et al.*, 2008), as well as showing interesting luminescence properties (Ferrari *et al.*, 2007). Herein, we report the crystal structure of a silver(I) thiocyanate complex containing triphenylphosphane. The title complex was prepared by reacting silver(I) thiocyanate and triphenylphosphane ( $\text{PPh}_3$ ), followed by the addition of 1-(4-nitrophenyl)-2-thiourea, NPTU, in acetonitrile. An unexpected complex,  $[\text{Ag}(\text{C}_{18}\text{H}_{15}\text{P})_3(\text{SCN})]$ , was formed in high yield (74%) with no NPTU (Fig. 1). In the mononuclear complex, the  $\text{Ag}^{\text{I}}$  center is in a slightly distorted tetrahedral coordination geometry formed by one S atom from the terminal thiocyanate ligand, and three P atoms from three triphenylphosphane ligands. The  $\text{Ag}-\text{S}$  bond length of 2.6128 (3) Å is slightly shorter than in  $[\text{Ag}(\text{SCN})\{\text{P}(4\text{-MeC}_6\text{H}_4)_3\}_3]$  [2.6613 (7) Å; Omondi *et al.*, 2009]. The angles at the  $\text{Ag}^{\text{I}}$  ion vary from 94.327 (10)° to 117.910 (10)°. In the crystal, the molecules are connected *via* weak  $\text{C}3-\text{H}3\cdots\text{N}1^{\text{i}}$ ,  $\text{C}40-\text{H}40\cdots\text{N}1^{\text{iii}}$  and  $\text{C}46-\text{H}46\cdots\text{N}1^{\text{iii}}$  hydrogen bonds, leading to the formation of a two-dimensional network parallel to  $(10\bar{1})$  (Fig. 2 and Table 1).



**Figure 1**  
The molecular structure, with displacement ellipsoids drawn at the 50% probability level. All H atoms and disordered component have been omitted for clarity.

### Synthesis and crystallization

Triphenylphosphane, PPh<sub>3</sub> (0.27 g, 1.03 mmol) was dissolved in acetonitrile (30 ml) at 339 K and then silver(I) thiocyanate, AgSCN (0.08 g, 0.48 mmol) was added. The mixture was stirred for 3 h after which 1-(4-nitrophenyl)-2-thiourea, NPTU (0.1 g, 0.51 mmol) was added. The resulting reaction mixture was heated under reflux for 6 h during which time the precipitate gradually disappeared. The resulting yellow solution was filtered and left to evaporate at room temperature. The crystalline complex, which deposited upon standing after a few



**Figure 2**  
Part of the crystal structure, showing the intermolecular C—H...N hydrogen bonds (shown as dashed lines) leading to the formation of a two-dimensional network parallel to (10 $\bar{1}$ ).

**Table 1**  
Hydrogen-bond geometry (Å, °).

D—H...A	D—H	H...A	D...A	D—H...A
C3—H3...N1 <sup>i</sup>	0.95	2.63	3.2987 (19)	128
C40—H40...N1 <sup>ii</sup>	0.95	2.68	3.5540 (18)	153
C46—H46...N1 <sup>iii</sup>	0.95	2.52	3.3460 (18)	145

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

**Table 2**  
Experimental details.

Crystal data	
Chemical formula	[Ag(NCS)(C <sub>18</sub> H <sub>15</sub> P) <sub>3</sub> ]
<i>M<sub>r</sub></i>	952.76
Crystal system, space group	Monoclinic, <i>P</i> <sub>2</sub> / <i>1</i> <i>n</i>
Temperature (K)	100
<i>a</i> , <i>b</i> , <i>c</i> (Å)	18.1884 (10), 13.5886 (7), 18.3224 (10)
$\beta$ (°)	94.711 (2)
<i>V</i> (Å <sup>3</sup> )	4513.2 (4)
<i>Z</i>	4
Radiation type	Mo <i>K</i> $\alpha$
$\mu$ (mm <sup>-1</sup> )	0.64
Crystal size (mm)	0.55 × 0.45 × 0.40
Data collection	
Diffractometer	Bruker AXS D8 Quest CMOS
Absorption correction	Multi-scan ( <i>APEX3</i> ; Bruker, 2016)
<i>T</i> <sub>min</sub> , <i>T</i> <sub>max</sub>	0.673, 0.747
No. of measured, independent and observed [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )] reflections	35349, 18408, 16598
<i>R</i> <sub>int</sub>	0.014
( <i>sin</i> $\theta$ / $\lambda$ ) <sub>max</sub> (Å <sup>-1</sup> )	0.834
Refinement	
<i>R</i> [ <i>F</i> <sup>2</sup> > 2 $\sigma$ ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i>	0.027, 0.068, 1.06
No. of reflections	18408
No. of parameters	597
No. of restraints	192
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$ , $\Delta\rho_{min}$ (e Å <sup>-3</sup> )	0.88, -0.95

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *Mercury* (Macrae *et al.*, 2008) and *pubCIF* (Westrip, 2010).

days, was filtered off and dried *in vacuo* (0.24 g, 74% yield). M.p. 445–447 K. IR bands (KBr, cm<sup>-1</sup>): 3375 (*m*), 3292 (*w*), 3179 (*m*), 3002 (*w*), 2368 (*m*), 2345 (*m*), 1509 (*w*), 1340 (*s*), 1243 (*m*), 1109 (*m*), 1056 (*m*), 879 (*w*), 830 (*w*), 808 (*m*), 748 (*w*), 692 (*m*), 511 (*w*), 418 (*m*).

### Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. A number of reflections, *i.e.* (202), (2 $\bar{1}$ 1), (012), (112), (202), (210), (141), ( $\bar{1}$ 12), ( $\bar{1}$ 21), (13,17,6), (16,13,10), ( $\bar{9}$ ,18,6), (5,4,12), (12,18,5), (14,15,10), (344), (571), (15,16,1), ( $\bar{8}$ ,19,3), (13,17,4), (103), (9,9,22), (9,7,15), (7,5,17), (5,4,10), (11,12,19), (234), ( $\bar{5}$ ,13,3) and (13,17,0) were omitted from the final refinement owing to poor agreement. Disorder in one of the phenyl was resolved over two positions with a refined occupancy ratio of 0.715 (16):0.285 (16). The C13/C13B atoms were common to both orientations. The *U*<sub>ij</sub>

components of the ADP's were restrained to be similar for atoms closer to each other than 1.7 Å (SIMU).

### Acknowledgements

Financial support from the Department of Chemistry, Faculty of Science, Prince of Songkla University, is gratefully acknowledged. We would like to thank Dr Matthias Zeller and Purdue University for assistance with the X-ray structure determination and use of structure refinement programs funding by The National Science Foundation of United States (CHE-1625543).

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## full crystallographic data

*IUCrData* (2017). **2**, x171185 [<https://doi.org/10.1107/S2414314617011853>]

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(Thiocyanato- $\kappa$ S)tris(triphenylphosphane- $\kappa$ P)silver(I)*Crystal data*

[Ag(NCS)(C<sub>18</sub>H<sub>15</sub>P)<sub>3</sub>]

$M_r = 952.76$

Monoclinic,  $P2_1/n$

$a = 18.1884$  (10) Å

$b = 13.5886$  (7) Å

$c = 18.3224$  (10) Å

$\beta = 94.711$  (2)°

$V = 4513.2$  (4) Å<sup>3</sup>

$Z = 4$

$F(000) = 1960$

$D_x = 1.402$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 9970 reflections

$\theta = 3.4\text{--}36.3^\circ$

$\mu = 0.64$  mm<sup>-1</sup>

$T = 100$  K

Block, colourless

$0.55 \times 0.45 \times 0.40$  mm

*Data collection*

Bruker AXS D8 Quest CMOS

diffractometer

Radiation source: sealed tube X-ray source

Triumph curved graphite crystal

monochromator

$\omega$  and  $\phi$ i scans

Absorption correction: multi-scan

(APEX3; Bruker, 2016)

$T_{\min} = 0.673$ ,  $T_{\max} = 0.747$

35349 measured reflections

18408 independent reflections

16598 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.014$

$\theta_{\max} = 36.4^\circ$ ,  $\theta_{\min} = 3.2^\circ$

$h = -22 \rightarrow 30$

$k = -18 \rightarrow 21$

$l = -30 \rightarrow 17$

*Refinement*

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.027$

$wR(F^2) = 0.068$

$S = 1.06$

18408 reflections

597 parameters

192 restraints

Primary atom site location: structure-invariant

direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0152P)^2 + 3.9007P]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.002$

$\Delta\rho_{\max} = 0.88$  e Å<sup>-3</sup>

$\Delta\rho_{\min} = -0.95$  e Å<sup>-3</sup>

Extinction correction: SHELXL2014

(Sheldrick, 2015),

$F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.000262

*Special details*

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

**Refinement.** One phenyl ring was refined as disordered. The two moieties were restrained to have similar geometries and Uij components of ADPs were restrained to be similar for atoms closer than 1.7 Angstrom. The ipso carbon atom was not included in the disorder. Occupancies refined to 0.715 (16) to 0.28 (5).

All H atoms attached to carbon atoms were positioned geometrically and constrained to ride on their parent atoms, with C—H = 0.95 Å.  $U_{\text{iso}}(\text{H})$  values were set to  $1.2U_{\text{eq}}(\text{C})$ .

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Ag1	0.26601 (2)	0.17828 (2)	0.00411 (2)	0.01458 (2)	
S1	0.32976 (2)	0.25597 (3)	0.12349 (2)	0.02206 (6)	
P1	0.23375 (2)	0.00665 (2)	0.04613 (2)	0.01421 (5)	
P2	0.15358 (2)	0.30707 (2)	−0.00563 (2)	0.01333 (5)	
P3	0.33118 (2)	0.18985 (2)	−0.11004 (2)	0.01245 (5)	
N1	0.47680 (7)	0.29965 (10)	0.09709 (9)	0.0324 (3)	
C1	0.30071 (6)	−0.09262 (8)	0.04243 (6)	0.01542 (18)	
C2	0.33764 (7)	−0.10148 (9)	−0.02128 (6)	0.01743 (19)	
H2	0.3274	−0.0562	−0.0603	0.021*	
C3	0.38914 (7)	−0.17563 (9)	−0.02825 (6)	0.01842 (19)	
H3	0.4137	−0.1810	−0.0719	0.022*	
C4	0.40473 (7)	−0.24203 (9)	0.02873 (6)	0.0188 (2)	
H4	0.4401	−0.2927	0.0243	0.023*	
C5	0.36828 (7)	−0.23374 (9)	0.09211 (6)	0.0204 (2)	
H5	0.3789	−0.2791	0.1310	0.024*	
C6	0.31640 (7)	−0.15979 (9)	0.09935 (6)	0.0186 (2)	
H6	0.2917	−0.1550	0.1429	0.022*	
C7	0.20648 (6)	−0.00109 (8)	0.13949 (6)	0.01578 (18)	
C8	0.25345 (7)	0.04010 (11)	0.19551 (6)	0.0237 (2)	
H8	0.2986	0.0695	0.1844	0.028*	
C9	0.23452 (8)	0.03820 (11)	0.26750 (7)	0.0265 (3)	
H9	0.2669	0.0657	0.3054	0.032*	
C10	0.16826 (7)	−0.00397 (10)	0.28404 (6)	0.0219 (2)	
H10	0.1549	−0.0043	0.3331	0.026*	
C11	0.12191 (7)	−0.04540 (10)	0.22893 (7)	0.0228 (2)	
H11	0.0768	−0.0745	0.2403	0.027*	
C12	0.14089 (7)	−0.04478 (10)	0.15683 (6)	0.0199 (2)	
H12	0.1090	−0.0743	0.1194	0.024*	
C13	0.15535 (7)	−0.03948 (9)	−0.01221 (6)	0.0184 (2)	0.715 (16)
C14	0.1448 (3)	−0.1397 (3)	−0.0261 (3)	0.0286 (7)	0.715 (16)
H14	0.1771	−0.1868	−0.0023	0.034*	0.715 (16)
C15	0.0864 (3)	−0.1706 (4)	−0.0751 (3)	0.0370 (8)	0.715 (16)
H15	0.0794	−0.2387	−0.0849	0.044*	0.715 (16)
C16	0.0392 (3)	−0.1035 (5)	−0.1090 (4)	0.0366 (10)	0.715 (16)

H16	-0.0011	-0.1253	-0.1413	0.044*	0.715 (16)
C17	0.0501 (2)	-0.0039 (4)	-0.0965 (3)	0.0346 (8)	0.715 (16)
H17	0.0179	0.0428	-0.1210	0.041*	0.715 (16)
C18	0.1081 (2)	0.0278 (3)	-0.0481 (3)	0.0255 (6)	0.715 (16)
H18	0.1153	0.0962	-0.0395	0.031*	0.715 (16)
C13B	0.15535 (7)	-0.03948 (9)	-0.01221 (6)	0.0184 (2)	0.285 (16)
C14B	0.1464 (7)	-0.1320 (8)	-0.0427 (6)	0.0288 (16)	0.285 (16)
H14B	0.1828	-0.1812	-0.0321	0.035*	0.285 (16)
C15B	0.0837 (8)	-0.1532 (10)	-0.0892 (7)	0.0358 (18)	0.285 (16)
H15B	0.0774	-0.2174	-0.1093	0.043*	0.285 (16)
C16B	0.0310 (10)	-0.0830 (11)	-0.1064 (11)	0.0330 (19)	0.285 (16)
H16B	-0.0104	-0.0978	-0.1396	0.040*	0.285 (16)
C17B	0.0383 (6)	0.0084 (7)	-0.0754 (7)	0.0328 (16)	0.285 (16)
H17B	0.0011	0.0566	-0.0857	0.039*	0.285 (16)
C18B	0.1000 (6)	0.0306 (8)	-0.0291 (7)	0.0275 (15)	0.285 (16)
H18B	0.1049	0.0945	-0.0083	0.033*	0.285 (16)
C19	0.12105 (6)	0.32699 (9)	0.08470 (6)	0.01555 (18)	
C20	0.13199 (7)	0.25301 (9)	0.13697 (6)	0.01797 (19)	
H20	0.1558	0.1936	0.1250	0.022*	
C21	0.10814 (8)	0.26562 (10)	0.20675 (6)	0.0229 (2)	
H21	0.1158	0.2148	0.2421	0.027*	
C22	0.07325 (8)	0.35212 (10)	0.22482 (6)	0.0230 (2)	
H22	0.0567	0.3604	0.2723	0.028*	
C23	0.06272 (8)	0.42658 (10)	0.17301 (7)	0.0242 (2)	
H23	0.0390	0.4859	0.1851	0.029*	
C24	0.08678 (7)	0.41458 (10)	0.10358 (6)	0.0217 (2)	
H24	0.0799	0.4661	0.0687	0.026*	
C25	0.06837 (6)	0.29596 (9)	-0.06609 (6)	0.01584 (18)	
C26	-0.00128 (7)	0.32053 (12)	-0.04485 (7)	0.0263 (3)	
H26	-0.0064	0.3422	0.0038	0.032*	
C27	-0.06330 (8)	0.31351 (13)	-0.09442 (9)	0.0306 (3)	
H27	-0.1104	0.3306	-0.0793	0.037*	
C28	-0.05700 (7)	0.28185 (10)	-0.16557 (8)	0.0242 (2)	
H28	-0.0994	0.2777	-0.1993	0.029*	
C29	0.01187 (7)	0.25637 (10)	-0.18700 (7)	0.0220 (2)	
H29	0.0166	0.2343	-0.2356	0.026*	
C30	0.07406 (7)	0.26298 (9)	-0.13763 (6)	0.0190 (2)	
H30	0.1209	0.2449	-0.1528	0.023*	
C31	0.18532 (6)	0.43102 (9)	-0.02609 (6)	0.01644 (18)	
C32	0.16240 (10)	0.48334 (11)	-0.08871 (7)	0.0318 (3)	
H32	0.1271	0.4555	-0.1239	0.038*	
C33	0.19094 (12)	0.57683 (12)	-0.10029 (8)	0.0415 (4)	
H33	0.1750	0.6124	-0.1434	0.050*	
C34	0.24236 (10)	0.61804 (11)	-0.04932 (8)	0.0303 (3)	
H34	0.2619	0.6816	-0.0574	0.036*	
C35	0.26504 (8)	0.56624 (10)	0.01329 (8)	0.0256 (2)	
H35	0.2999	0.5946	0.0486	0.031*	
C36	0.23721 (7)	0.47303 (10)	0.02494 (7)	0.0219 (2)	

H36	0.2536	0.4376	0.0679	0.026*
C37	0.26260 (6)	0.18834 (9)	-0.18794 (6)	0.01470 (17)
C38	0.21575 (6)	0.10661 (9)	-0.19572 (6)	0.0187 (2)
H38	0.2210	0.0546	-0.1611	0.022*
C39	0.16174 (7)	0.10095 (10)	-0.25368 (7)	0.0220 (2)
H39	0.1312	0.0443	-0.2593	0.026*
C40	0.15213 (7)	0.17778 (11)	-0.30343 (7)	0.0226 (2)
H40	0.1150	0.1740	-0.3430	0.027*
C41	0.19707 (7)	0.26011 (10)	-0.29506 (6)	0.0220 (2)
H41	0.1899	0.3133	-0.3285	0.026*
C42	0.25269 (7)	0.26558 (9)	-0.23798 (6)	0.01769 (19)
H42	0.2837	0.3218	-0.2332	0.021*
C43	0.38650 (6)	0.29955 (8)	-0.12092 (6)	0.01403 (17)
C44	0.38381 (7)	0.37536 (9)	-0.07008 (6)	0.01840 (19)
H44	0.3519	0.3702	-0.0317	0.022*
C45	0.42769 (7)	0.45866 (10)	-0.07527 (7)	0.0228 (2)
H45	0.4252	0.5105	-0.0408	0.027*
C46	0.47497 (7)	0.46606 (9)	-0.13071 (7)	0.0220 (2)
H46	0.5054	0.5225	-0.1338	0.026*
C47	0.47766 (7)	0.39092 (9)	-0.18164 (7)	0.0210 (2)
H47	0.5097	0.3963	-0.2198	0.025*
C48	0.43372 (6)	0.30783 (9)	-0.17714 (6)	0.01781 (19)
H48	0.4358	0.2567	-0.2122	0.021*
C49	0.39554 (6)	0.09351 (8)	-0.13276 (5)	0.01357 (17)
C50	0.45835 (6)	0.08074 (9)	-0.08460 (6)	0.01700 (19)
H50	0.4652	0.1204	-0.0419	0.020*
C51	0.51089 (7)	0.01063 (9)	-0.09859 (7)	0.0194 (2)
H51	0.5540	0.0037	-0.0661	0.023*
C52	0.50052 (7)	-0.04948 (9)	-0.16009 (6)	0.0187 (2)
H52	0.5363	-0.0977	-0.1696	0.022*
C53	0.43760 (7)	-0.03841 (9)	-0.20743 (6)	0.0188 (2)
H53	0.4299	-0.0801	-0.2490	0.023*
C54	0.38552 (6)	0.03338 (9)	-0.19448 (6)	0.01629 (18)
H54	0.3431	0.0414	-0.2278	0.020*
C55	0.41587 (7)	0.28107 (9)	0.10648 (7)	0.0206 (2)

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Ag1	0.01684 (4)	0.01539 (4)	0.01166 (3)	-0.00341 (3)	0.00210 (2)	-0.00063 (2)
S1	0.02313 (14)	0.02779 (15)	0.01479 (10)	-0.00642 (11)	-0.00123 (10)	-0.00447 (10)
P1	0.01547 (12)	0.01409 (12)	0.01254 (10)	-0.00292 (9)	-0.00198 (9)	0.00205 (9)
P2	0.01477 (11)	0.01392 (12)	0.01151 (10)	-0.00087 (9)	0.00237 (8)	-0.00050 (8)
P3	0.01244 (11)	0.01482 (12)	0.01006 (9)	-0.00165 (9)	0.00071 (8)	-0.00044 (8)
N1	0.0219 (5)	0.0280 (6)	0.0460 (7)	-0.0024 (4)	-0.0053 (5)	-0.0027 (5)
C1	0.0180 (5)	0.0142 (5)	0.0136 (4)	-0.0023 (4)	-0.0013 (3)	0.0014 (3)
C2	0.0208 (5)	0.0169 (5)	0.0141 (4)	-0.0032 (4)	-0.0009 (4)	0.0014 (3)
C3	0.0208 (5)	0.0180 (5)	0.0163 (4)	-0.0035 (4)	0.0003 (4)	-0.0018 (4)

C4	0.0208 (5)	0.0158 (5)	0.0191 (4)	-0.0012 (4)	-0.0026 (4)	-0.0021 (4)
C5	0.0263 (6)	0.0173 (5)	0.0167 (4)	0.0003 (4)	-0.0031 (4)	0.0020 (4)
C6	0.0229 (5)	0.0185 (5)	0.0142 (4)	0.0008 (4)	-0.0003 (4)	0.0032 (4)
C7	0.0177 (5)	0.0152 (5)	0.0141 (4)	-0.0006 (4)	-0.0007 (3)	0.0023 (3)
C8	0.0249 (6)	0.0308 (7)	0.0149 (4)	-0.0105 (5)	-0.0021 (4)	0.0020 (4)
C9	0.0312 (7)	0.0335 (7)	0.0140 (4)	-0.0079 (5)	-0.0034 (4)	0.0021 (4)
C10	0.0283 (6)	0.0216 (6)	0.0161 (4)	0.0022 (4)	0.0027 (4)	0.0029 (4)
C11	0.0223 (5)	0.0263 (6)	0.0203 (5)	-0.0025 (4)	0.0051 (4)	-0.0001 (4)
C12	0.0187 (5)	0.0229 (6)	0.0181 (4)	-0.0040 (4)	0.0015 (4)	-0.0014 (4)
C13	0.0185 (5)	0.0218 (5)	0.0142 (4)	-0.0070 (4)	-0.0024 (3)	0.0032 (4)
C14	0.0375 (13)	0.0239 (11)	0.0223 (15)	-0.0125 (9)	-0.0104 (13)	0.0014 (10)
C15	0.0478 (15)	0.0327 (16)	0.0280 (16)	-0.0222 (13)	-0.0124 (13)	0.0030 (11)
C16	0.0317 (19)	0.052 (2)	0.0239 (11)	-0.0253 (18)	-0.0106 (14)	0.0073 (18)
C17	0.0235 (12)	0.0497 (18)	0.0283 (15)	-0.0089 (11)	-0.0113 (10)	0.0094 (13)
C18	0.0217 (10)	0.0295 (11)	0.0236 (14)	-0.0053 (8)	-0.0072 (10)	0.0073 (11)
C13B	0.0185 (5)	0.0218 (5)	0.0142 (4)	-0.0070 (4)	-0.0024 (3)	0.0032 (4)
C14B	0.036 (3)	0.030 (3)	0.019 (3)	-0.002 (2)	-0.004 (3)	-0.004 (2)
C15B	0.043 (3)	0.037 (4)	0.026 (3)	-0.015 (3)	-0.006 (3)	-0.004 (3)
C16B	0.032 (3)	0.039 (4)	0.026 (3)	-0.006 (3)	-0.014 (2)	0.012 (3)
C17B	0.029 (3)	0.034 (3)	0.033 (3)	-0.005 (2)	-0.014 (3)	0.005 (3)
C18B	0.024 (3)	0.031 (3)	0.026 (3)	-0.004 (2)	-0.011 (2)	0.007 (3)
C19	0.0168 (4)	0.0174 (5)	0.0128 (4)	-0.0011 (4)	0.0029 (3)	-0.0011 (3)
C20	0.0227 (5)	0.0171 (5)	0.0145 (4)	-0.0016 (4)	0.0037 (4)	0.0003 (4)
C21	0.0325 (6)	0.0225 (6)	0.0144 (4)	-0.0023 (5)	0.0051 (4)	0.0018 (4)
C22	0.0279 (6)	0.0272 (6)	0.0146 (4)	-0.0021 (5)	0.0063 (4)	-0.0022 (4)
C23	0.0305 (6)	0.0245 (6)	0.0186 (5)	0.0049 (5)	0.0084 (4)	-0.0021 (4)
C24	0.0280 (6)	0.0211 (6)	0.0168 (4)	0.0051 (4)	0.0066 (4)	0.0010 (4)
C25	0.0158 (4)	0.0164 (5)	0.0154 (4)	-0.0018 (4)	0.0021 (3)	0.0007 (3)
C26	0.0181 (5)	0.0391 (8)	0.0217 (5)	0.0022 (5)	0.0019 (4)	-0.0047 (5)
C27	0.0172 (5)	0.0431 (8)	0.0311 (6)	0.0042 (5)	-0.0001 (5)	-0.0022 (6)
C28	0.0203 (5)	0.0246 (6)	0.0265 (5)	-0.0030 (4)	-0.0050 (4)	0.0035 (5)
C29	0.0234 (5)	0.0239 (6)	0.0179 (4)	-0.0045 (4)	-0.0025 (4)	0.0006 (4)
C30	0.0185 (5)	0.0224 (5)	0.0162 (4)	-0.0026 (4)	0.0015 (4)	-0.0018 (4)
C31	0.0199 (5)	0.0154 (5)	0.0144 (4)	-0.0027 (4)	0.0041 (3)	-0.0010 (3)
C32	0.0530 (9)	0.0230 (6)	0.0176 (5)	-0.0137 (6)	-0.0072 (5)	0.0045 (4)
C33	0.0750 (13)	0.0251 (7)	0.0223 (6)	-0.0184 (8)	-0.0079 (7)	0.0087 (5)
C34	0.0488 (9)	0.0186 (6)	0.0243 (5)	-0.0114 (6)	0.0072 (6)	0.0001 (5)
C35	0.0294 (6)	0.0190 (6)	0.0284 (6)	-0.0071 (5)	0.0023 (5)	-0.0033 (5)
C36	0.0239 (5)	0.0182 (5)	0.0230 (5)	-0.0035 (4)	-0.0014 (4)	0.0003 (4)
C37	0.0127 (4)	0.0187 (5)	0.0126 (4)	0.0001 (3)	0.0002 (3)	-0.0009 (3)
C38	0.0170 (5)	0.0206 (5)	0.0181 (4)	-0.0027 (4)	-0.0012 (4)	-0.0002 (4)
C39	0.0185 (5)	0.0256 (6)	0.0213 (5)	-0.0032 (4)	-0.0027 (4)	-0.0047 (4)
C40	0.0184 (5)	0.0320 (7)	0.0166 (4)	0.0026 (4)	-0.0037 (4)	-0.0043 (4)
C41	0.0227 (5)	0.0266 (6)	0.0160 (4)	0.0042 (4)	-0.0033 (4)	0.0016 (4)
C42	0.0186 (5)	0.0197 (5)	0.0145 (4)	0.0005 (4)	-0.0003 (4)	0.0014 (4)
C43	0.0146 (4)	0.0138 (4)	0.0136 (4)	-0.0011 (3)	0.0002 (3)	-0.0001 (3)
C44	0.0196 (5)	0.0185 (5)	0.0170 (4)	-0.0025 (4)	0.0014 (4)	-0.0033 (4)
C45	0.0257 (6)	0.0170 (5)	0.0250 (5)	-0.0042 (4)	-0.0010 (4)	-0.0038 (4)



C46	0.0193 (5)	0.0170 (5)	0.0291 (6)	-0.0035 (4)	-0.0024 (4)	0.0041 (4)
C47	0.0189 (5)	0.0197 (5)	0.0249 (5)	-0.0017 (4)	0.0046 (4)	0.0052 (4)
C48	0.0184 (5)	0.0175 (5)	0.0181 (4)	-0.0013 (4)	0.0046 (4)	0.0004 (4)
C49	0.0144 (4)	0.0143 (4)	0.0119 (3)	-0.0015 (3)	0.0007 (3)	0.0005 (3)
C50	0.0161 (4)	0.0185 (5)	0.0159 (4)	-0.0017 (4)	-0.0015 (3)	-0.0008 (4)
C51	0.0159 (5)	0.0217 (5)	0.0201 (4)	0.0004 (4)	-0.0011 (4)	0.0021 (4)
C52	0.0198 (5)	0.0161 (5)	0.0207 (4)	0.0022 (4)	0.0047 (4)	0.0032 (4)
C53	0.0228 (5)	0.0176 (5)	0.0163 (4)	0.0012 (4)	0.0029 (4)	-0.0017 (4)
C54	0.0174 (5)	0.0185 (5)	0.0127 (4)	0.0004 (4)	-0.0003 (3)	-0.0008 (3)
C55	0.0243 (5)	0.0131 (5)	0.0230 (5)	0.0009 (4)	-0.0070 (4)	-0.0010 (4)

*Geometric parameters (Å, °)*

Ag1—P3	2.4923 (3)	C20—H20	0.9500
Ag1—P1	2.5399 (3)	C21—C22	1.3886 (19)
Ag1—S1	2.6128 (3)	C21—H21	0.9500
Ag1—P2	2.6863 (3)	C22—C23	1.3900 (19)
S1—C55	1.6574 (14)	C22—H22	0.9500
P1—C13B	1.8216 (12)	C23—C24	1.3884 (16)
P1—C13	1.8216 (12)	C23—H23	0.9500
P1—C1	1.8224 (12)	C24—H24	0.9500
P1—C7	1.8228 (11)	C25—C26	1.3959 (17)
P2—C19	1.8231 (10)	C25—C30	1.3972 (16)
P2—C31	1.8293 (12)	C26—C27	1.3922 (19)
P2—C25	1.8358 (12)	C26—H26	0.9500
P3—C37	1.8169 (11)	C27—C28	1.386 (2)
P3—C43	1.8184 (11)	C27—H27	0.9500
P3—C49	1.8269 (11)	C28—C29	1.3871 (19)
N1—C55	1.1630 (18)	C28—H28	0.9500
C1—C6	1.3976 (15)	C29—C30	1.3920 (17)
C1—C2	1.3989 (15)	C29—H29	0.9500
C2—C3	1.3888 (17)	C30—H30	0.9500
C2—H2	0.9500	C31—C32	1.3846 (18)
C3—C4	1.3913 (17)	C31—C36	1.3950 (17)
C3—H3	0.9500	C32—C33	1.395 (2)
C4—C5	1.3883 (17)	C32—H32	0.9500
C4—H4	0.9500	C33—C34	1.385 (2)
C5—C6	1.3922 (18)	C33—H33	0.9500
C5—H5	0.9500	C34—C35	1.380 (2)
C6—H6	0.9500	C34—H34	0.9500
C7—C12	1.3924 (16)	C35—C36	1.3870 (18)
C7—C8	1.3974 (16)	C35—H35	0.9500
C8—C9	1.3905 (17)	C36—H36	0.9500
C8—H8	0.9500	C37—C42	1.3956 (16)
C9—C10	1.3902 (19)	C37—C38	1.4000 (16)
C9—H9	0.9500	C38—C39	1.3884 (17)
C10—C11	1.3811 (19)	C38—H38	0.9500
C10—H10	0.9500	C39—C40	1.3875 (19)

C11—C12	1.3926 (17)	C39—H39	0.9500
C11—H11	0.9500	C40—C41	1.3865 (19)
C12—H12	0.9500	C40—H40	0.9500
C13—C18	1.384 (4)	C41—C42	1.3960 (16)
C13—C14	1.396 (4)	C41—H41	0.9500
C14—C15	1.398 (5)	C42—H42	0.9500
C14—H14	0.9500	C43—C44	1.3924 (15)
C15—C16	1.366 (6)	C43—C48	1.3989 (15)
C15—H15	0.9500	C44—C45	1.3927 (17)
C16—C17	1.385 (5)	C44—H44	0.9500
C16—H16	0.9500	C45—C46	1.3875 (19)
C17—C18	1.390 (4)	C45—H45	0.9500
C17—H17	0.9500	C46—C47	1.3868 (19)
C18—H18	0.9500	C46—H46	0.9500
C13B—C14B	1.380 (10)	C47—C48	1.3896 (17)
C13B—C18B	1.402 (9)	C47—H47	0.9500
C14B—C15B	1.397 (12)	C48—H48	0.9500
C14B—H14B	0.9500	C49—C54	1.3948 (15)
C15B—C16B	1.369 (12)	C49—C50	1.3959 (15)
C15B—H15B	0.9500	C50—C51	1.3880 (17)
C16B—C17B	1.367 (12)	C50—H50	0.9500
C16B—H16B	0.9500	C51—C52	1.3920 (18)
C17B—C18B	1.383 (10)	C51—H51	0.9500
C17B—H17B	0.9500	C52—C53	1.3861 (17)
C18B—H18B	0.9500	C52—H52	0.9500
C19—C20	1.3913 (16)	C53—C54	1.3936 (16)
C19—C24	1.4001 (17)	C53—H53	0.9500
C20—C21	1.3941 (16)	C54—H54	0.9500
P3—Ag1—P1	116.740 (10)	C21—C20—H20	119.8
P3—Ag1—S1	117.910 (10)	C22—C21—C20	120.37 (11)
P1—Ag1—S1	102.412 (10)	C22—C21—H21	119.8
P3—Ag1—P2	108.367 (9)	C20—C21—H21	119.8
P1—Ag1—P2	115.139 (10)	C21—C22—C23	119.56 (11)
S1—Ag1—P2	94.327 (10)	C21—C22—H22	120.2
C55—S1—Ag1	106.68 (4)	C23—C22—H22	120.2
C13B—P1—C1	102.52 (6)	C24—C23—C22	120.28 (12)
C13—P1—C1	102.52 (6)	C24—C23—H23	119.9
C13B—P1—C7	105.70 (5)	C22—C23—H23	119.9
C13—P1—C7	105.70 (5)	C23—C24—C19	120.43 (11)
C1—P1—C7	103.09 (5)	C23—C24—H24	119.8
C13B—P1—Ag1	109.11 (4)	C19—C24—H24	119.8
C13—P1—Ag1	109.11 (4)	C26—C25—C30	118.51 (11)
C1—P1—Ag1	119.78 (4)	C26—C25—P2	123.54 (9)
C7—P1—Ag1	115.14 (4)	C30—C25—P2	117.94 (9)
C19—P2—C31	100.41 (5)	C27—C26—C25	120.45 (12)
C19—P2—C25	103.84 (5)	C27—C26—H26	119.8
C31—P2—C25	102.54 (5)	C25—C26—H26	119.8

C19—P2—Ag1	109.78 (4)	C28—C27—C26	120.65 (13)
C31—P2—Ag1	111.23 (4)	C28—C27—H27	119.7
C25—P2—Ag1	125.94 (4)	C26—C27—H27	119.7
C37—P3—C43	105.88 (5)	C27—C28—C29	119.33 (12)
C37—P3—C49	102.96 (5)	C27—C28—H28	120.3
C43—P3—C49	101.06 (5)	C29—C28—H28	120.3
C37—P3—Ag1	108.38 (3)	C28—C29—C30	120.30 (12)
C43—P3—Ag1	116.69 (3)	C28—C29—H29	119.9
C49—P3—Ag1	120.25 (3)	C30—C29—H29	119.9
C6—C1—C2	118.94 (11)	C29—C30—C25	120.76 (11)
C6—C1—P1	123.49 (9)	C29—C30—H30	119.6
C2—C1—P1	117.57 (8)	C25—C30—H30	119.6
C3—C2—C1	120.86 (10)	C32—C31—C36	119.10 (11)
C3—C2—H2	119.6	C32—C31—P2	124.34 (10)
C1—C2—H2	119.6	C36—C31—P2	116.55 (9)
C2—C3—C4	119.93 (11)	C31—C32—C33	120.21 (13)
C2—C3—H3	120.0	C31—C32—H32	119.9
C4—C3—H3	120.0	C33—C32—H32	119.9
C5—C4—C3	119.55 (11)	C34—C33—C32	120.32 (14)
C5—C4—H4	120.2	C34—C33—H33	119.8
C3—C4—H4	120.2	C32—C33—H33	119.8
C4—C5—C6	120.81 (11)	C35—C34—C33	119.58 (13)
C4—C5—H5	119.6	C35—C34—H34	120.2
C6—C5—H5	119.6	C33—C34—H34	120.2
C5—C6—C1	119.92 (11)	C34—C35—C36	120.39 (13)
C5—C6—H6	120.0	C34—C35—H35	119.8
C1—C6—H6	120.0	C36—C35—H35	119.8
C12—C7—C8	119.12 (10)	C35—C36—C31	120.40 (12)
C12—C7—P1	122.89 (9)	C35—C36—H36	119.8
C8—C7—P1	117.98 (9)	C31—C36—H36	119.8
C9—C8—C7	120.35 (12)	C42—C37—C38	119.01 (10)
C9—C8—H8	119.8	C42—C37—P3	123.43 (9)
C7—C8—H8	119.8	C38—C37—P3	117.51 (8)
C10—C9—C8	120.07 (12)	C39—C38—C37	120.56 (11)
C10—C9—H9	120.0	C39—C38—H38	119.7
C8—C9—H9	120.0	C37—C38—H38	119.7
C11—C10—C9	119.77 (11)	C40—C39—C38	120.25 (12)
C11—C10—H10	120.1	C40—C39—H39	119.9
C9—C10—H10	120.1	C38—C39—H39	119.9
C10—C11—C12	120.48 (12)	C41—C40—C39	119.55 (11)
C10—C11—H11	119.8	C41—C40—H40	120.2
C12—C11—H11	119.8	C39—C40—H40	120.2
C7—C12—C11	120.19 (11)	C40—C41—C42	120.67 (12)
C7—C12—H12	119.9	C40—C41—H41	119.7
C11—C12—H12	119.9	C42—C41—H41	119.7
C18—C13—C14	119.2 (3)	C37—C42—C41	119.92 (11)
C18—C13—P1	118.50 (19)	C37—C42—H42	120.0
C14—C13—P1	122.1 (2)	C41—C42—H42	120.0

C13—C14—C15	119.7 (4)	C44—C43—C48	119.38 (10)
C13—C14—H14	120.2	C44—C43—P3	118.88 (8)
C15—C14—H14	120.2	C48—C43—P3	121.69 (8)
C16—C15—C14	120.6 (4)	C43—C44—C45	120.25 (11)
C16—C15—H15	119.7	C43—C44—H44	119.9
C14—C15—H15	119.7	C45—C44—H44	119.9
C15—C16—C17	120.1 (4)	C46—C45—C44	120.13 (12)
C15—C16—H16	120.0	C46—C45—H45	119.9
C17—C16—H16	120.0	C44—C45—H45	119.9
C16—C17—C18	120.0 (4)	C47—C46—C45	119.84 (11)
C16—C17—H17	120.0	C47—C46—H46	120.1
C18—C17—H17	120.0	C45—C46—H46	120.1
C13—C18—C17	120.5 (3)	C46—C47—C48	120.39 (11)
C13—C18—H18	119.7	C46—C47—H47	119.8
C17—C18—H18	119.7	C48—C47—H47	119.8
C14B—C13B—C18B	118.0 (6)	C47—C48—C43	120.00 (11)
C14B—C13B—P1	127.7 (5)	C47—C48—H48	120.0
C18B—C13B—P1	114.2 (4)	C43—C48—H48	120.0
C13B—C14B—C15B	119.9 (9)	C54—C49—C50	119.03 (10)
C13B—C14B—H14B	120.1	C54—C49—P3	124.13 (8)
C15B—C14B—H14B	120.1	C50—C49—P3	116.84 (8)
C16B—C15B—C14B	121.1 (11)	C51—C50—C49	120.58 (10)
C16B—C15B—H15B	119.4	C51—C50—H50	119.7
C14B—C15B—H15B	119.4	C49—C50—H50	119.7
C17B—C16B—C15B	119.7 (12)	C50—C51—C52	120.17 (11)
C17B—C16B—H16B	120.2	C50—C51—H51	119.9
C15B—C16B—H16B	120.2	C52—C51—H51	119.9
C16B—C17B—C18B	119.9 (9)	C53—C52—C51	119.53 (11)
C16B—C17B—H17B	120.0	C53—C52—H52	120.2
C18B—C17B—H17B	120.0	C51—C52—H52	120.2
C17B—C18B—C13B	121.3 (8)	C52—C53—C54	120.48 (11)
C17B—C18B—H18B	119.4	C52—C53—H53	119.8
C13B—C18B—H18B	119.4	C54—C53—H53	119.8
C20—C19—C24	119.05 (10)	C53—C54—C49	120.18 (10)
C20—C19—P2	118.61 (9)	C53—C54—H54	119.9
C24—C19—P2	122.33 (9)	C49—C54—H54	119.9
C19—C20—C21	120.31 (11)	N1—C55—S1	177.60 (13)
C19—C20—H20	119.8		
C13B—P1—C1—C6	-103.90 (10)	C20—C19—C24—C23	-1.31 (19)
C13—P1—C1—C6	-103.90 (10)	P2—C19—C24—C23	179.88 (11)
C7—P1—C1—C6	5.75 (11)	C19—P2—C25—C26	12.39 (13)
Ag1—P1—C1—C6	135.21 (9)	C31—P2—C25—C26	-91.82 (12)
C13B—P1—C1—C2	75.74 (10)	Ag1—P2—C25—C26	139.91 (10)
C13—P1—C1—C2	75.74 (10)	C19—P2—C25—C30	-168.95 (9)
C7—P1—C1—C2	-174.62 (9)	C31—P2—C25—C30	86.84 (10)
Ag1—P1—C1—C2	-45.15 (10)	Ag1—P2—C25—C30	-41.43 (11)
C6—C1—C2—C3	0.00 (17)	C30—C25—C26—C27	-0.9 (2)

P1—C1—C2—C3	-179.65 (9)	P2—C25—C26—C27	177.74 (12)
C1—C2—C3—C4	-0.25 (18)	C25—C26—C27—C28	0.1 (2)
C2—C3—C4—C5	0.27 (18)	C26—C27—C28—C29	0.5 (2)
C3—C4—C5—C6	-0.05 (19)	C27—C28—C29—C30	-0.3 (2)
C4—C5—C6—C1	-0.21 (19)	C28—C29—C30—C25	-0.5 (2)
C2—C1—C6—C5	0.23 (18)	C26—C25—C30—C29	1.09 (19)
P1—C1—C6—C5	179.86 (9)	P2—C25—C30—C29	-177.64 (10)
C13B—P1—C7—C12	6.14 (12)	C19—P2—C31—C32	-125.88 (13)
C13—P1—C7—C12	6.14 (12)	C25—P2—C31—C32	-19.02 (13)
C1—P1—C7—C12	-101.11 (11)	Ag1—P2—C31—C32	117.98 (12)
Ag1—P1—C7—C12	126.64 (10)	C19—P2—C31—C36	55.53 (10)
C13B—P1—C7—C8	-172.97 (10)	C25—P2—C31—C36	162.39 (9)
C13—P1—C7—C8	-172.97 (10)	Ag1—P2—C31—C36	-60.61 (10)
C1—P1—C7—C8	79.78 (11)	C36—C31—C32—C33	-0.1 (2)
Ag1—P1—C7—C8	-52.48 (11)	P2—C31—C32—C33	-178.61 (14)
C12—C7—C8—C9	-0.6 (2)	C31—C32—C33—C34	0.0 (3)
P1—C7—C8—C9	178.56 (11)	C32—C33—C34—C35	-0.3 (3)
C7—C8—C9—C10	-0.6 (2)	C33—C34—C35—C36	0.7 (2)
C8—C9—C10—C11	1.1 (2)	C34—C35—C36—C31	-0.7 (2)
C9—C10—C11—C12	-0.3 (2)	C32—C31—C36—C35	0.4 (2)
C8—C7—C12—C11	1.33 (19)	P2—C31—C36—C35	179.11 (10)
P1—C7—C12—C11	-177.77 (10)	C43—P3—C37—C42	-7.22 (11)
C10—C11—C12—C7	-0.9 (2)	C49—P3—C37—C42	-112.89 (10)
C1—P1—C13—C18	-152.3 (3)	Ag1—P3—C37—C42	118.70 (9)
C7—P1—C13—C18	100.1 (3)	C43—P3—C37—C38	175.41 (9)
Ag1—P1—C13—C18	-24.3 (3)	C49—P3—C37—C38	69.74 (9)
C1—P1—C13—C14	22.8 (3)	Ag1—P3—C37—C38	-58.67 (9)
C7—P1—C13—C14	-84.8 (3)	C42—C37—C38—C39	2.04 (17)
Ag1—P1—C13—C14	150.8 (3)	P3—C37—C38—C39	179.54 (9)
C18—C13—C14—C15	-0.7 (5)	C37—C38—C39—C40	-1.93 (19)
P1—C13—C14—C15	-175.8 (3)	C38—C39—C40—C41	0.29 (19)
C13—C14—C15—C16	-0.5 (7)	C39—C40—C41—C42	1.22 (19)
C14—C15—C16—C17	1.6 (9)	C38—C37—C42—C41	-0.54 (17)
C15—C16—C17—C18	-1.4 (9)	P3—C37—C42—C41	-177.87 (9)
C14—C13—C18—C17	0.9 (4)	C40—C41—C42—C37	-1.09 (18)
P1—C13—C18—C17	176.2 (2)	C37—P3—C43—C44	113.98 (9)
C16—C17—C18—C13	0.1 (5)	C49—P3—C43—C44	-138.98 (9)
C1—P1—C13B—C14B	7.8 (7)	Ag1—P3—C43—C44	-6.68 (11)
C7—P1—C13B—C14B	-99.8 (7)	C37—P3—C43—C48	-68.66 (10)
Ag1—P1—C13B—C14B	135.8 (7)	C49—P3—C43—C48	38.39 (10)
C1—P1—C13B—C18B	-169.6 (6)	Ag1—P3—C43—C48	170.68 (8)
C7—P1—C13B—C18B	82.8 (6)	C48—C43—C44—C45	0.08 (18)
Ag1—P1—C13B—C18B	-41.6 (6)	P3—C43—C44—C45	177.50 (10)
C18B—C13B—C14B—C15B	0.3 (11)	C43—C44—C45—C46	-0.72 (19)
P1—C13B—C14B—C15B	-177.0 (7)	C44—C45—C46—C47	0.9 (2)
C13B—C14B—C15B—C16B	1.2 (18)	C45—C46—C47—C48	-0.5 (2)
C14B—C15B—C16B—C17B	-2 (3)	C46—C47—C48—C43	-0.10 (19)
C15B—C16B—C17B—C18B	2 (2)	C44—C43—C48—C47	0.33 (18)

C16B—C17B—C18B—C13B	-0.8 (16)	P3—C43—C48—C47	-177.02 (9)
C14B—C13B—C18B—C17B	-0.5 (10)	C37—P3—C49—C54	-3.88 (11)
P1—C13B—C18B—C17B	177.1 (6)	C43—P3—C49—C54	-113.22 (10)
C31—P2—C19—C20	-143.05 (10)	Ag1—P3—C49—C54	116.70 (9)
C25—P2—C19—C20	111.13 (10)	C37—P3—C49—C50	175.99 (8)
Ag1—P2—C19—C20	-25.83 (10)	C43—P3—C49—C50	66.66 (9)
C31—P2—C19—C24	35.76 (11)	Ag1—P3—C49—C50	-63.42 (9)
C25—P2—C19—C24	-70.05 (11)	C54—C49—C50—C51	1.30 (17)
Ag1—P2—C19—C24	152.98 (9)	P3—C49—C50—C51	-178.58 (9)
C24—C19—C20—C21	0.92 (18)	C49—C50—C51—C52	-1.58 (18)
P2—C19—C20—C21	179.77 (10)	C50—C51—C52—C53	0.37 (18)
C19—C20—C21—C22	0.0 (2)	C51—C52—C53—C54	1.09 (18)
C20—C21—C22—C23	-0.5 (2)	C52—C53—C54—C49	-1.36 (17)
C21—C22—C23—C24	0.1 (2)	C50—C49—C54—C53	0.16 (16)
C22—C23—C24—C19	0.8 (2)	P3—C49—C54—C53	-179.96 (9)

*Hydrogen-bond geometry (Å, °)*

<i>D—H...A</i>	<i>D—H</i>	<i>H...A</i>	<i>D...A</i>	<i>D—H...A</i>
C3—H3...N1 <sup>i</sup>	0.95	2.63	3.2987 (19)	128
C40—H40...N1 <sup>ii</sup>	0.95	2.68	3.5540 (18)	153
C46—H46...N1 <sup>iii</sup>	0.95	2.52	3.3460 (18)	145

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