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(Triphenylphosphine-κP)[tris(indazol-1-yl)borato-$\kappa^3 N,N',N''$]silver(I)

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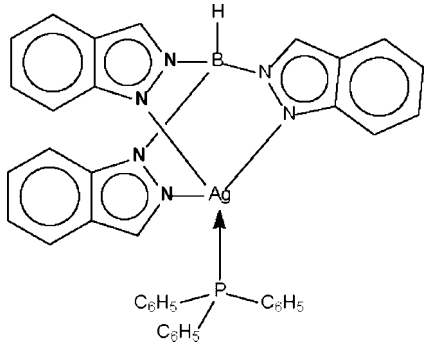
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.009 Å; R factor = 0.044; wR factor = 0.159; data-to-parameter ratio = 18.3.

The phosphine-coordinated Ag^I atom in the title compound, $[Ag(C_{21}H_{17}BN_6)(C_{18}H_{15}P)]$, is also N,N',N''-chelated by the tris(indazolyl)borate anion. The resultant N_3P coordination geometry is tetrahedral.

Related literature

For related literature; see Janiak *et al.* (2000).



Experimental

Crystal data

$[Ag(C_{21}H_{17}BN_6)(C_{18}H_{15}P)]$
M_r = 734.36
Triclinic, $P\overline{1}$
a = 10.2950 (6) Å
b = 12.6644 (6) Å
c = 13.9555 (7) Å
α = 87.003 (1)°
β = 77.966 (2)°
γ = 79.903 (1)°
V = 1751.7 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.66 mm^{-1}
T = 295 (2) K
0.31 × 0.28 × 0.15 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.551, T_{max} = 0.908
17380 measured reflections
7925 independent reflections
4255 reflections with $I > 2\sigma(I)$
R_{int} = 0.038

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.159
S = 1.08
7925 reflections
433 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.87 e Å^{-3}
$\Delta\rho_{min}$ = −0.95 e Å^{-3}

Data collection: *RAPID-AUTO* (Rigaku Corporation, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2225).

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supplementary materials

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(Triphenylphosphine-κP)[tris(indazol-1-yl)borato-$\kappa^3 N,N',N''$]silver(I)

M. H. Sadr, S. A. Niaz, S. Gorbani, S. Gao and S. W. Ng

Comment

Hydrotris(indazolyl)borate, Tp^{4Bo}, is suggested to be a suitable tripodal ligand for supramolecular assembly (Janiak *et al.*, 2000). In the title silver derivative, $Ag(C_{21}H_{17}N_6B)(C_{18}H_{15}P)$, the Tp^{4Bo} anion functions as a tridentate ligand (Fig. 1). The triphenylphosphine ligand completes the N_3P coordination geometry for Ag. The Ag center is tetrahedrally coordinated, but the N–Ag–N angles are significantly less than 90°, *i.e.* range from 82.3 (1) to 83.8 (2)°.

Experimental

Under a dry nitrogen atmosphere, K[HB(Indazolyl)$_3$] (0.2 g, 1 mmol) was added to a mixture of $AgNO_3$ (0.17 g, 1 mmol) and PPh_3 (0.26 g, 2 mmol) in methanol (40 ml). After being stirred for 3 h, the colorless solution was filtered. Crystals were obtained from the filtrate after a week.

Refinement

The H atoms were included in the refinement in the riding model approximation with = C–H 0.93, and with U(H) = 1.2U_{eq}(C).

Figures

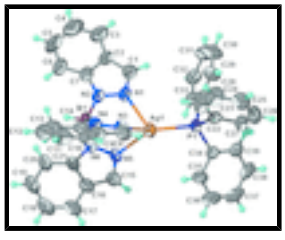


Fig. 1. The molecular structure of (I) showing atom numbering scheme, displacement ellipsoids at the 50% probability level and H atoms as spheres of arbitrary radii.

(Triphenylphosphine-κP)[tris(indazol-1-yl)borato- κ^{3}N,\<i>N',N'']silver(I)

Crystal data

$[Ag(C_{21}H_{17}BN_6)(C_{18}H_{15}P)]$	$Z = 2$
$M_r = 734.36$	$F(000) = 750$
Triclinic, $P\overline{1}$	$D_x = 1.392$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 10.2950$ (6) Å	Cell parameters from 10642 reflections
$b = 12.6644$ (6) Å	$\theta = 3.0$–$27.5°$

c = 13.9555 (7) Å	μ = 0.66 mm^{-1}
α = 87.003 (1)°	T = 295 K
β = 77.966 (2)°	Block, colorless
γ = 79.903 (1)°	0.31 × 0.28 × 0.15 mm
V = 1751.7 (2) Å^3	

Data collection

Rigaku R-AXIS RAPID IP diffractometer	7925 independent reflections
Radiation source: fine-focus sealed tube	4255 reflections with $I > 2\sigma(I)$
graphite	R_{int} = 0.038
ω scans	θ_{max} = 27.5°, θ_{min} = 3.0°
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	h = −13→13
T_{min} = 0.551, T_{max} = 0.908	k = −16→14
17380 measured reflections	l = −18→17

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)]$ = 0.044	Hydrogen site location: inferred from neighbouring sites
$wR(F^2)$ = 0.159	H-atom parameters constrained
S = 1.08	$w = 1/[\sigma^2(F_o^2) + (0.0652P)^2 + 1.2113P]$ where $P = (F_o^2 + 2F_c^2)/3$
7925 reflections	$(\Delta/\sigma)_{max}$ = 0.001
433 parameters	$\Delta\rho_{max}$ = 0.87 e Å^{-3}
0 restraints	$\Delta\rho_{min}$ = −0.95 e Å^{-3}

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

	x	y	z	U_{iso}*/U_{eq}
Ag1	0.46371 (4)	0.69276 (3)	0.81804 (3)	0.06680 (17)
P1	0.28241 (12)	0.80700 (9)	0.90871 (9)	0.0525 (3)
N1	0.5981 (4)	0.7791 (3)	0.6910 (3)	0.0682 (11)
N2	0.7025 (4)	0.7136 (3)	0.6353 (3)	0.0587 (9)
N3	0.4898 (4)	0.5627 (3)	0.7017 (3)	0.0660 (11)
N4	0.6162 (4)	0.5350 (3)	0.6461 (3)	0.0610 (10)
N5	0.6709 (4)	0.5973 (3)	0.8415 (3)	0.0637 (10)
N6	0.7627 (4)	0.5686 (3)	0.7583 (3)	0.0590 (9)
C1	0.6028 (6)	0.8787 (4)	0.6578 (4)	0.0772 (15)
H1	0.5422	0.9386	0.6837	0.093*
C2	0.7101 (6)	0.8818 (4)	0.5794 (4)	0.0704 (14)
C3	0.7642 (8)	0.9632 (6)	0.5185 (5)	0.105 (2)
H3	0.7241	1.0349	0.5260	0.126*

C4	0.8754 (10)	0.9333 (8)	0.4497 (6)	0.132 (3)
H4	0.9140	0.9858	0.4102	0.158*
C5	0.9350 (8)	0.8255 (8)	0.4357 (6)	0.125 (3)
H5	1.0101	0.8080	0.3856	0.150*
C6	0.8851 (6)	0.7453 (6)	0.4941 (4)	0.0890 (17)
H6	0.9253	0.6739	0.4849	0.107*
C7	0.7729 (5)	0.7747 (4)	0.5670 (4)	0.0638 (12)
C8	0.4152 (6)	0.4946 (4)	0.6823 (4)	0.0736 (14)
H8	0.3245	0.4971	0.7101	0.088*
C9	0.4908 (6)	0.4181 (4)	0.6143 (4)	0.0672 (13)
C10	0.4641 (8)	0.3292 (5)	0.5697 (5)	0.0900 (19)
H10	0.3785	0.3108	0.5828	0.108*
C11	0.5667 (10)	0.2717 (5)	0.5075 (5)	0.104 (2)
H11	0.5511	0.2126	0.4774	0.125*
C12	0.6947 (9)	0.2981 (5)	0.4871 (4)	0.100 (2)
H12	0.7627	0.2556	0.4442	0.120*
C13	0.7254 (7)	0.3861 (4)	0.5285 (4)	0.0816 (17)
H13	0.7589	0.4337	0.4760	0.098*
H13B	0.7977	0.3609	0.5632	0.098*
C14	0.6182 (6)	0.4457 (4)	0.5935 (3)	0.0615 (12)
C15	0.7202 (6)	0.5533 (4)	0.9166 (4)	0.0696 (13)
H15	0.6759	0.5614	0.9817	0.083*
C16	0.8488 (5)	0.4923 (4)	0.8855 (4)	0.0686 (13)
C17	0.9442 (6)	0.4265 (4)	0.9313 (5)	0.0844 (17)
H17	0.9291	0.4168	0.9990	0.101*
C18	1.0592 (7)	0.3777 (5)	0.8726 (7)	0.101 (2)
H18	1.1232	0.3333	0.9011	0.121*
C19	1.0845 (6)	0.3920 (5)	0.7716 (6)	0.096 (2)
H19	1.1655	0.3584	0.7344	0.115*
C20	0.9923 (5)	0.4547 (4)	0.7253 (5)	0.0768 (15)
H20	1.0093	0.4637	0.6575	0.092*
C21	0.8725 (5)	0.5043 (3)	0.7836 (4)	0.0619 (12)
C22	0.1187 (5)	0.7991 (3)	0.8834 (3)	0.0576 (11)
C23	0.1166 (6)	0.7634 (5)	0.7923 (4)	0.0804 (15)
H23	0.1973	0.7414	0.7486	0.096*
C24	−0.0051 (7)	0.7600 (6)	0.7647 (5)	0.099 (2)
H24	−0.0047	0.7364	0.7027	0.119*
C25	−0.1241 (7)	0.7907 (5)	0.8274 (5)	0.0873 (17)
H25	−0.2053	0.7902	0.8083	0.105*
C26	−0.1224 (5)	0.8227 (5)	0.9196 (5)	0.0811 (16)
H26	−0.2033	0.8413	0.9640	0.097*
C27	−0.0024 (5)	0.8276 (4)	0.9475 (4)	0.0654 (12)
H27	−0.0034	0.8504	1.0100	0.079*
C28	0.3049 (4)	0.9449 (3)	0.8736 (3)	0.0495 (10)
C29	0.2260 (6)	1.0098 (4)	0.8192 (4)	0.0774 (15)
H29	0.1512	0.9871	0.8048	0.093*
C30	0.2568 (7)	1.1094 (4)	0.7852 (5)	0.094 (2)
H30	0.2043	1.1516	0.7461	0.113*
C31	0.3624 (7)	1.1457 (4)	0.8083 (5)	0.0825 (16)

H31	0.3813	1.2130	0.7865	0.099*
C32	0.4409 (6)	1.0826 (4)	0.8639 (4)	0.0731 (14)
H32	0.5135	1.1071	0.8801	0.088*
C33	0.4127 (5)	0.9823 (4)	0.8963 (4)	0.0626 (12)
H33	0.4670	0.9396	0.9338	0.075*
C34	0.2676 (5)	0.8030 (4)	1.0407 (3)	0.0563 (11)
C35	0.3329 (5)	0.7129 (4)	1.0828 (4)	0.0667 (13)
H35	0.3793	0.6558	1.0435	0.080*
C36	0.3300 (7)	0.7069 (5)	1.1818 (5)	0.0879 (18)
H36	0.3739	0.6458	1.2090	0.105*
C37	0.2629 (7)	0.7904 (6)	1.2403 (4)	0.093 (2)
H37	0.2615	0.7861	1.3072	0.111*
C38	0.1973 (6)	0.8808 (6)	1.2007 (4)	0.0872 (17)
H38	0.1517	0.9376	1.2408	0.105*
C39	0.1992 (5)	0.8872 (4)	1.1014 (4)	0.0692 (13)
H39	0.1545	0.9484	1.0749	0.083*
B1	0.7306 (5)	0.5929 (4)	0.6564 (4)	0.0608 (14)
H1B	0.8105	0.5624	0.6084	0.073*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.0566 (2)	0.0586 (2)	0.0756 (3)	−0.00108 (16)	0.00227 (18)	−0.00611 (17)
P1	0.0478 (7)	0.0523 (6)	0.0537 (7)	−0.0065 (5)	−0.0036 (5)	−0.0012 (5)
N1	0.068 (3)	0.059 (2)	0.066 (3)	−0.0076 (19)	0.008 (2)	−0.0010 (19)
N2	0.054 (2)	0.064 (2)	0.055 (2)	−0.0135 (18)	−0.0013 (18)	−0.0005 (18)
N3	0.060 (3)	0.060 (2)	0.079 (3)	−0.0117 (19)	−0.013 (2)	−0.010 (2)
N4	0.061 (3)	0.059 (2)	0.062 (2)	−0.0072 (18)	−0.013 (2)	−0.0086 (19)
N5	0.056 (2)	0.066 (2)	0.064 (2)	0.0058 (18)	−0.014 (2)	−0.0028 (19)
N6	0.045 (2)	0.065 (2)	0.064 (2)	−0.0014 (17)	−0.0100 (19)	−0.0067 (18)
C1	0.089 (4)	0.055 (3)	0.079 (4)	−0.007 (3)	−0.001 (3)	−0.001 (3)
C2	0.075 (4)	0.076 (3)	0.059 (3)	−0.024 (3)	−0.003 (3)	0.004 (2)
C3	0.130 (6)	0.096 (5)	0.083 (4)	−0.035 (4)	0.003 (4)	0.012 (4)
C4	0.143 (8)	0.134 (7)	0.112 (6)	−0.054 (6)	0.008 (6)	0.034 (5)
C5	0.104 (6)	0.160 (8)	0.093 (5)	−0.036 (5)	0.029 (4)	0.018 (5)
C6	0.075 (4)	0.107 (4)	0.075 (4)	−0.016 (3)	0.007 (3)	−0.003 (3)
C7	0.057 (3)	0.078 (3)	0.058 (3)	−0.016 (2)	−0.009 (2)	−0.006 (2)
C8	0.065 (3)	0.069 (3)	0.091 (4)	−0.014 (3)	−0.025 (3)	0.003 (3)
C9	0.083 (4)	0.063 (3)	0.066 (3)	−0.017 (3)	−0.037 (3)	0.004 (2)
C10	0.125 (6)	0.076 (4)	0.085 (4)	−0.027 (4)	−0.052 (4)	0.002 (3)
C11	0.165 (8)	0.081 (4)	0.085 (5)	−0.029 (5)	−0.058 (5)	−0.008 (4)
C12	0.153 (7)	0.083 (4)	0.060 (4)	0.002 (4)	−0.027 (4)	−0.021 (3)
C13	0.117 (5)	0.078 (3)	0.046 (3)	0.001 (3)	−0.023 (3)	−0.001 (3)
C14	0.080 (4)	0.057 (3)	0.050 (3)	−0.004 (2)	−0.026 (3)	0.000 (2)
C15	0.073 (4)	0.064 (3)	0.072 (3)	−0.009 (3)	−0.019 (3)	−0.004 (2)
C16	0.069 (3)	0.051 (3)	0.092 (4)	−0.014 (2)	−0.027 (3)	0.003 (3)
C17	0.087 (4)	0.066 (3)	0.109 (5)	−0.015 (3)	−0.041 (4)	0.013 (3)
C18	0.074 (4)	0.077 (4)	0.153 (7)	−0.003 (3)	−0.039 (5)	0.017 (4)

C19	0.061 (4)	0.070 (4)	0.147 (7)	0.003 (3)	−0.011 (4)	0.004 (4)
C20	0.058 (3)	0.067 (3)	0.102 (4)	−0.004 (2)	−0.011 (3)	−0.005 (3)
C21	0.051 (3)	0.049 (2)	0.088 (4)	−0.011 (2)	−0.016 (3)	−0.004 (2)
C22	0.070 (3)	0.051 (2)	0.052 (3)	−0.016 (2)	−0.008 (2)	0.000 (2)
C23	0.073 (4)	0.103 (4)	0.069 (4)	−0.024 (3)	−0.011 (3)	−0.018 (3)
C24	0.100 (5)	0.127 (5)	0.085 (4)	−0.036 (4)	−0.035 (4)	−0.024 (4)
C25	0.084 (4)	0.085 (4)	0.107 (5)	−0.028 (3)	−0.038 (4)	−0.005 (4)
C26	0.045 (3)	0.088 (4)	0.110 (5)	−0.019 (3)	−0.006 (3)	−0.006 (3)
C27	0.055 (3)	0.074 (3)	0.067 (3)	−0.012 (2)	−0.008 (2)	−0.010 (2)
C28	0.044 (2)	0.057 (2)	0.046 (2)	−0.0053 (18)	−0.0074 (19)	−0.0032 (18)
C29	0.079 (4)	0.065 (3)	0.098 (4)	−0.014 (3)	−0.041 (3)	0.009 (3)
C30	0.104 (5)	0.062 (3)	0.132 (6)	−0.022 (3)	−0.060 (4)	0.026 (3)
C31	0.098 (4)	0.058 (3)	0.095 (4)	−0.022 (3)	−0.025 (4)	0.019 (3)
C32	0.074 (4)	0.074 (3)	0.075 (3)	−0.032 (3)	−0.008 (3)	0.002 (3)
C33	0.057 (3)	0.073 (3)	0.059 (3)	−0.018 (2)	−0.012 (2)	0.005 (2)
C34	0.051 (3)	0.062 (3)	0.056 (3)	−0.014 (2)	−0.008 (2)	0.004 (2)
C35	0.070 (3)	0.060 (3)	0.075 (3)	−0.019 (2)	−0.021 (3)	0.014 (2)
C36	0.099 (5)	0.096 (4)	0.081 (4)	−0.040 (4)	−0.036 (4)	0.032 (4)
C37	0.096 (5)	0.136 (6)	0.057 (3)	−0.055 (4)	−0.019 (3)	0.022 (4)
C38	0.077 (4)	0.125 (5)	0.057 (3)	−0.023 (4)	0.000 (3)	−0.006 (3)
C39	0.064 (3)	0.081 (3)	0.060 (3)	−0.011 (3)	−0.009 (3)	0.003 (3)
B1	0.041 (3)	0.071 (3)	0.068 (4)	−0.003 (2)	−0.006 (3)	−0.014 (3)

Geometric parameters (Å, °)

Ag1—N1	2.358 (4)	C15—H15	0.9300
Ag1—N3	2.316 (4)	C16—C21	1.397 (7)
Ag1—N5	2.337 (4)	C16—C17	1.410 (7)
Ag1—P1	2.332 (1)	C17—C18	1.359 (9)
P1—C22	1.814 (5)	C17—H17	0.9300
P1—C34	1.814 (5)	C18—C19	1.387 (10)
P1—C28	1.830 (4)	C18—H18	0.9300
N1—C1	1.326 (6)	C19—C20	1.373 (8)
N1—N2	1.361 (5)	C19—H19	0.9300
N2—C7	1.365 (6)	C20—C21	1.394 (7)
N2—B1	1.529 (7)	C20—H20	0.9300
N3—C8	1.322 (6)	C22—C27	1.377 (7)
N3—N4	1.366 (5)	C22—C23	1.377 (7)
N4—C14	1.375 (6)	C23—C24	1.393 (8)
N4—B1	1.526 (7)	C23—H23	0.9300
N5—C15	1.316 (6)	C24—C25	1.356 (9)
N5—N6	1.356 (5)	C24—H24	0.9300
N6—C21	1.370 (6)	C25—C26	1.373 (8)
N6—B1	1.531 (7)	C25—H25	0.9300
C1—C2	1.388 (7)	C26—C27	1.383 (7)
C1—H1	0.9300	C26—H26	0.9300
C2—C7	1.400 (7)	C27—H27	0.9300
C2—C3	1.416 (8)	C28—C29	1.368 (6)
C3—C4	1.343 (11)	C28—C33	1.379 (6)

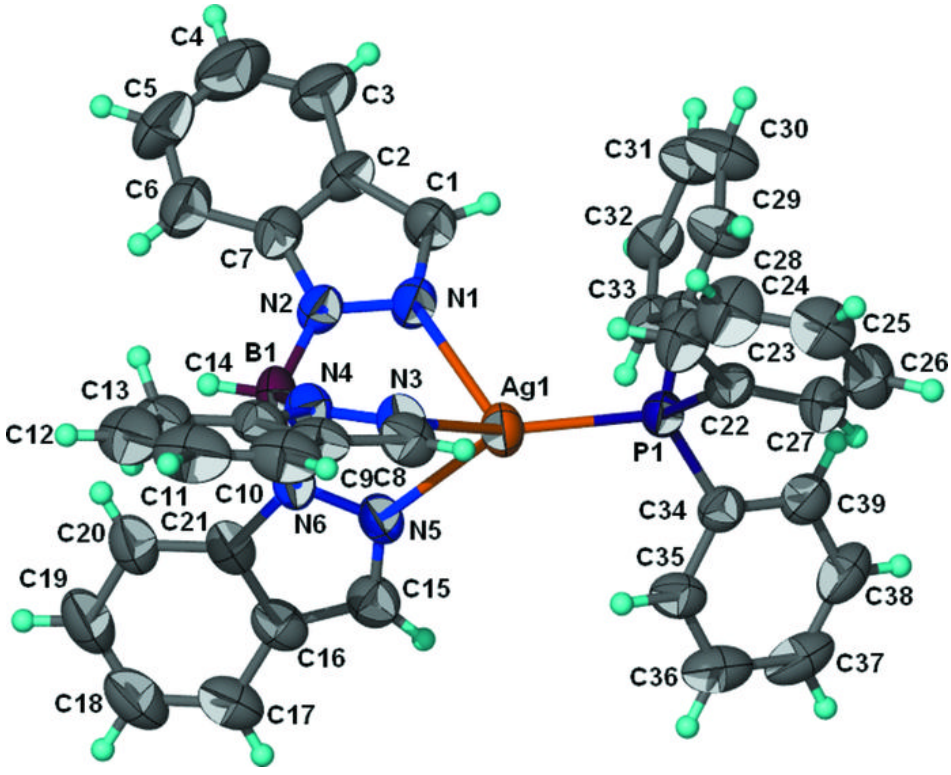
C3—H3	0.9300	C29—C30	1.390 (7)
C4—C5	1.401 (11)	C29—H29	0.9300
C4—H4	0.9300	C30—C31	1.354 (8)
C5—C6	1.372 (9)	C30—H30	0.9300
C5—H5	0.9300	C31—C32	1.365 (8)
C6—C7	1.382 (7)	C31—H31	0.9300
C6—H6	0.9300	C32—C33	1.385 (7)
C8—C9	1.403 (7)	C32—H32	0.9300
C8—H8	0.9300	C33—H33	0.9300
C9—C14	1.386 (7)	C34—C39	1.391 (7)
C9—C10	1.408 (7)	C34—C35	1.387 (6)
C10—C11	1.347 (10)	C35—C36	1.374 (8)
C10—H10	0.9300	C35—H35	0.9300
C11—C12	1.385 (10)	C36—C37	1.364 (9)
C11—H11	0.9300	C36—H36	0.9300
C12—C13	1.394 (8)	C37—C38	1.376 (9)
C12—H12	0.9300	C37—H37	0.9300
C13—C14	1.404 (7)	C38—C39	1.380 (7)
C13—H13	0.9700	C38—H38	0.9300
C13—H13B	0.9700	C39—H39	0.9300
C15—C16	1.405 (7)	B1—H1B	0.9800
N1—Ag1—N3	83.8 (2)	C21—C16—C15	103.7 (4)
N1—Ag1—N5	83.7 (2)	C21—C16—C17	120.4 (5)
N1—Ag1—P1	114.3 (1)	C15—C16—C17	135.8 (6)
N3—Ag1—N5	82.3 (1)	C18—C17—C16	117.3 (6)
N3—Ag1—P1	135.6 (1)	C18—C17—H17	121.3
N5—Ag1—P1	137.2 (1)	C16—C17—H17	121.3
C22—P1—C34	108.0 (2)	C17—C18—C19	122.3 (6)
C22—P1—C28	103.7 (2)	C17—C18—H18	118.9
C34—P1—C28	104.0 (2)	C19—C18—H18	118.9
C22—P1—Ag1	115.48 (15)	C20—C19—C18	121.4 (6)
C34—P1—Ag1	116.65 (15)	C20—C19—H19	119.3
C28—P1—Ag1	107.61 (14)	C18—C19—H19	119.3
C1—N1—N2	107.6 (4)	C19—C20—C21	117.5 (6)
C1—N1—Ag1	137.0 (3)	C19—C20—H20	121.2
N2—N1—Ag1	115.3 (3)	C21—C20—H20	121.2
N1—N2—C7	108.7 (4)	N6—C21—C20	130.5 (5)
N1—N2—B1	121.5 (4)	N6—C21—C16	108.5 (4)
C7—N2—B1	129.7 (4)	C20—C21—C16	121.0 (5)
C8—N3—N4	107.6 (4)	C27—C22—C23	118.2 (5)
C8—N3—Ag1	135.3 (4)	C27—C22—P1	124.9 (4)
N4—N3—Ag1	116.4 (3)	C23—C22—P1	116.9 (4)
N3—N4—C14	108.3 (4)	C22—C23—C24	120.7 (6)
N3—N4—B1	121.1 (4)	C22—C23—H23	119.6
C14—N4—B1	130.3 (4)	C24—C23—H23	119.6
C15—N5—N6	108.3 (4)	C25—C24—C23	120.8 (6)
C15—N5—Ag1	136.0 (4)	C25—C24—H24	119.6
N6—N5—Ag1	115.3 (3)	C23—C24—H24	119.6
N5—N6—C21	108.4 (4)	C24—C25—C26	118.7 (6)

N5—N6—B1	122.2 (4)	C24—C25—H25	120.7
C21—N6—B1	128.7 (4)	C26—C25—H25	120.7
N1—C1—C2	111.2 (5)	C27—C26—C25	121.2 (6)
N1—C1—H1	124.4	C27—C26—H26	119.4
C2—C1—H1	124.4	C25—C26—H26	119.4
C1—C2—C7	104.3 (4)	C22—C27—C26	120.4 (5)
C1—C2—C3	135.7 (6)	C22—C27—H27	119.8
C7—C2—C3	120.0 (6)	C26—C27—H27	119.8
C4—C3—C2	117.7 (7)	C29—C28—C33	118.3 (4)
C4—C3—H3	121.2	C29—C28—P1	122.9 (4)
C2—C3—H3	121.2	C33—C28—P1	118.6 (3)
C3—C4—C5	121.9 (7)	C28—C29—C30	120.5 (5)
C3—C4—H4	119.0	C28—C29—H29	119.7
C5—C4—H4	119.0	C30—C29—H29	119.7
C6—C5—C4	121.5 (7)	C31—C30—C29	120.7 (5)
C6—C5—H5	119.3	C31—C30—H30	119.7
C4—C5—H5	119.3	C29—C30—H30	119.7
C5—C6—C7	117.5 (6)	C30—C31—C32	119.5 (5)
C5—C6—H6	121.3	C30—C31—H31	120.2
C7—C6—H6	121.3	C32—C31—H31	120.2
N2—C7—C6	130.4 (5)	C31—C32—C33	120.1 (5)
N2—C7—C2	108.2 (4)	C31—C32—H32	119.9
C6—C7—C2	121.4 (5)	C33—C32—H32	119.9
N3—C8—C9	111.3 (5)	C28—C33—C32	120.8 (5)
N3—C8—H8	124.4	C28—C33—H33	119.6
C9—C8—H8	124.4	C32—C33—H33	119.6
C14—C9—C8	104.1 (4)	C39—C34—C35	118.1 (5)
C14—C9—C10	120.7 (6)	C39—C34—P1	123.5 (4)
C8—C9—C10	135.2 (6)	C35—C34—P1	118.3 (4)
C11—C10—C9	117.8 (7)	C36—C35—C34	121.0 (5)
C11—C10—H10	121.1	C36—C35—H35	119.5
C9—C10—H10	121.1	C34—C35—H35	119.5
C10—C11—C12	121.8 (6)	C37—C36—C35	120.1 (6)
C10—C11—H11	119.1	C37—C36—H36	119.9
C12—C11—H11	119.1	C35—C36—H36	119.9
C11—C12—C13	122.4 (6)	C36—C37—C38	120.3 (6)
C11—C12—H12	118.8	C36—C37—H37	119.9
C13—C12—H12	118.8	C38—C37—H37	119.9
C12—C13—C14	115.6 (6)	C39—C38—C37	119.9 (6)
C12—C13—H13	108.4	C39—C38—H38	120.0
C14—C13—H13	108.4	C37—C38—H38	120.0
C12—C13—H13B	108.4	C38—C39—C34	120.5 (5)
C14—C13—H13B	108.4	C38—C39—H39	119.7
H13—C13—H13B	107.4	C34—C39—H39	119.7
N4—C14—C9	108.8 (4)	N4—B1—N2	113.6 (4)
N4—C14—C13	129.6 (5)	N4—B1—N6	108.9 (4)
C9—C14—C13	121.7 (5)	N2—B1—N6	111.7 (4)
N5—C15—C16	111.0 (5)	N4—B1—H1B	107.4
N5—C15—H15	124.5	N2—B1—H1B	107.4

C16—C15—H15	124.5	N6—B1—H1B	107.4
N3—Ag1—P1—C22	−2.1 (2)	C12—C13—C14—N4	179.4 (5)
N5—Ag1—P1—C22	−147.2 (2)	C12—C13—C14—C9	−0.2 (7)
N1—Ag1—P1—C22	104.8 (2)	N6—N5—C15—C16	−0.2 (6)
N3—Ag1—P1—C34	126.3 (2)	Ag1—N5—C15—C16	171.9 (3)
N5—Ag1—P1—C34	−18.7 (2)	N5—C15—C16—C21	0.2 (6)
N1—Ag1—P1—C34	−126.8 (2)	N5—C15—C16—C17	−177.2 (6)
N3—Ag1—P1—C28	−117.4 (2)	C21—C16—C17—C18	1.1 (8)
N5—Ag1—P1—C28	97.6 (2)	C15—C16—C17—C18	178.1 (6)
N1—Ag1—P1—C28	−10.5 (2)	C16—C17—C18—C19	0.7 (10)
N3—Ag1—N1—C1	141.2 (6)	C17—C18—C19—C20	−1.5 (11)
P1—Ag1—N1—C1	3.5 (6)	C18—C19—C20—C21	0.5 (9)
N5—Ag1—N1—C1	−136.0 (6)	N5—N6—C21—C20	179.9 (5)
N3—Ag1—N1—N2	−40.6 (3)	B1—N6—C21—C20	9.3 (8)
P1—Ag1—N1—N2	−178.3 (3)	N5—N6—C21—C16	0.1 (5)
N5—Ag1—N1—N2	42.2 (3)	B1—N6—C21—C16	−170.5 (5)
C1—N1—N2—C7	0.4 (6)	C19—C20—C21—N6	−178.5 (5)
Ag1—N1—N2—C7	−178.4 (3)	C19—C20—C21—C16	1.3 (8)
C1—N1—N2—B1	177.5 (5)	C15—C16—C21—N6	−0.1 (5)
Ag1—N1—N2—B1	−1.2 (5)	C17—C16—C21—N6	177.7 (4)
P1—Ag1—N3—C8	−29.4 (6)	C15—C16—C21—C20	180.0 (5)
N5—Ag1—N3—C8	127.4 (5)	C17—C16—C21—C20	−2.1 (7)
N1—Ag1—N3—C8	−148.1 (5)	C34—P1—C22—C27	23.4 (5)
P1—Ag1—N3—N4	161.9 (2)	C28—P1—C22—C27	−86.5 (4)
N5—Ag1—N3—N4	−41.2 (3)	Ag1—P1—C22—C27	156.0 (4)
N1—Ag1—N3—N4	43.3 (3)	C34—P1—C22—C23	−157.7 (4)
C8—N3—N4—C14	−1.6 (5)	C28—P1—C22—C23	92.4 (4)
Ag1—N3—N4—C14	170.0 (3)	Ag1—P1—C22—C23	−25.1 (4)
C8—N3—N4—B1	−175.6 (4)	C27—C22—C23—C24	2.3 (8)
Ag1—N3—N4—B1	−3.9 (5)	P1—C22—C23—C24	−176.7 (5)
N3—Ag1—N5—C15	−127.3 (5)	C22—C23—C24—C25	−0.7 (10)
P1—Ag1—N5—C15	28.9 (6)	C23—C24—C25—C26	−1.7 (10)
N1—Ag1—N5—C15	148.2 (5)	C24—C25—C26—C27	2.5 (9)
N3—Ag1—N5—N6	44.4 (3)	C23—C22—C27—C26	−1.5 (7)
P1—Ag1—N5—N6	−159.5 (2)	P1—C22—C27—C26	177.4 (4)
N1—Ag1—N5—N6	−40.2 (3)	C25—C26—C27—C22	−0.9 (8)
C15—N5—N6—C21	0.1 (5)	C22—P1—C28—C29	−14.0 (5)
Ag1—N5—N6—C21	−173.8 (3)	C34—P1—C28—C29	−126.8 (4)
C15—N5—N6—B1	171.4 (4)	Ag1—P1—C28—C29	108.8 (4)
Ag1—N5—N6—B1	−2.5 (5)	C22—P1—C28—C33	171.2 (4)
N2—N1—C1—C2	0.1 (7)	C34—P1—C28—C33	58.4 (4)
Ag1—N1—C1—C2	178.4 (4)	Ag1—P1—C28—C33	−65.9 (4)
N1—C1—C2—C7	−0.4 (7)	C33—C28—C29—C30	2.1 (8)
N1—C1—C2—C3	−178.4 (7)	P1—C28—C29—C30	−172.7 (5)
C1—C2—C3—C4	178.1 (8)	C28—C29—C30—C31	−2.5 (10)
C7—C2—C3—C4	0.4 (10)	C29—C30—C31—C32	1.4 (10)
C2—C3—C4—C5	1.8 (14)	C30—C31—C32—C33	0.1 (9)
C3—C4—C5—C6	−2.3 (15)	C29—C28—C33—C32	−0.7 (7)
C4—C5—C6—C7	0.5 (12)	P1—C28—C33—C32	174.4 (4)

N1—N2—C7—C6	−179.3 (6)	C31—C32—C33—C28	−0.4 (8)
B1—N2—C7—C6	3.8 (9)	C22—P1—C34—C39	−71.4 (5)
N1—N2—C7—C2	−0.6 (6)	C28—P1—C34—C39	38.3 (5)
B1—N2—C7—C2	−177.5 (5)	Ag1—P1—C34—C39	156.6 (4)
C5—C6—C7—N2	−179.8 (6)	C22—P1—C34—C35	111.5 (4)
C5—C6—C7—C2	1.7 (9)	C28—P1—C34—C35	−138.7 (4)
C1—C2—C7—N2	0.6 (6)	Ag1—P1—C34—C35	−20.5 (4)
C3—C2—C7—N2	179.0 (5)	C39—C34—C35—C36	0.1 (8)
C1—C2—C7—C6	179.4 (5)	P1—C34—C35—C36	177.3 (4)
C3—C2—C7—C6	−2.2 (9)	C34—C35—C36—C37	−0.3 (9)
N4—N3—C8—C9	1.1 (6)	C35—C36—C37—C38	0.2 (10)
Ag1—N3—C8—C9	−168.2 (3)	C36—C37—C38—C39	0.1 (10)
N3—C8—C9—C14	−0.2 (6)	C37—C38—C39—C34	−0.3 (9)
N3—C8—C9—C10	179.2 (6)	C35—C34—C39—C38	0.2 (8)
C14—C9—C10—C11	0.8 (8)	P1—C34—C39—C38	−176.9 (4)
C8—C9—C10—C11	−178.6 (6)	N3—N4—B1—N2	−59.2 (6)
C9—C10—C11—C12	−0.1 (9)	C14—N4—B1—N2	128.3 (5)
C10—C11—C12—C13	−0.7 (10)	N3—N4—B1—N6	66.0 (5)
C11—C12—C13—C14	0.8 (9)	C14—N4—B1—N6	−106.5 (5)
N3—N4—C14—C9	1.5 (5)	N1—N2—B1—N4	62.3 (6)
B1—N4—C14—C9	174.7 (5)	C7—N2—B1—N4	−121.2 (5)
N3—N4—C14—C13	−178.2 (5)	N1—N2—B1—N6	−61.5 (6)
B1—N4—C14—C13	−5.0 (8)	C7—N2—B1—N6	115.1 (5)
C8—C9—C14—N4	−0.8 (5)	N5—N6—B1—N4	−61.8 (5)
C10—C9—C14—N4	179.7 (4)	C21—N6—B1—N4	107.6 (5)
C8—C9—C14—C13	178.9 (4)	N5—N6—B1—N2	64.5 (6)
C10—C9—C14—C13	−0.6 (7)	C21—N6—B1—N2	−126.1 (5)

Fig. 1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