

Poly[[μ_3 -tris[2-(4-phenyl-1,2,3-triazol-1-yl)ethyl]amine]silver(I)] hexafluoridophosphate]

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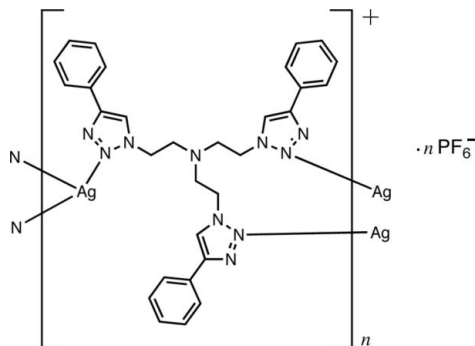
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Key indicators: single-crystal X-ray study; $T = 193$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.054; wR factor = 0.056; data-to-parameter ratio = 15.8.

The title compound, $\{[\text{Ag}(L)]\text{PF}_6\}_n$ [L is tris[2-(4-phenyl-1,2,3-triazol-1-yl)ethyl]amine, $\text{C}_{30}\text{H}_{30}\text{N}_{10}$], consists of alternating two-dimensional cationic layers of $[\text{Ag}(L)]^+$ and anionic PF_6^- layers. Each Ag^{I} atom is three coordinated in a T-shaped geometry by three N atoms from three ligands. Each ligand links three Ag^{I} atoms, generating a two-dimensional network structure with two different metallacycles, A and B . In A , eight coordination units from four ligands connect four Ag^{I} atoms, forming a 48-membered ring. In B , four coordination units from two ligands link two Ag^{I} atoms, forming a 24-membered ring. Each B ring is surrounded by four A rings, and each A ring has four A and four B rings as neighbours. This cationic layer thus generates a 4.8^2 topology network, with each Ag^{I} centre and ligand acting as a three-connected topological node.

Related literature

For related literature, see: Newkome *et al.* (1999); Robin & Fromm (2006); Ohi *et al.* (2004, 2005); Obata *et al.* (2008).



Experimental

Crystal data

$[\text{Ag}(\text{C}_{30}\text{H}_{30}\text{N}_{10})]\text{PF}_6$
 $M_r = 783.47$
 Monoclinic, $P2_1/n$
 $a = 14.893$ (3) Å
 $b = 14.935$ (3) Å
 $c = 15.735$ (3) Å
 $\beta = 112.646$ (5)°

$V = 3230.2$ (12) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.75$ mm⁻¹
 $T = 193.1$ K
 $0.30 \times 0.15 \times 0.05$ mm

Data collection

Rigaku Mercury diffractometer
 Absorption correction: multi-scan (Jacobson, 1998)
 $T_{\text{min}} = 0.776$, $T_{\text{max}} = 0.963$

31971 measured reflections
 7326 independent reflections
 4647 reflections with $F^2 > 2\sigma(F^2)$
 $R_{\text{int}} = 0.075$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.054$
 $wR(F^2) = 0.055$
 $S = 1.03$
 7326 reflections

463 parameters
 All H-atom parameters refined
 $\Delta\rho_{\text{max}} = 3.48$ e Å⁻³
 $\Delta\rho_{\text{min}} = -2.33$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Ag1—N4	2.208 (2)	Ag1—N10 ⁱⁱ	2.268 (2)
Ag1—N7 ⁱ	2.210 (3)		
N4—Ag1—N7 ⁱ	132.43 (10)	N7 ⁱ —Ag1—N10 ⁱⁱ	113.51 (10)
N4—Ag1—N10 ⁱⁱ	114.02 (10)		

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

Data collection: *CrystalClear* (Rigaku/MSC & Rigaku, 2006); cell refinement: *CrystalClear*; data reduction: *CrystalStructure*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *ORTEP III* (Burnett & Johnson, 1996); software used to prepare material for publication: *CrystalStructure* (Rigaku/MSC & Rigaku, 2006).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2780).

References

- Altomare, A., Burla, M. C., Camalli, M., Cascarano, G. L., Giacovazzo, C., Guagliardi, A., Moliterni, A. G. G., Polidori, G. & Spagna, R. (1999). *J. Appl. Cryst.* **32**, 115–119.
 Betteridge, P. W., Carruthers, J. R., Cooper, R. I., Prout, K. & Watkin, D. J. (2003). *J. Appl. Cryst.* **36**, 1487.
 Burnett, M. N. & Johnson, C. K. (1996). *ORTEP III*. Report ORNL-6895. Oak Ridge National Laboratory, Tennessee, USA.

- Jacobson, R. (1998). Private communication to the Rigaku Corporation, Tokyo, Japan.
- Newkome, G. R., He, E. & Moorefield, C. N. (1999). *Chem. Rev.* **183**, 1689–1746.
- Obata, M., Kitamura, A., Mori, A., Kameyama, C., Czaplewska, J. A., Tanaka, R., Kinoshita, I., Kusumoto, T., Hashimoto, H., Harada, M., Mikata, Y., Funabiki, T. & Yano, S. (2008). *Dalton Trans.* pp. 3292–3300.
- Ohi, H., Tachi, Y., Kunimoto, T. & Itoh, S. (2005). *Dalton Trans.* pp. 3146–3147.
- Rigaku/MSD & Rigaku (2006). *CrystalClear* and *CrystalStructure*. Rigaku/MSD, The Woodlands, Texas, USA, and Rigaku Corporation, Tokyo, Japan.
- Robin, A. & Fromm, K. (2006). *Coord. Chem. Rev.* **250**, 2127–2157.

supplementary materials

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Poly[[μ_3 -tris[2-(4-phenyl-1,2,3-triazol-1-yl)ethyl]amine}silver(I)] hexafluoridophosphate]

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Comment

Coordination polymer complexes have attracted much attention due to their various intriguing framework topologies and their unique properties such as magnetism, physical gas adsorption, ion-exchange, heterogeneous catalysis, and so on (Newkome *et al.*, 1999; Robin *et al.*, 2006). We have recently demonstrated that a C_3 symmetric tripodal tripyridine ligand consisting of a 1,3,5-triethylbenzene spacer can be adopted in coordination polymer chemistry to give one- and/or two-dimensional coordination polymer complexes with a variety of network topology (Ohi *et al.*, 2004, 2005). In this study, we synthesized a new C_3 symmetric ligand (L) consisting of triethylamine as the spacer and three 1,2,3-triazole groups as the metal binding site by using Huisgen reaction and used this ligand to synthesize a new Ag^{I} complex, $[\text{Ag}^{\text{I}}(L)](\text{PF}_6)_n$ (I). We report here the crystal structure of Ag^{I} complex.

In the title compound (I), the asymmetric unit contained one ligand molecular, one Ag^{I} ion, and one PF_6^- counterion. No solvent molecules were incorporated in the structure. As shown in Fig. 1, each Ag^{I} ion features a T-shaped coordination geometry, being coordinated by three nitrogen atoms from three ligands [$\text{Ag}-\text{N}$: 2.208 (2)–2.268 (2) Å; $\text{N}-\text{Ag}-\text{N}$: 113.51 (10)–132.43 (10)°], and each ligand links three Ag^{I} atoms to generate a two-dimensional network structure with two different metallacycles A and B. In A, eight coordination moieties from four ligands connected four Ag^{I} atoms to form a 48-membered ring. In B, four coordination moieties from two ligands link two Ag^{I} atoms to form 24-membered ring. Each B ring is surrounded by four A rings, and each A ring neighbors upon four A and four B rings. Thus, this sheet generates a rare 4.8^2 topology network with each Ag^{I} center and ligand acting as a three-connected topological node (Fig. 2a). The two-dimensional polymer sheets are stacked alternate arranging cationic two-dimensional layers of $[\text{Ag}^{\text{I}}(L)]^+$ and anionic (PF_6^-) layers to form laminated structure (Fig. 2b), where no specific interaction is probably between the sheets.

Experimental

The ligand tris((4-phenyl-1,2,3-triazole-1-yl)ethyl)amine (L) was synthesized by using Huisgen reaction, which is known as cycloaddition of azide and acetylene derivatives to give 1,2,3-triazole unit (Obata *et al.*, 2008). The title coordination complex, (I), was synthesized according to the following method. An acetone/ CHCl_3 ($v/v = 1/1$, 5 ml) solution of $\text{Ag}^{\text{I}}\text{PF}_6$ (50.6 mg, 2.0×10^{-4} mol) was added slowly to an acetone/ CHCl_3 ($v/v = 1/1$, 45 ml) solution of L (104.6 mg, 2.0×10^{-4} mol). After the mixture was stirred for 1 day under dark, the precipitate was collected by filtration to give white powder. This powder was dissolved in CH_3CN and insoluble materials were removed by filtration. The filtrate was concentrated under reduced pressure to give white powder (98.6 mg, yield 64%). Single crystals suitable for X-ray crystallographic analysis were obtained by recrystallization from $\text{CH}_3\text{CN}/\text{CHCl}_3$ ($v/v = 2/1$)/ Et_2O . Anal. Calcd. for $\text{C}_{30}\text{H}_{30}\text{AgF}_6\text{N}_{10}\text{P}$: C 45.99, H 3.86, N 17.88. Found: C 46.17, H 4.00, N 17.80.

Refinement

Hydrogen atoms were positioned geometrically (C—H = 0.95 Å) and refined using a riding model with $U(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Figures

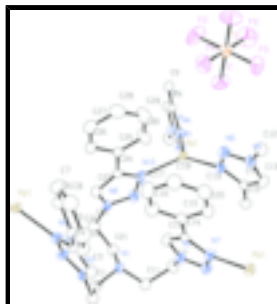


Fig. 1. The coordination geometry of the Ag^{I} atom and the ligated mode of L in the title compound. Displacement ellipsoids are drawn at the 50% probability level. H atoms omitted for clarity.

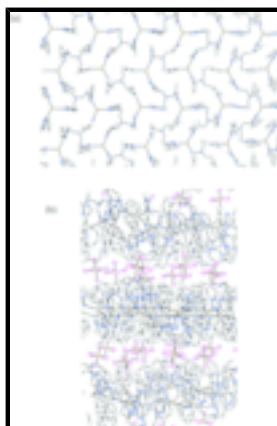


Fig. 2. (a) Two-dimensional 4.8^2 topology network with 24-membered and 48-membered metallacycles. (b). Three-dimensional packing diagram, showing the alternate arrangement of cationic layers (black) and anionic layers (pink).

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Crystal data

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$M_r = 783.47$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 14.893(3) \text{ \AA}$

$b = 14.935(3) \text{ \AA}$

$c = 15.735(3) \text{ \AA}$

$\beta = 112.646(5)^\circ$

$V = 3230.2(12) \text{ \AA}^3$

$Z = 4$

$F_{000} = 1584.00$

$D_x = 1.611 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71070 \text{ \AA}$

Cell parameters from 9566 reflections

$\theta = 4.0\text{--}27.5^\circ$

$\mu = 0.75 \text{ mm}^{-1}$

$T = 193.1 \text{ K}$

Platelet, colourless

$0.30 \times 0.15 \times 0.05 \text{ mm}$

Data collection

Rigaku Mercury diffractometer	4647 reflections with $F^2 > 2\sigma(F^2)$
Detector resolution: 7.31 pixels mm^{-1}	$R_{\text{int}} = 0.075$
ω scans	$\theta_{\text{max}} = 27.5^\circ$
Absorption correction: multi-scan (Jacobson, 1998)	$h = -19 \rightarrow 16$
$T_{\text{min}} = 0.776$, $T_{\text{max}} = 0.963$	$k = -19 \rightarrow 19$
31971 measured reflections	$l = -20 \rightarrow 20$
7326 independent reflections	

Refinement

Refinement on F^2	All H-atom parameters refined
$R[F^2 > 2\sigma(F^2)] = 0.054$	$w = 1/[1.0000\sigma(F_o^2)]/(4F_o^2)$
$wR(F^2) = 0.055$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.03$	$\Delta\rho_{\text{max}} = 3.48 \text{ e } \text{\AA}^{-3}$
7326 reflections	$\Delta\rho_{\text{min}} = -2.33 \text{ e } \text{\AA}^{-3}$
463 parameters	Extinction correction: none

Special details

Experimental. The ligand tris((4-phenyl-1,2,3-triazole-1-yl)ethyl)amine (*L*) was synthesized by using Huisgen reaction, which is known as cycloaddition of azide and acetylene derivatives to give 1,2,3-triazole unit. The conversion of tris(2-chloroethyl)amine (2.21 g, 10.9 mmol) into tris(2-azidoethyl)amine was achieved by addition of 3 mole equivalents of sodium azide to tris(2-chloroethyl)amine in dimethylformamide under stirring at 80 °C. To the THF (100 ml) and water (100 ml) solution of crude tris(2-azidoethyl)amine obtained and phenylacetylene (2.57 g, 25.2 mmol) was added 1 *M* sodium ascorbate (aq) (0.9 ml) and 7.5 wt% CuSO_4 (aq) (2.5 ml) and the mixture was stirred at 50 °C for 1 day. After concentration under reduced pressure, the resulting residue was then suspended in CHCl_3 , to which an aqueous solution of NH_3 was successively added. After washing the organic layer with the NH_3 aqueous solution, the organic layer was dried over anhydrous Na_2SO_4 and concentrated by evaporation. The resulting residue was purified by silica gel column chromatography (eluent; from CHCl_3 to ethyl acetate). The organic materials having $R_f = 0.21$ (eluent; ethyl acetate) were collected (1.73 g, yield 37%). ^1H NMR (CDCl_3 , 400 MHz): δ 3.33 (dt, 6H, $J = 4.8, 2.4$ Hz, N— CH_2CH_2 –), 4.10 (dt, 6H, $J = 4.8, 2.4$ Hz, N— CH_2CH_2 –), 6.80 (s, 3H, triazole-*H*), 7.00 (t, 6H, $J = 7.6$ Hz Ar-3*H*, 5*H*), 7.18 (tt, 3H, $J = 7.6, 1.2$ Hz, Ar-4*H*), 7.27 (d, 3H, $J = 7.6$ Hz, Ar-2*H* or 6*H*), 7.28 (d, 3H, $J = 7.6$ Hz, Ar-2*H* or 6*H*). HRMS (FAB, pos): $m/z = 531.2729$ calcd for $[\text{L} + \text{H}]^+$, $\text{C}_{30}\text{H}_{31}\text{N}_{10}$, 531.2733.

Geometry. ENTER SPECIAL DETAILS OF THE MOLECULAR GEOMETRY

Refinement. Refinement was performed using all reflections. The weighted *R*-factor (wR) and goodness of fit (*S*) are based on F^2 . *R*-factor (gt) are based on *F*. The threshold expression of $F^2 > 2.0 \sigma(F^2)$ is used only for calculating *R*-factor (gt).

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Ag(1)	0.45614 (2)	0.23636 (2)	0.47433 (2)	0.02556 (7)
P(1)	0.72081 (8)	0.21389 (8)	0.19893 (9)	0.0300 (3)

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F(1)	0.78327 (16)	0.23364 (19)	0.13875 (17)	0.0552 (8)
F(2)	0.65821 (18)	0.19439 (16)	0.25993 (18)	0.0492 (9)
F(3)	0.7415 (2)	0.31311 (17)	0.2382 (2)	0.0583 (10)
F(4)	0.81644 (17)	0.17994 (18)	0.28073 (17)	0.0477 (8)
F(5)	0.70048 (18)	0.11394 (16)	0.15986 (17)	0.0475 (8)
F(6)	0.62526 (17)	0.2473 (2)	0.11681 (17)	0.0628 (9)
N(1)	0.0406 (2)	0.4073 (2)	0.3528 (2)	0.0209 (9)
N(2)	0.2601 (2)	0.4507 (2)	0.4393 (2)	0.0264 (10)
N(3)	0.2869 (2)	0.3656 (2)	0.4548 (2)	0.0249 (10)
N(4)	0.3631 (2)	0.3565 (2)	0.4315 (2)	0.0223 (9)
N(5)	-0.0085 (2)	0.5197 (2)	0.1746 (2)	0.0258 (10)
N(6)	-0.0277 (2)	0.5971 (2)	0.1282 (2)	0.0303 (10)
N(7)	0.0412 (2)	0.6093 (2)	0.0966 (2)	0.0242 (9)
N(8)	0.0859 (2)	0.2467 (2)	0.26377 (19)	0.0231 (9)
N(9)	0.0191 (2)	0.2593 (2)	0.1787 (2)	0.0265 (9)
N(10)	0.06704 (19)	0.2581 (2)	0.1214 (2)	0.0214 (8)
C(1)	0.1011 (2)	0.4214 (2)	0.4501 (2)	0.0245 (11)
C(2)	0.1823 (3)	0.4872 (2)	0.4670 (3)	0.0290 (13)
C(3)	0.3162 (3)	0.4970 (2)	0.4061 (2)	0.0258 (12)
C(4)	0.3837 (2)	0.4368 (2)	0.4008 (2)	0.0196 (10)
C(5)	0.4644 (2)	0.4490 (2)	0.3710 (2)	0.0216 (11)
C(6)	0.5077 (3)	0.3770 (2)	0.3441 (3)	0.0320 (13)
C(7)	0.5821 (3)	0.3898 (2)	0.3148 (3)	0.0355 (13)
C(8)	0.6151 (3)	0.4762 (2)	0.3095 (3)	0.0339 (13)
C(9)	0.5733 (3)	0.5481 (2)	0.3355 (3)	0.0334 (13)
C(10)	0.4994 (2)	0.5343 (2)	0.3659 (2)	0.0262 (12)
C(11)	-0.0307 (2)	0.4794 (2)	0.3191 (2)	0.0275 (12)
C(12)	-0.0760 (3)	0.4862 (2)	0.2144 (2)	0.0292 (12)
C(13)	0.0726 (3)	0.4829 (2)	0.1727 (2)	0.0289 (12)
C(14)	0.1058 (2)	0.5395 (2)	0.1229 (2)	0.0213 (11)
C(15)	0.1908 (3)	0.5339 (2)	0.0964 (3)	0.0260 (12)
C(16)	0.2701 (3)	0.4828 (2)	0.1481 (3)	0.0338 (13)
C(17)	0.3512 (3)	0.4771 (3)	0.1237 (3)	0.0435 (15)
C(18)	0.3528 (3)	0.5245 (3)	0.0501 (3)	0.0378 (14)
C(19)	0.2756 (3)	0.5757 (2)	-0.0014 (3)	0.0373 (14)
C(20)	0.1933 (3)	0.5808 (2)	0.0213 (3)	0.0330 (13)
C(21)	-0.0095 (2)	0.3209 (2)	0.3415 (2)	0.0264 (12)
C(22)	0.0557 (2)	0.2428 (2)	0.3421 (2)	0.0305 (11)
C(23)	0.1756 (2)	0.2375 (2)	0.2625 (2)	0.0246 (10)
C(24)	0.1642 (2)	0.2460 (2)	0.1730 (2)	0.0186 (9)
C(25)	0.2370 (2)	0.2422 (2)	0.1313 (2)	0.0229 (10)
C(26)	0.3333 (2)	0.2192 (2)	0.1856 (2)	0.0300 (12)
C(27)	0.4044 (2)	0.2207 (2)	0.1484 (2)	0.0348 (13)
C(28)	0.3802 (2)	0.2411 (3)	0.0577 (3)	0.0398 (13)
C(29)	0.2856 (3)	0.2615 (3)	0.0021 (2)	0.0463 (14)
C(30)	0.2140 (2)	0.2632 (3)	0.0378 (2)	0.0371 (12)
H(1)	0.0609	0.4411	0.4809	0.031*
H(2)	0.1300	0.3657	0.4752	0.031*
H(3)	0.2097	0.5019	0.5306	0.035*

H(4)	0.1560	0.5396	0.4320	0.035*
H(5)	0.3109	0.5585	0.3894	0.030*
H(6)	0.4843	0.3180	0.3456	0.038*
H(7)	0.6119	0.3401	0.2984	0.043*
H(8)	0.6660	0.4853	0.2882	0.042*
H(9)	0.5956	0.6070	0.3318	0.039*
H(10)	0.4713	0.5841	0.3842	0.032*
H(11)	-0.0812	0.4703	0.3410	0.033*
H(12)	0.0015	0.5343	0.3426	0.033*
H(13)	-0.1302	0.5256	0.1973	0.034*
H(14)	-0.0975	0.4283	0.1902	0.035*
H(15)	0.1018	0.4283	0.2008	0.034*
H(16)	0.2699	0.4520	0.2009	0.042*
H(17)	0.4051	0.4408	0.1587	0.051*
H(18)	0.4077	0.5204	0.0335	0.046*
H(19)	0.2777	0.6090	-0.0521	0.046*
H(20)	0.1390	0.6162	-0.0148	0.038*
H(21)	-0.0344	0.3136	0.3883	0.033*
H(22)	-0.0618	0.3215	0.2829	0.033*
H(23)	0.0215	0.1885	0.3391	0.038*
H(24)	0.1117	0.2447	0.3979	0.038*
H(25)	0.2345	0.2270	0.3140	0.029*
H(26)	0.3498	0.2023	0.2480	0.033*
H(27)	0.4700	0.2075	0.1866	0.041*
H(28)	0.4292	0.2411	0.0330	0.049*
H(29)	0.2695	0.2747	-0.0612	0.056*
H(30)	0.1488	0.2782	-0.0003	0.043*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag(1)	0.02591 (16)	0.01924 (15)	0.02906 (17)	0.00118 (17)	0.00786 (13)	-0.00264 (17)
P(1)	0.0251 (6)	0.0333 (7)	0.0370 (7)	0.0018 (5)	0.0179 (5)	-0.0044 (5)
F(1)	0.0571 (16)	0.0648 (18)	0.0679 (18)	0.0167 (16)	0.0508 (15)	0.0146 (17)
F(2)	0.0509 (16)	0.0533 (17)	0.066 (2)	-0.0082 (13)	0.0474 (15)	-0.0081 (14)
F(3)	0.059 (2)	0.0343 (16)	0.100 (2)	-0.0089 (14)	0.0517 (19)	-0.0210 (15)
F(4)	0.0291 (15)	0.0657 (19)	0.0396 (16)	-0.0025 (13)	0.0036 (13)	-0.0018 (13)
F(5)	0.0530 (17)	0.0392 (16)	0.0500 (17)	-0.0004 (13)	0.0195 (14)	-0.0172 (13)
F(6)	0.0385 (14)	0.073 (2)	0.0681 (18)	0.0214 (17)	0.0110 (13)	0.0161 (18)
N(1)	0.0190 (18)	0.0246 (19)	0.0191 (18)	0.0041 (14)	0.0073 (15)	0.0046 (14)
N(2)	0.0191 (19)	0.027 (2)	0.032 (2)	0.0078 (15)	0.0085 (17)	-0.0015 (16)
N(3)	0.025 (2)	0.0202 (19)	0.028 (2)	0.0007 (15)	0.0092 (17)	-0.0004 (15)
N(4)	0.0207 (18)	0.0194 (18)	0.027 (2)	-0.0013 (14)	0.0091 (16)	-0.0030 (15)
N(5)	0.027 (2)	0.024 (2)	0.024 (2)	-0.0012 (16)	0.0073 (17)	0.0025 (16)
N(6)	0.033 (2)	0.028 (2)	0.027 (2)	0.0027 (17)	0.0082 (18)	0.0069 (16)
N(7)	0.029 (2)	0.0230 (19)	0.0200 (19)	0.0010 (15)	0.0080 (16)	0.0034 (15)
N(8)	0.0319 (18)	0.0146 (19)	0.0206 (17)	0.0029 (15)	0.0076 (15)	0.0042 (15)
N(9)	0.0206 (16)	0.0262 (19)	0.0275 (18)	-0.0016 (16)	0.0035 (14)	0.0025 (17)

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N(10)	0.0153 (15)	0.0141 (17)	0.0324 (18)	-0.0031 (14)	0.0065 (14)	-0.0005 (15)
C(1)	0.023 (2)	0.036 (2)	0.019 (2)	0.0077 (19)	0.0132 (19)	0.0000 (19)
C(2)	0.026 (2)	0.037 (2)	0.026 (2)	0.009 (2)	0.012 (2)	-0.002 (2)
C(3)	0.029 (2)	0.021 (2)	0.025 (2)	-0.0017 (18)	0.008 (2)	0.0042 (18)
C(4)	0.020 (2)	0.016 (2)	0.019 (2)	0.0022 (16)	0.0027 (18)	0.0006 (16)
C(5)	0.022 (2)	0.017 (2)	0.024 (2)	0.0005 (17)	0.0068 (19)	-0.0013 (17)
C(6)	0.033 (2)	0.023 (2)	0.039 (2)	-0.0044 (19)	0.012 (2)	-0.004 (2)
C(7)	0.028 (2)	0.034 (2)	0.045 (3)	0.003 (2)	0.015 (2)	-0.006 (2)
C(8)	0.024 (2)	0.041 (2)	0.040 (2)	-0.004 (2)	0.016 (2)	0.001 (2)
C(9)	0.028 (2)	0.026 (2)	0.044 (2)	-0.007 (2)	0.011 (2)	-0.002 (2)
C(10)	0.026 (2)	0.022 (2)	0.033 (2)	0.0018 (18)	0.013 (2)	0.0001 (19)
C(11)	0.023 (2)	0.030 (2)	0.029 (2)	0.0057 (19)	0.0093 (19)	0.0033 (19)
C(12)	0.026 (2)	0.034 (2)	0.026 (2)	0.0013 (19)	0.009 (2)	0.003 (2)
C(13)	0.034 (2)	0.020 (2)	0.031 (2)	0.0055 (19)	0.010 (2)	0.0060 (19)
C(14)	0.028 (2)	0.016 (2)	0.016 (2)	-0.0004 (18)	0.0034 (19)	-0.0009 (16)
C(15)	0.030 (2)	0.020 (2)	0.025 (2)	-0.0051 (19)	0.006 (2)	-0.0044 (18)
C(16)	0.037 (2)	0.032 (2)	0.035 (2)	-0.002 (2)	0.018 (2)	0.007 (2)
C(17)	0.037 (2)	0.048 (3)	0.042 (3)	0.010 (2)	0.012 (2)	0.009 (2)
C(18)	0.029 (2)	0.046 (3)	0.040 (2)	0.002 (2)	0.014 (2)	0.000 (2)
C(19)	0.049 (3)	0.031 (2)	0.036 (2)	-0.006 (2)	0.020 (2)	0.003 (2)
C(20)	0.040 (2)	0.026 (2)	0.029 (2)	0.000 (2)	0.009 (2)	0.006 (2)
C(21)	0.025 (2)	0.031 (2)	0.026 (2)	0.0000 (19)	0.0136 (19)	0.0095 (19)
C(22)	0.041 (2)	0.027 (2)	0.028 (2)	-0.001 (2)	0.018 (2)	0.004 (2)
C(23)	0.020 (2)	0.029 (2)	0.024 (2)	0.004 (2)	0.0074 (17)	0.003 (2)
C(24)	0.0205 (19)	0.009 (2)	0.0212 (19)	-0.0041 (16)	0.0022 (16)	-0.0047 (16)
C(25)	0.0212 (19)	0.021 (2)	0.023 (2)	-0.0004 (18)	0.0052 (16)	-0.0066 (19)
C(26)	0.026 (2)	0.026 (2)	0.030 (2)	0.0029 (19)	0.003 (2)	0.0026 (19)
C(27)	0.020 (2)	0.041 (2)	0.040 (2)	0.005 (2)	0.008 (2)	-0.005 (2)
C(28)	0.030 (2)	0.051 (3)	0.042 (2)	-0.004 (2)	0.019 (2)	-0.011 (2)
C(29)	0.039 (2)	0.072 (3)	0.029 (2)	-0.006 (2)	0.014 (2)	0.002 (2)
C(30)	0.025 (2)	0.058 (2)	0.024 (2)	-0.005 (2)	0.0050 (18)	0.003 (2)

Geometric parameters (Å, °)

Ag(1)—N(4)	2.208 (2)	C(17)—C(18)	1.365 (7)
Ag(1)—N(7) ⁱ	2.210 (3)	C(18)—C(19)	1.359 (5)
Ag(1)—N(10) ⁱⁱ	2.268 (2)	C(19)—C(20)	1.405 (8)
P(1)—F(1)	1.590 (3)	C(21)—C(22)	1.516 (5)
P(1)—F(2)	1.601 (3)	C(23)—C(24)	1.359 (5)
P(1)—F(3)	1.590 (2)	C(24)—C(25)	1.468 (6)
P(1)—F(4)	1.591 (2)	C(25)—C(26)	1.401 (4)
P(1)—F(5)	1.598 (2)	C(25)—C(30)	1.410 (5)
P(1)—F(6)	1.590 (2)	C(26)—C(27)	1.395 (7)
N(1)—C(1)	1.462 (4)	C(27)—C(28)	1.365 (6)
N(1)—C(11)	1.462 (4)	C(28)—C(29)	1.376 (5)
N(1)—C(21)	1.466 (4)	C(29)—C(30)	1.385 (7)
N(2)—N(3)	1.327 (4)	C(1)—H(1)	0.950
N(2)—C(2)	1.489 (6)	C(1)—H(2)	0.950
N(2)—C(3)	1.336 (6)	C(2)—H(3)	0.950

N(3)—N(4)	1.327 (5)	C(2)—H(4)	0.950
N(4)—C(4)	1.372 (5)	C(3)—H(5)	0.950
N(5)—N(6)	1.338 (4)	C(6)—H(6)	0.950
N(5)—C(12)	1.463 (6)	C(7)—H(7)	0.950
N(5)—C(13)	1.337 (6)	C(8)—H(8)	0.950
N(6)—N(7)	1.314 (6)	C(9)—H(9)	0.950
N(7)—C(14)	1.370 (4)	C(10)—H(10)	0.950
N(8)—N(9)	1.339 (3)	C(11)—H(11)	0.950
N(8)—C(22)	1.466 (5)	C(11)—H(12)	0.950
N(8)—C(23)	1.350 (5)	C(12)—H(13)	0.950
N(9)—N(10)	1.349 (5)	C(12)—H(14)	0.950
N(10)—C(24)	1.372 (3)	C(13)—H(15)	0.950
C(1)—C(2)	1.501 (5)	C(16)—H(16)	0.950
C(3)—C(4)	1.375 (6)	C(17)—H(17)	0.950
C(4)—C(5)	1.460 (6)	C(18)—H(18)	0.950
C(5)—C(6)	1.402 (6)	C(19)—H(19)	0.950
C(5)—C(10)	1.390 (5)	C(20)—H(20)	0.950
C(6)—C(7)	1.368 (7)	C(21)—H(21)	0.950
C(7)—C(8)	1.394 (6)	C(21)—H(22)	0.950
C(8)—C(9)	1.381 (6)	C(22)—H(23)	0.950
C(9)—C(10)	1.374 (7)	C(22)—H(24)	0.950
C(11)—C(12)	1.524 (5)	C(23)—H(25)	0.950
C(13)—C(14)	1.368 (6)	C(26)—H(26)	0.950
C(14)—C(15)	1.479 (7)	C(27)—H(27)	0.950
C(15)—C(16)	1.379 (5)	C(28)—H(28)	0.950
C(15)—C(20)	1.386 (6)	C(29)—H(29)	0.950
C(16)—C(17)	1.404 (8)	C(30)—H(30)	0.950
F(1)···N(3) ⁱⁱⁱ	3.271 (4)	N(10)···H(20) ^{ix}	3.433
F(1)···N(9) ^{iv}	3.343 (3)	C(4)···H(10) ^{vii}	3.253
F(1)···C(9) ^v	3.427 (5)	C(7)···H(3) ^{vii}	3.513
F(1)···C(19) ^{vi}	3.477 (5)	C(8)···H(3) ^{vii}	2.863
F(2)···N(6) ⁱ	3.409 (5)	C(9)···H(3) ^{vii}	3.195
F(2)···C(7)	3.362 (5)	C(11)···H(1) ^{xiii}	3.550
F(2)···C(12) ⁱ	3.421 (5)	C(12)···H(19) ^{ix}	3.414
F(2)···C(27)	3.523 (4)	C(12)···H(20) ^{ix}	3.289
F(3)···C(7)	3.256 (6)	C(13)···H(20) ^{ix}	3.502
F(3)···C(8)	3.516 (5)	C(19)···H(13) ^{ix}	3.368
F(3)···C(21) ^{iv}	3.430 (4)	C(19)···H(14) ^{ix}	3.131
F(4)···C(9) ^v	3.498 (5)	C(20)···H(13) ^{ix}	3.572
F(4)···C(21) ^{iv}	3.188 (4)	C(20)···H(14) ^{ix}	3.079
F(4)···C(22) ^{iv}	3.445 (4)	C(21)···H(28) ^{viii}	3.591
F(5)···C(1) ⁱⁱⁱ	3.099 (4)	C(28)···H(21) ⁱⁱⁱ	3.465
F(5)···C(2) ⁱⁱⁱ	3.307 (5)	H(1)···F(5) ^{viii}	2.901
F(5)···C(8) ^v	3.316 (5)	H(1)···F(6) ^{viii}	3.440
F(5)···C(9) ^v	3.484 (5)	H(1)···C(11) ^{xiii}	3.550

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F(5)···C(11) ⁱ	3.345 (5)	H(1)···H(1) ^{xiii}	2.754
F(6)···C(1) ⁱⁱⁱ	3.554 (4)	H(1)···H(11) ^{xiii}	3.006
F(6)···C(27)	3.533 (5)	H(1)···H(12) ^{xiii}	3.271
F(6)···C(28)	3.403 (4)	H(2)···P(1) ^{viii}	3.460
N(2)···C(9) ^{vii}	3.456 (4)	H(2)···F(1) ^{viii}	3.084
N(3)···F(1) ^{viii}	3.271 (4)	H(2)···F(5) ^{viii}	2.700
N(3)···C(9) ^{vii}	3.405 (4)	H(2)···F(6) ^{viii}	2.818
N(4)···C(10) ^{vii}	3.463 (4)	H(3)···F(5) ^{viii}	2.714
N(5)···C(20) ^{ix}	3.578 (4)	H(3)···C(7) ^{vii}	3.513
N(6)···F(2) ^x	3.409 (5)	H(3)···C(8) ^{vii}	2.863
N(9)···F(1) ^{xi}	3.343 (3)	H(3)···C(9) ^{vii}	3.195
C(1)···F(5) ^{viii}	3.099 (4)	H(3)···H(8) ^{vii}	2.744
C(1)···F(6) ^{viii}	3.554 (4)	H(3)···H(9) ^{vii}	3.303
C(2)···F(5) ^{viii}	3.307 (5)	H(3)···H(11) ^{xiii}	3.300
C(4)···C(10) ^{vii}	3.431 (5)	H(7)···P(1)	3.254
C(7)···F(2)	3.362 (5)	H(7)···F(2)	2.429
C(7)···F(3)	3.256 (6)	H(7)···F(3)	2.489
C(8)···F(3)	3.516 (5)	H(7)···F(6)	3.251
C(8)···F(5) ^{xii}	3.316 (5)	H(8)···F(3)	3.030
C(9)···F(1) ^{xii}	3.427 (5)	H(8)···F(4) ^{xii}	3.148
C(9)···F(4) ^{xii}	3.498 (5)	H(8)···F(5) ^{xii}	2.657
C(9)···F(5) ^{xii}	3.484 (5)	H(8)···H(3) ^{vii}	2.744
C(9)···N(2) ^{vii}	3.456 (4)	H(8)···H(11) ^{iv}	3.536
C(9)···N(3) ^{vii}	3.405 (4)	H(9)···P(1) ^{xii}	3.358
C(10)···N(4) ^{vii}	3.463 (4)	H(9)···F(1) ^{xii}	2.530
C(10)···C(4) ^{vii}	3.431 (5)	H(9)···F(4) ^{xii}	2.797
C(11)···F(5) ^x	3.345 (5)	H(9)···F(5) ^{xii}	2.990
C(12)···F(2) ^x	3.421 (5)	H(9)···N(2) ^{vii}	3.517
C(12)···C(20) ^{ix}	3.582 (5)	H(9)···N(3) ^{vii}	3.159
C(19)···F(1) ^{vi}	3.477 (5)	H(9)···N(4) ^{vii}	3.576
C(20)···N(5) ^{ix}	3.578 (4)	H(9)···H(3) ^{vii}	3.303
C(20)···C(12) ^{ix}	3.582 (5)	H(10)···Ag(1) ^{vii}	3.386
C(21)···F(3) ^{xi}	3.430 (4)	H(10)···N(3) ^{vii}	3.595
C(21)···F(4) ^{xi}	3.188 (4)	H(10)···N(4) ^{vii}	3.127
C(22)···F(4) ^{xi}	3.445 (4)	H(10)···C(4) ^{vii}	3.253
C(27)···F(2)	3.523 (4)	H(11)···F(3) ^{xi}	3.437
C(27)···F(6)	3.533 (5)	H(11)···F(5) ^x	2.782
C(28)···F(6)	3.403 (4)	H(11)···H(1) ^{xiii}	3.006
Ag(1)···H(10) ^{vii}	3.386	H(11)···H(3) ^{xiii}	3.300
P(1)···H(2) ⁱⁱⁱ	3.460	H(11)···H(8) ^{xi}	3.536
P(1)···H(7)	3.254	H(12)···F(2) ^x	3.320

P(1)···H(9) ^v	3.358	H(12)···F(5) ^x	3.221
P(1)···H(19) ^{vi}	3.519	H(12)···H(1) ^{xiii}	3.271
P(1)···H(22) ^{iv}	3.394	H(13)···F(2) ^x	2.682
P(1)···H(29) ⁱⁱ	3.564	H(13)···F(5) ^x	3.114
F(1)···H(2) ⁱⁱⁱ	3.084	H(13)···C(19) ^{ix}	3.368
F(1)···H(9) ^v	2.530	H(13)···C(20) ^{ix}	3.572
F(1)···H(14) ^{iv}	3.340	H(13)···H(19) ^{ix}	3.198
F(1)···H(19) ^{vi}	2.694	H(13)···H(20) ^{ix}	3.530
F(1)···H(20) ^{vi}	3.451	H(14)···F(1) ^{xi}	3.340
F(1)···H(22) ^{iv}	2.857	H(14)···F(3) ^{xi}	3.267
F(2)···H(7)	2.429	H(14)···C(19) ^{ix}	3.131
F(2)···H(12) ⁱ	3.320	H(14)···C(20) ^{ix}	3.079
F(2)···H(13) ⁱ	2.682	H(14)···H(19) ^{ix}	2.783
F(2)···H(27)	2.595	H(14)···H(20) ^{ix}	2.670
F(2)···H(29) ⁱⁱ	2.700	H(18)···H(18) ^{vi}	3.360
F(3)···H(7)	2.489	H(19)···P(1) ^{vi}	3.519
F(3)···H(8)	3.030	H(19)···F(1) ^{vi}	2.694
F(3)···H(11) ^{iv}	3.437	H(19)···F(3) ^{vi}	3.062
F(3)···H(14) ^{iv}	3.267	H(19)···F(6) ^{vi}	2.978
F(3)···H(19) ^{vi}	3.062	H(19)···C(12) ^{ix}	3.414
F(3)···H(21) ^{iv}	3.263	H(19)···H(13) ^{ix}	3.198
F(3)···H(22) ^{iv}	2.740	H(19)···H(14) ^{ix}	2.783
F(3)···H(29) ⁱⁱ	3.293	H(20)···F(1) ^{vi}	3.451
F(4)···H(8) ^v	3.148	H(20)···N(5) ^{ix}	3.234
F(4)···H(9) ^v	2.797	H(20)···N(9) ^{ix}	3.312
F(4)···H(21) ^{iv}	2.981	H(20)···N(10) ^{ix}	3.433
F(4)···H(22) ^{iv}	2.777	H(20)···C(12) ^{ix}	3.289
F(4)···H(23) ^{iv}	2.833	H(20)···C(13) ^{ix}	3.502
F(4)···H(29) ⁱⁱ	2.912	H(20)···H(13) ^{ix}	3.530
F(5)···H(1) ⁱⁱⁱ	2.901	H(20)···H(14) ^{ix}	2.670
F(5)···H(2) ⁱⁱⁱ	2.700	H(21)···F(3) ^{xi}	3.263
F(5)···H(3) ⁱⁱⁱ	2.714	H(21)···F(4) ^{xi}	2.981
F(5)···H(8) ^v	2.657	H(21)···F(6) ^{viii}	3.582
F(5)···H(9) ^v	2.990	H(21)···C(28) ^{viii}	3.465
F(5)···H(11) ⁱ	2.782	H(21)···H(28) ^{viii}	2.664
F(5)···H(12) ⁱ	3.221	H(21)···H(29) ^{viii}	3.563
F(5)···H(13) ⁱ	3.114	H(22)···P(1) ^{xi}	3.394
F(6)···H(1) ⁱⁱⁱ	3.440	H(22)···F(1) ^{xi}	2.857
F(6)···H(2) ⁱⁱⁱ	2.818	H(22)···F(3) ^{xi}	2.740
F(6)···H(7)	3.251	H(22)···F(4) ^{xi}	2.777
F(6)···H(19) ^{vi}	2.978	H(23)···F(4) ^{xi}	2.833

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F(6)···H(21) ⁱⁱⁱ	3.582	H(24)···F(6) ^{viii}	3.374
F(6)···H(24) ⁱⁱⁱ	3.374	H(27)···F(2)	2.595
F(6)···H(27)	2.977	H(27)···F(6)	2.977
F(6)···H(28)	2.703	H(28)···F(6)	2.703
N(2)···H(9) ^{vii}	3.517	H(28)···C(21) ⁱⁱⁱ	3.591
N(3)···H(9) ^{vii}	3.159	H(28)···H(21) ⁱⁱⁱ	2.664
N(3)···H(10) ^{vii}	3.595	H(29)···P(1) ^{xiv}	3.564
N(4)···H(9) ^{vii}	3.576	H(29)···F(2) ^{xiv}	2.700
N(4)···H(10) ^{vii}	3.127	H(29)···F(3) ^{xiv}	3.293
N(5)···H(20) ^{ix}	3.234	H(29)···F(4) ^{xiv}	2.912
N(6)···H(30) ^{ix}	2.825	H(29)···H(21) ⁱⁱⁱ	3.563
N(7)···H(30) ^{ix}	3.136	H(30)···N(6) ^{ix}	2.825
N(9)···H(20) ^{ix}	3.312	H(30)···N(7) ^{ix}	3.136
N(4)—Ag(1)—N(7) ⁱ	132.43 (10)	C(23)—C(24)—C(25)	129.9 (2)
N(4)—Ag(1)—N(10) ⁱⁱ	114.02 (10)	C(24)—C(25)—C(26)	119.7 (3)
N(7) ⁱ —Ag(1)—N(10) ⁱⁱ	113.51 (10)	C(24)—C(25)—C(30)	122.2 (3)
F(1)—P(1)—F(2)	179.70 (15)	C(26)—C(25)—C(30)	118.1 (4)
F(1)—P(1)—F(3)	89.34 (18)	C(25)—C(26)—C(27)	120.3 (3)
F(1)—P(1)—F(4)	89.67 (14)	C(26)—C(27)—C(28)	120.3 (3)
F(1)—P(1)—F(5)	90.68 (16)	C(27)—C(28)—C(29)	120.6 (4)
F(1)—P(1)—F(6)	90.20 (15)	C(28)—C(29)—C(30)	120.4 (4)
F(2)—P(1)—F(3)	90.39 (17)	C(25)—C(30)—C(29)	120.2 (3)
F(2)—P(1)—F(4)	90.20 (15)	N(1)—C(1)—H(1)	108.9
F(2)—P(1)—F(5)	89.59 (15)	N(1)—C(1)—H(2)	107.9
F(2)—P(1)—F(6)	89.93 (14)	C(2)—C(1)—H(1)	109.2
F(3)—P(1)—F(4)	90.18 (14)	C(2)—C(1)—H(2)	107.1
F(3)—P(1)—F(5)	179.69 (15)	H(1)—C(1)—H(2)	109.5
F(3)—P(1)—F(6)	90.13 (15)	N(2)—C(2)—H(3)	109.0
F(4)—P(1)—F(5)	89.51 (13)	N(2)—C(2)—H(4)	109.0
F(4)—P(1)—F(6)	179.66 (16)	C(1)—C(2)—H(3)	109.2
F(5)—P(1)—F(6)	90.17 (14)	C(1)—C(2)—H(4)	108.3
C(1)—N(1)—C(11)	110.0 (3)	H(3)—C(2)—H(4)	109.5
C(1)—N(1)—C(21)	109.5 (3)	N(2)—C(3)—H(5)	127.7
C(11)—N(1)—C(21)	109.9 (2)	C(4)—C(3)—H(5)	126.8
N(3)—N(2)—C(2)	120.7 (3)	C(5)—C(6)—H(6)	119.2
N(3)—N(2)—C(3)	112.2 (3)	C(7)—C(6)—H(6)	119.4
C(2)—N(2)—C(3)	126.8 (3)	C(6)—C(7)—H(7)	120.3
N(2)—N(3)—N(4)	106.0 (3)	C(8)—C(7)—H(7)	119.7
Ag(1)—N(4)—N(3)	120.1 (2)	C(7)—C(8)—H(8)	120.1
Ag(1)—N(4)—C(4)	128.3 (2)	C(9)—C(8)—H(8)	120.4
N(3)—N(4)—C(4)	109.8 (3)	C(8)—C(9)—H(9)	119.5
N(6)—N(5)—C(12)	119.4 (3)	C(10)—C(9)—H(9)	120.5
N(6)—N(5)—C(13)	110.4 (3)	C(5)—C(10)—H(10)	118.8
C(12)—N(5)—C(13)	130.1 (3)	C(9)—C(10)—H(10)	119.5
N(5)—N(6)—N(7)	106.9 (3)	N(1)—C(11)—H(11)	109.2
Ag(1) ^x —N(7)—N(6)	118.6 (2)	N(1)—C(11)—H(12)	107.9

Ag(1) ^x —N(7)—C(14)	131.2 (3)	C(12)—C(11)—H(11)	108.6
N(6)—N(7)—C(14)	110.0 (3)	C(12)—C(11)—H(12)	108.0
N(9)—N(8)—C(22)	119.7 (3)	H(11)—C(11)—H(12)	109.5
N(9)—N(8)—C(23)	111.0 (3)	N(5)—C(12)—H(13)	108.4
C(22)—N(8)—C(23)	129.3 (2)	N(5)—C(12)—H(14)	108.7
N(8)—N(9)—N(10)	106.6 (2)	C(11)—C(12)—H(13)	108.8
Ag(1) ^{xiv} —N(10)—N(9)	108.43 (17)	C(11)—C(12)—H(14)	108.2
Ag(1) ^{xiv} —N(10)—C(24)	142.8 (2)	H(13)—C(12)—H(14)	109.5
N(9)—N(10)—C(24)	108.4 (2)	N(5)—C(13)—H(15)	126.8
N(1)—C(1)—C(2)	114.2 (3)	C(14)—C(13)—H(15)	126.5
N(2)—C(2)—C(1)	111.9 (3)	C(15)—C(16)—H(16)	119.6
N(2)—C(3)—C(4)	105.5 (3)	C(17)—C(16)—H(16)	120.2
N(4)—C(4)—C(3)	106.4 (4)	C(16)—C(17)—H(17)	120.0
N(4)—C(4)—C(5)	123.0 (3)	C(18)—C(17)—H(17)	120.1
C(3)—C(4)—C(5)	130.5 (3)	C(17)—C(18)—H(18)	119.8
C(4)—C(5)—C(6)	122.2 (3)	C(19)—C(18)—H(18)	119.5
C(4)—C(5)—C(10)	120.4 (3)	C(18)—C(19)—H(19)	120.1
C(6)—C(5)—C(10)	117.3 (4)	C(20)—C(19)—H(19)	119.9
C(5)—C(6)—C(7)	121.4 (4)	C(15)—C(20)—H(20)	119.7
C(6)—C(7)—C(8)	120.0 (4)	C(19)—C(20)—H(20)	120.2
C(7)—C(8)—C(9)	119.5 (4)	N(1)—C(21)—H(21)	109.8
C(8)—C(9)—C(10)	120.0 (4)	N(1)—C(21)—H(22)	107.4
C(5)—C(10)—C(9)	121.7 (4)	C(22)—C(21)—H(21)	110.3
N(1)—C(11)—C(12)	113.5 (3)	C(22)—C(21)—H(22)	107.3
N(5)—C(12)—C(11)	113.2 (3)	H(21)—C(21)—H(22)	109.5
N(5)—C(13)—C(14)	106.7 (3)	N(8)—C(22)—H(23)	109.0
N(7)—C(14)—C(13)	106.0 (4)	N(8)—C(22)—H(24)	109.4
N(7)—C(14)—C(15)	122.4 (3)	C(21)—C(22)—H(23)	109.0
C(13)—C(14)—C(15)	131.6 (3)	C(21)—C(22)—H(24)	108.3
C(14)—C(15)—C(16)	119.7 (4)	H(23)—C(22)—H(24)	109.5
C(14)—C(15)—C(20)	121.2 (3)	N(8)—C(23)—H(25)	126.8
C(16)—C(15)—C(20)	119.0 (4)	C(24)—C(23)—H(25)	127.2
C(15)—C(16)—C(17)	120.2 (4)	C(25)—C(26)—H(26)	119.6
C(16)—C(17)—C(18)	119.9 (4)	C(27)—C(26)—H(26)	120.1
C(17)—C(18)—C(19)	120.7 (5)	C(26)—C(27)—H(27)	119.6
C(18)—C(19)—C(20)	120.0 (4)	C(28)—C(27)—H(27)	120.1
C(15)—C(20)—C(19)	120.1 (3)	C(27)—C(28)—H(28)	119.5
N(1)—C(21)—C(22)	112.4 (3)	C(29)—C(28)—H(28)	120.0
N(8)—C(22)—C(21)	111.5 (3)	C(28)—C(29)—H(29)	119.8
N(8)—C(23)—C(24)	106.1 (2)	C(30)—C(29)—H(29)	119.8
N(10)—C(24)—C(23)	107.9 (3)	C(25)—C(30)—H(30)	119.3
N(10)—C(24)—C(25)	122.2 (3)	C(29)—C(30)—H(30)	120.5
N(4)—Ag(1)—N(7) ⁱ —N(6) ⁱ	104.7 (2)	Ag(1) ^{xiv} —N(10)—C(24)—C(23)	-170.2 (3)
N(4)—Ag(1)—N(7) ⁱ —C(14) ⁱ	-68.5 (3)	Ag(1) ^{xiv} —N(10)—C(24)—C(25)	8.7 (5)
N(7) ⁱ —Ag(1)—N(4)—N(3)	96.6 (2)	N(9)—N(10)—C(24)—C(23)	1.4 (3)
N(7) ⁱ —Ag(1)—N(4)—C(4)	-100.5 (3)	N(9)—N(10)—C(24)—C(25)	-179.6 (3)
N(4)—Ag(1)—N(10) ⁱⁱ —N(9) ⁱⁱ	66.5 (2)	N(1)—C(1)—C(2)—N(2)	-70.9 (4)

supplementary materials

N(4)—Ag(1)—N(10) ⁱⁱ —C(24) ⁱⁱ	-105.2 (3)	N(2)—C(3)—C(4)—N(4)	0.2 (3)
N(10) ⁱⁱ —Ag(1)—N(4)—N(3)	-80.8 (2)	N(2)—C(3)—C(4)—C(5)	-178.9 (3)
N(10) ⁱⁱ —Ag(1)—N(4)—C(4)	82.1 (3)	N(4)—C(4)—C(5)—C(6)	20.4 (5)
N(7) ⁱ —Ag(1)—N(10) ⁱⁱ —N(9) ⁱⁱ	-111.4 (2)	N(4)—C(4)—C(5)—C(10)	-161.5 (3)
N(7) ⁱ —Ag(1)—N(10) ⁱⁱ —C(24) ⁱⁱ	76.9 (4)	C(3)—C(4)—C(5)—C(6)	-160.5 (3)
N(10) ⁱⁱ —Ag(1)—N(7) ⁱ —N(6) ⁱ	-77.9 (2)	C(3)—C(4)—C(5)—C(10)	17.6 (5)
N(10) ⁱⁱ —Ag(1)—N(7) ⁱ —C(14) ⁱ	108.9 (3)	C(4)—C(5)—C(6)—C(7)	178.8 (3)
C(1)—N(1)—C(11)—C(12)	162.9 (3)	C(4)—C(5)—C(10)—C(9)	-178.0 (3)
C(11)—N(1)—C(1)—C(2)	-80.9 (4)	C(6)—C(5)—C(10)—C(9)	0.2 (4)
C(1)—N(1)—C(21)—C(22)	-79.6 (4)	C(10)—C(5)—C(6)—C(7)	0.6 (5)
C(21)—N(1)—C(1)—C(2)	158.2 (3)	C(5)—C(6)—C(7)—C(8)	-1.3 (5)
C(11)—N(1)—C(21)—C(22)	159.5 (3)	C(6)—C(7)—C(8)—C(9)	1.1 (5)
C(21)—N(1)—C(11)—C(12)	-76.5 (4)	C(7)—C(8)—C(9)—C(10)	-0.3 (5)
N(3)—N(2)—C(2)—C(1)	-39.0 (4)	C(8)—C(9)—C(10)—C(5)	-0.3 (5)
C(2)—N(2)—N(3)—N(4)	-173.8 (2)	N(1)—C(11)—C(12)—N(5)	-71.1 (4)
N(3)—N(2)—C(3)—C(4)	-0.4 (4)	N(5)—C(13)—C(14)—N(7)	-0.0 (3)
C(3)—N(2)—N(3)—N(4)	0.4 (3)	N(5)—C(13)—C(14)—C(15)	-179.0 (3)
C(2)—N(2)—C(3)—C(4)	173.3 (3)	N(7)—C(14)—C(15)—C(16)	157.3 (3)
C(3)—N(2)—C(2)—C(1)	147.8 (3)	N(7)—C(14)—C(15)—C(20)	-21.3 (5)
N(2)—N(3)—N(4)—Ag(1)	165.6 (2)	C(13)—C(14)—C(15)—C(16)	-23.9 (6)
N(2)—N(3)—N(4)—C(4)	-0.2 (3)	C(13)—C(14)—C(15)—C(20)	157.5 (4)
Ag(1)—N(4)—C(4)—C(3)	-164.4 (2)	C(14)—C(15)—C(16)—C(17)	-180.0 (3)
Ag(1)—N(4)—C(4)—C(5)	14.9 (4)	C(14)—C(15)—C(20)—C(19)	178.9 (3)
N(3)—N(4)—C(4)—C(3)	-0.0 (3)	C(16)—C(15)—C(20)—C(19)	0.2 (5)
N(3)—N(4)—C(4)—C(5)	179.2 (3)	C(20)—C(15)—C(16)—C(17)	-1.3 (6)
N(6)—N(5)—C(12)—C(11)	-117.3 (3)	C(15)—C(16)—C(17)—C(18)	2.1 (6)
C(12)—N(5)—N(6)—N(7)	-177.2 (2)	C(16)—C(17)—C(18)—C(19)	-1.7 (6)
N(6)—N(5)—C(13)—C(14)	-0.1 (3)	C(17)—C(18)—C(19)—C(20)	0.6 (6)
C(13)—N(5)—N(6)—N(7)	0.1 (3)	C(18)—C(19)—C(20)—C(15)	0.2 (5)
C(12)—N(5)—C(13)—C(14)	176.9 (3)	N(1)—C(21)—C(22)—N(8)	-63.9 (3)
C(13)—N(5)—C(12)—C(11)	66.0 (5)	N(8)—C(23)—C(24)—N(10)	-1.4 (4)
N(5)—N(6)—N(7)—Ag(1) ^x	-174.7 (2)	N(8)—C(23)—C(24)—C(25)	179.7 (3)
N(5)—N(6)—N(7)—C(14)	-0.1 (3)	N(10)—C(24)—C(25)—C(26)	-172.5 (3)
Ag(1) ^x —N(7)—C(14)—C(13)	173.7 (2)	N(10)—C(24)—C(25)—C(30)	9.1 (5)
Ag(1) ^x —N(7)—C(14)—C(15)	-7.2 (5)	C(23)—C(24)—C(25)—C(26)	6.2 (6)
N(6)—N(7)—C(14)—C(13)	0.1 (3)	C(23)—C(24)—C(25)—C(30)	-172.2 (4)
N(6)—N(7)—C(14)—C(15)	179.2 (3)	C(24)—C(25)—C(26)—C(27)	-176.0 (3)
N(9)—N(8)—C(22)—C(21)	-49.6 (4)	C(24)—C(25)—C(30)—C(29)	177.9 (4)
C(22)—N(8)—N(9)—N(10)	-178.8 (2)	C(26)—C(25)—C(30)—C(29)	-0.5 (6)
N(9)—N(8)—C(23)—C(24)	0.9 (4)	C(30)—C(25)—C(26)—C(27)	2.4 (5)
C(23)—N(8)—N(9)—N(10)	-0.0 (3)	C(25)—C(26)—C(27)—C(28)	-2.5 (6)
C(22)—N(8)—C(23)—C(24)	179.5 (3)	C(26)—C(27)—C(28)—C(29)	0.7 (6)
C(23)—N(8)—C(22)—C(21)	131.9 (3)	C(27)—C(28)—C(29)—C(30)	1.3 (7)
N(8)—N(9)—N(10)—Ag(1) ^{xiv}	173.8 (2)	C(28)—C(29)—C(30)—C(25)	-1.3 (7)
N(8)—N(9)—N(10)—C(24)	-0.9 (3)		

Symmetry codes: (i) $-x+1/2, y-1/2, -z+1/2$; (ii) $x+1/2, -y+1/2, z+1/2$; (iii) $x+1/2, -y+1/2, z-1/2$; (iv) $x+1, y, z$; (v) $-x+3/2, y-1/2, -z+1/2$; (vi) $-x+1, -y+1, -z$; (vii) $-x+1, -y+1, -z+1$; (viii) $x-1/2, -y+1/2, z+1/2$; (ix) $-x, -y+1, -z$; (x) $-x+1/2, y+1/2, -z+1/2$; (xi) $x-1, y, z$; (xii) $-x+3/2, y+1/2, -z+1/2$; (xiii) $-x, -y+1, -z+1$; (xiv) $x-1/2, -y+1/2, z-1/2$.

Fig. 1

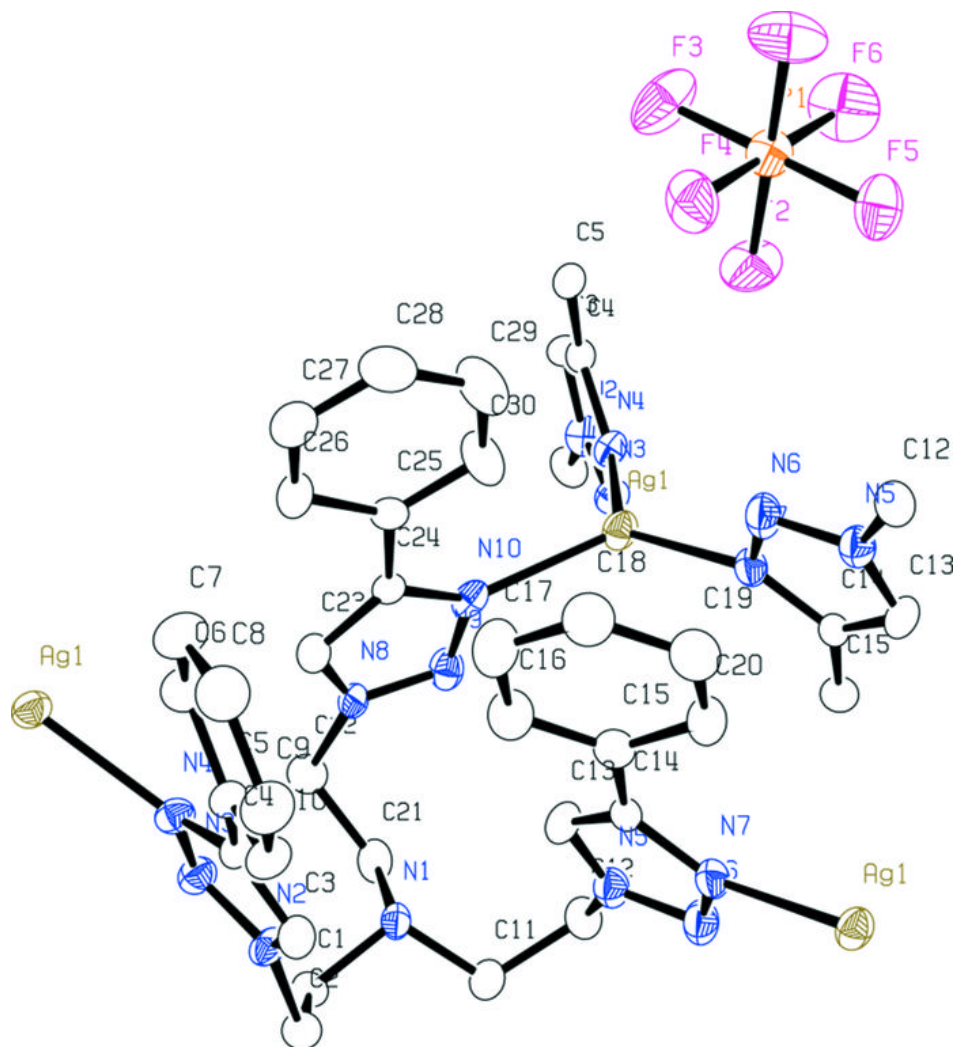


Fig. 2

