

Bis{tris[μ -2-(1*H*-pyrazol-3-yl- κ N¹: κ N²)-pyridinato- κ N]trisilver(I)}(2 Ag—Ag)

Rong Li

College of Chemistry and Chemical Engineering, China West Normal University, Nanchong 637002, People's Republic of China
Correspondence e-mail: ronglinc@yahoo.com.cn

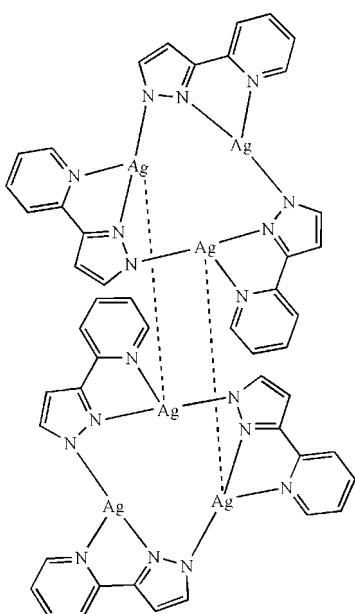
Received 7 May 2007; accepted 8 May 2007

Key indicators: single-crystal X-ray study; $T = 294$ K; mean $\sigma(\text{C}-\text{C}) = 0.006$ Å; R factor = 0.026; wR factor = 0.056; data-to-parameter ratio = 13.1.

The asymmetric unit of the title complex, $[\text{Ag}_6(\text{C}_8\text{H}_6\text{N}_3)_6]$, contains one half-molecule; the molecule is centrosymmetric. The Ag atoms form two nearly equilateral triangles, with $\text{Ag}\cdots\text{Ag}$ distances of 3.725 (3), 3.741 (3) and 3.843 (2) Å.

Related literature

For general background, see: Singh *et al.* (1997); Allen *et al.* (1987).



Experimental

Crystal data

$[\text{Ag}_6(\text{C}_8\text{H}_6\text{N}_3)_6]$	$V = 2441.3$ (7) Å ³
$M_r = 1512.17$	$Z = 2$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 11.5599$ (17) Å	$\mu = 2.42$ mm ⁻¹
$b = 8.5424$ (13) Å	$T = 294$ (2) K
$c = 25.389$ (4) Å	$0.22 \times 0.20 \times 0.10$ mm
$\beta = 103.16$ (3)°	

Data collection

Bruker SMART CCD area-detector diffractometer	11942 measured reflections
Absorption correction: multi-scan (<i>SADABS</i> ; Sheldrick, 1996)	4272 independent reflections
$T_{\min} = 0.619$, $T_{\max} = 0.794$	3045 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.034$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.027$	326 parameters
$wR(F^2) = 0.056$	H-atom parameters constrained
$S = 1.04$	$\Delta\rho_{\text{max}} = 0.32$ e Å ⁻³
4272 reflections	$\Delta\rho_{\text{min}} = -0.28$ e Å ⁻³

Table 1
Selected bond lengths (Å).

Ag1—N9	2.103 (3)	Ag2—N4	2.539 (3)
Ag1—N2	2.132 (3)	Ag2—Ag3	3.1144 (6)
Ag1—N1	2.603 (3)	Ag3—N6 ⁱ	2.107 (3)
Ag2—N3	2.124 (3)	Ag3—N8	2.144 (3)
Ag2—N5	2.160 (3)	Ag3—N7	2.586 (3)

Symmetry code: (i) $-x, -y + 1, -z$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2246).

References

- Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Bruker (1998). *SMART*, *SAINT* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Singh, K., Long, J. R. & Stavropoulos, P. (1997). *J. Am. Chem. Soc.* **119**, 2942–2943.

supplementary materials

Acta Cryst. (2007). E63, m1640 [doi:10.1107/S1600536807022581]

Bis{tris[μ -2-(1H-pyrazol-3-yl- κN^1 : κN^2)pyridinato- κN]trisilver(I)}(2 Ag-Ag)

R. Li

Comment

The compound, $[Ag_3(C_8H_6N_3)_3]_2\cdot 2py$, (II), (where py is pyridine), first synthesized and characterized by X-ray structure analysis at 295 K (Singh *et al.*, 1997). It was obtained by the reaction of $Ag(O_3SCF_3)$ with deprotonated 3-(2-pyridyl)pyrazole in methanol. The title complex, $[Ag_3(C_8H_6N_3)_3]_2$, (I), is obtained by the reaction of $AgNO_3$ with 3-(2-pyridyl)pyrazole in water, under hydrothermal conditions. We herein report its crystal structure.

The asymmetric unit of (I) contains one half molecule (Fig. 1). The bond lengths and angles (Table 1) are within normal ranges (Allen *et al.*, 1987). The $Ag_2\cdots Ag_3$ [3.1144 (6) Å] distance is shorter than the corresponding one [3.227 (2) Å] in (II). In the molecule of (I), the silver atoms form two nearly equilateral triangles with $Ag_1\cdots Ag_{3A}$ [3.725 (3) Å], $Ag_1\cdots Ag_2$ [3.741 (3) Å] and $Ag_2\cdots Ag_{3A}$ [3.843 (2) Å] (symmetry code A: $-x, 1 - y, -z$) distances, they are reported as 3.655, 3.702 and 3.835 Å, respectively, in (II).

Experimental

The title complex was obtained by the reaction of $AgNO_3$ with 3-(2-pyridyl)pyrazole in the molar ratio of 1:1 mixed with water (15 ml), under hydrothermal conditions at 413 K for 2 d. The colorless crystals were washed by water and acetone, and dried in air (yield: 0.452 g, 50%).

Refinement

H atoms were positioned geometrically, with C—H = 0.93 Å for aromatic H and constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

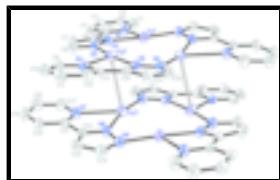


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level [symmetry code for unlabelled atoms: $-x, 1 - y, -z$].

Bis{tris[μ -2-(1H-pyrazol-3-yl- κN^1 : κN^2)pyridinato- κN]trisilver(I)}(2 Ag—Ag)

Crystal data

$[Ag_6(C_8H_6N_3)_6]$

$F_{000} = 1464$

supplementary materials

$M_r = 1512.17$	$D_x = 2.057 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
Hall symbol: -P 2ybc	$\lambda = 0.71073 \text{ \AA}$
$a = 11.5599 (17) \text{ \AA}$	Cell parameters from 4311 reflections
$b = 8.5424 (13) \text{ \AA}$	$\theta = 2.5\text{--}25.9^\circ$
$c = 25.389 (4) \text{ \AA}$	$\mu = 2.42 \text{ mm}^{-1}$
$\beta = 103.16 (3)^\circ$	$T = 294 (2) \text{ K}$
$V = 2441.3 (7) \text{ \AA}^3$	Block, colourless
$Z = 2$	$0.22 \times 0.20 \times 0.10 \text{ mm}$

Data collection

Bruker SMART CCD area-detector diffractometer	4272 independent reflections
Radiation source: fine-focus sealed tube	3045 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.034$
$T = 294(2) \text{ K}$	$\theta_{\max} = 25.0^\circ$
φ and ω scans	$\theta_{\min} = 2.5^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -10 \rightarrow 13$
$T_{\min} = 0.619$, $T_{\max} = 0.794$	$k = -10 \rightarrow 10$
11942 measured reflections	$l = -30 \rightarrow 28$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.027$	$w = 1/[\sigma^2(F_o^2) + (0.0176P)^2 + 0.4151P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.056$	$(\Delta/\sigma)_{\max} = 0.001$
$S = 1.04$	$\Delta\rho_{\max} = 0.32 \text{ e \AA}^{-3}$
4272 reflections	$\Delta\rho_{\min} = -0.28 \text{ e \AA}^{-3}$
326 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997), $F_c^* = kF_c[1 + 0.001xF_c^2\lambda^3/\sin(2\theta)]^{1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.00435 (13)
Secondary atom site location: difference Fourier map	

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) etc. and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Ag1	0.22972 (3)	0.51678 (4)	0.144579 (13)	0.05937 (12)
Ag2	0.13707 (3)	0.75885 (4)	0.019264 (12)	0.05891 (12)
Ag3	0.08700 (3)	0.50068 (3)	-0.069650 (12)	0.05764 (11)
C1	0.4993 (4)	0.4002 (5)	0.24241 (17)	0.0697 (12)
H1	0.4499	0.3419	0.2591	0.084*
C2	0.6178 (4)	0.3998 (5)	0.26535 (17)	0.0667 (12)
H2	0.6482	0.3438	0.2969	0.080*
C3	0.6911 (4)	0.4843 (5)	0.24049 (17)	0.0623 (11)
H3	0.7727	0.4855	0.2547	0.075*
C4	0.6425 (3)	0.5671 (4)	0.19450 (15)	0.0518 (10)
H4	0.6908	0.6255	0.1772	0.062*
C5	0.5205 (3)	0.5630 (4)	0.17397 (15)	0.0449 (9)
C6	0.4638 (3)	0.6537 (4)	0.12573 (14)	0.0450 (9)
C7	0.5113 (4)	0.7506 (5)	0.09238 (17)	0.0661 (12)
H7	0.5910	0.7732	0.0948	0.079*
C8	0.4152 (4)	0.8060 (5)	0.05497 (17)	0.0668 (12)
H8	0.4192	0.8742	0.0269	0.080*
C9	0.1409 (4)	1.0506 (5)	-0.08115 (18)	0.0613 (11)
H9	0.2225	1.0554	-0.0672	0.074*
C10	0.0920 (4)	1.1513 (5)	-0.12247 (18)	0.0694 (12)
H10	0.1390	1.2216	-0.1362	0.083*
C11	-0.0289 (4)	1.1445 (5)	-0.14278 (17)	0.0721 (13)
H11	-0.0653	1.2105	-0.1708	0.087*
C12	-0.0954 (4)	1.0389 (5)	-0.12118 (16)	0.0621 (11)
H12	-0.1773	1.0346	-0.1340	0.075*
C13	-0.0396 (3)	0.9396 (4)	-0.08040 (14)	0.0449 (9)
C14	-0.1060 (3)	0.8254 (4)	-0.05652 (14)	0.0457 (9)
C15	-0.2251 (3)	0.7862 (5)	-0.06899 (16)	0.0601 (11)
H15	-0.2847	0.8297	-0.0959	0.072*
C16	-0.2374 (3)	0.6695 (5)	-0.03332 (17)	0.0622 (12)
H16	-0.3083	0.6196	-0.0322	0.075*
C17	0.3620 (4)	0.6835 (6)	-0.0800 (2)	0.0778 (14)
H17	0.3966	0.6296	-0.0485	0.093*
C18	0.4308 (5)	0.7882 (7)	-0.1007 (3)	0.0953 (17)
H18	0.5093	0.8064	-0.0830	0.114*
C19	0.3823 (5)	0.8637 (6)	-0.1472 (3)	0.0904 (17)
H19	0.4279	0.9328	-0.1623	0.109*
C20	0.2645 (4)	0.8382 (5)	-0.1722 (2)	0.0720 (13)
H20	0.2296	0.8900	-0.2041	0.086*
C21	0.1997 (3)	0.7331 (5)	-0.14861 (17)	0.0537 (10)

supplementary materials

C22	0.0750 (3)	0.6993 (4)	-0.17222 (15)	0.0475 (9)
C23	-0.0011 (4)	0.7552 (5)	-0.21866 (17)	0.0630 (11)
H23	0.0162	0.8268	-0.2434	0.076*
C24	0.1065 (4)	0.3171 (5)	0.22022 (16)	0.0602 (11)
H24	0.1751	0.3028	0.2472	0.072*
N1	0.4490 (3)	0.4793 (4)	0.19730 (13)	0.0556 (8)
N2	0.3454 (2)	0.6541 (3)	0.10872 (12)	0.0486 (8)
N3	0.3155 (3)	0.7482 (4)	0.06472 (12)	0.0550 (8)
N4	0.0787 (3)	0.9466 (3)	-0.05986 (12)	0.0502 (8)
N5	-0.0509 (3)	0.7343 (3)	-0.01512 (11)	0.0463 (7)
N6	-0.1315 (3)	0.6389 (4)	-0.00049 (12)	0.0522 (8)
N7	0.2489 (3)	0.6559 (4)	-0.10277 (14)	0.0598 (9)
N8	0.0148 (3)	0.5983 (3)	-0.14802 (12)	0.0497 (8)
N9	0.0978 (3)	0.4114 (4)	0.17768 (12)	0.0521 (8)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.04537 (19)	0.0684 (2)	0.0623 (2)	-0.01088 (15)	0.00801 (15)	0.00317 (17)
Ag2	0.04773 (18)	0.0656 (2)	0.0541 (2)	0.00651 (15)	-0.00783 (13)	-0.00370 (16)
Ag3	0.0634 (2)	0.0568 (2)	0.0507 (2)	0.00115 (16)	0.00852 (15)	0.00713 (15)
C1	0.064 (3)	0.075 (3)	0.067 (3)	-0.002 (2)	0.007 (2)	0.021 (2)
C2	0.062 (3)	0.068 (3)	0.061 (3)	0.003 (2)	-0.006 (2)	0.012 (2)
C3	0.047 (2)	0.065 (3)	0.067 (3)	0.003 (2)	-0.004 (2)	0.000 (2)
C4	0.048 (2)	0.052 (2)	0.053 (3)	-0.0042 (19)	0.0052 (19)	-0.005 (2)
C5	0.040 (2)	0.044 (2)	0.047 (2)	-0.0014 (17)	0.0032 (18)	-0.0067 (18)
C6	0.042 (2)	0.045 (2)	0.043 (2)	-0.0031 (17)	-0.0003 (18)	-0.0042 (18)
C7	0.050 (2)	0.077 (3)	0.067 (3)	-0.019 (2)	0.005 (2)	0.017 (2)
C8	0.063 (3)	0.068 (3)	0.066 (3)	-0.015 (2)	0.008 (2)	0.021 (2)
C9	0.056 (3)	0.060 (3)	0.070 (3)	-0.002 (2)	0.020 (2)	-0.009 (2)
C10	0.091 (4)	0.057 (3)	0.069 (3)	0.002 (3)	0.035 (3)	0.006 (2)
C11	0.091 (4)	0.076 (3)	0.051 (3)	0.016 (3)	0.019 (3)	0.018 (2)
C12	0.064 (3)	0.074 (3)	0.044 (3)	0.008 (2)	0.003 (2)	0.005 (2)
C13	0.052 (2)	0.048 (2)	0.035 (2)	0.0066 (18)	0.0100 (18)	-0.0025 (18)
C14	0.045 (2)	0.051 (2)	0.038 (2)	0.0070 (18)	0.0016 (18)	-0.0059 (18)
C15	0.043 (2)	0.077 (3)	0.056 (3)	0.004 (2)	0.0007 (19)	0.008 (2)
C16	0.043 (2)	0.073 (3)	0.067 (3)	-0.006 (2)	0.005 (2)	0.003 (2)
C17	0.056 (3)	0.090 (3)	0.088 (4)	-0.004 (3)	0.018 (3)	-0.012 (3)
C18	0.063 (3)	0.107 (4)	0.124 (5)	-0.024 (3)	0.037 (3)	-0.025 (4)
C19	0.084 (4)	0.083 (4)	0.122 (5)	-0.029 (3)	0.057 (4)	-0.011 (3)
C20	0.076 (3)	0.062 (3)	0.088 (4)	-0.015 (2)	0.042 (3)	-0.007 (2)
C21	0.055 (2)	0.051 (2)	0.061 (3)	-0.002 (2)	0.026 (2)	-0.009 (2)
C22	0.057 (2)	0.044 (2)	0.045 (2)	0.0015 (19)	0.020 (2)	-0.0020 (18)
C23	0.084 (3)	0.057 (3)	0.053 (3)	-0.003 (2)	0.026 (2)	0.006 (2)
C24	0.062 (3)	0.066 (3)	0.046 (3)	0.007 (2)	-0.001 (2)	0.006 (2)
N1	0.0451 (18)	0.062 (2)	0.056 (2)	-0.0043 (16)	0.0041 (16)	0.0135 (18)
N2	0.0418 (19)	0.0523 (19)	0.046 (2)	-0.0045 (15)	-0.0014 (14)	0.0033 (16)
N3	0.049 (2)	0.059 (2)	0.050 (2)	-0.0078 (17)	-0.0045 (15)	0.0077 (17)

N4	0.048 (2)	0.0505 (19)	0.051 (2)	0.0005 (15)	0.0079 (16)	-0.0045 (15)
N5	0.0472 (18)	0.0476 (18)	0.0407 (18)	0.0019 (16)	0.0034 (14)	-0.0006 (15)
N6	0.0469 (19)	0.057 (2)	0.048 (2)	-0.0035 (16)	0.0004 (16)	0.0031 (16)
N7	0.045 (2)	0.067 (2)	0.069 (2)	-0.0060 (17)	0.0169 (18)	-0.0045 (19)
N8	0.048 (2)	0.0511 (19)	0.049 (2)	-0.0028 (15)	0.0099 (16)	0.0069 (16)
N9	0.049 (2)	0.058 (2)	0.049 (2)	-0.0032 (16)	0.0087 (16)	0.0051 (17)

Geometric parameters (\AA , $^\circ$)

Ag1—N9	2.103 (3)	C12—C13	1.380 (5)
Ag1—N2	2.132 (3)	C12—H12	0.9300
Ag1—N1	2.603 (3)	C13—N4	1.350 (4)
Ag2—N3	2.124 (3)	C13—C14	1.456 (5)
Ag2—N5	2.160 (3)	C14—N5	1.346 (4)
Ag2—N4	2.539 (3)	C14—C15	1.382 (5)
Ag2—Ag3	3.1144 (6)	C15—C16	1.376 (5)
Ag3—N6 ⁱ	2.107 (3)	C15—H15	0.9300
Ag3—N8	2.144 (3)	C16—N6	1.341 (4)
Ag3—N7	2.586 (3)	C16—H16	0.9300
C1—N1	1.343 (5)	C17—N7	1.324 (5)
C1—C2	1.361 (5)	C17—C18	1.379 (7)
C1—H1	0.9300	C17—H17	0.9300
C2—C3	1.371 (6)	C18—C19	1.349 (7)
C2—H2	0.9300	C18—H18	0.9300
C3—C4	1.371 (5)	C19—C20	1.382 (6)
C3—H3	0.9300	C19—H19	0.9300
C4—C5	1.387 (5)	C20—C21	1.390 (5)
C4—H4	0.9300	C20—H20	0.9300
C5—N1	1.330 (5)	C21—N7	1.346 (5)
C5—C6	1.471 (5)	C21—C22	1.458 (5)
C6—N2	1.338 (4)	C22—N8	1.342 (4)
C6—C7	1.384 (5)	C22—C23	1.385 (5)
C7—C8	1.371 (5)	C23—C24 ⁱ	1.359 (5)
C7—H7	0.9300	C23—H23	0.9300
C8—N3	1.328 (5)	C24—N9	1.333 (5)
C8—H8	0.9300	C24—C23 ⁱ	1.359 (5)
C9—N4	1.333 (5)	C24—H24	0.9300
C9—C10	1.375 (6)	N2—N3	1.356 (4)
C9—H9	0.9300	N5—N6	1.352 (4)
C10—C11	1.376 (6)	N6—Ag3 ⁱ	2.107 (3)
C10—H10	0.9300	N8—N9 ⁱ	1.350 (4)
C11—C12	1.377 (6)	N9—N8 ⁱ	1.350 (4)
C11—H11	0.9300		
N9—Ag1—N2	171.11 (12)	C16—C15—C14	105.7 (3)
N9—Ag1—N1	116.85 (11)	C16—C15—H15	127.1
N2—Ag1—N1	69.83 (10)	C14—C15—H15	127.1
N3—Ag2—N5	168.18 (12)	N6—C16—C15	109.5 (4)
N3—Ag2—N4	120.48 (11)	N6—C16—H16	125.2

supplementary materials

N5—Ag2—N4	71.33 (10)	C15—C16—H16	125.2
N3—Ag2—Ag3	111.15 (9)	N7—C17—C18	123.2 (5)
N5—Ag2—Ag3	68.55 (7)	N7—C17—H17	118.4
N4—Ag2—Ag3	84.36 (7)	C18—C17—H17	118.4
N6 ⁱ —Ag3—N8	166.69 (12)	C19—C18—C17	118.8 (5)
N6 ⁱ —Ag3—N7	120.62 (11)	C19—C18—H18	120.6
N8—Ag3—N7	69.91 (11)	C17—C18—H18	120.6
N6 ⁱ —Ag3—Ag2	79.55 (9)	C18—C19—C20	119.8 (5)
N8—Ag3—Ag2	111.48 (8)	C18—C19—H19	120.1
N7—Ag3—Ag2	81.01 (7)	C20—C19—H19	120.1
N1—C1—C2	124.4 (4)	C19—C20—C21	118.4 (5)
N1—C1—H1	117.8	C19—C20—H20	120.8
C2—C1—H1	117.8	C21—C20—H20	120.8
C1—C2—C3	117.9 (4)	N7—C21—C20	121.7 (4)
C1—C2—H2	121.0	N7—C21—C22	116.3 (3)
C3—C2—H2	121.0	C20—C21—C22	122.0 (4)
C2—C3—C4	119.2 (4)	N8—C22—C23	108.4 (3)
C2—C3—H3	120.4	N8—C22—C21	120.4 (3)
C4—C3—H3	120.4	C23—C22—C21	131.2 (4)
C3—C4—C5	119.4 (4)	C24 ⁱ —C23—C22	105.0 (4)
C3—C4—H4	120.3	C24 ⁱ —C23—H23	127.5
C5—C4—H4	120.3	C22—C23—H23	127.5
N1—C5—C4	121.9 (3)	N9—C24—C23 ⁱ	110.5 (4)
N1—C5—C6	116.7 (3)	N9—C24—H24	124.8
C4—C5—C6	121.4 (3)	C23 ⁱ —C24—H24	124.8
N2—C6—C7	108.7 (3)	C5—N1—C1	117.2 (3)
N2—C6—C5	119.9 (3)	C5—N1—Ag1	109.7 (2)
C7—C6—C5	131.4 (3)	C1—N1—Ag1	133.0 (3)
C8—C7—C6	105.0 (3)	C6—N2—N3	108.5 (3)
C8—C7—H7	127.5	C6—N2—Ag1	123.8 (2)
C6—C7—H7	127.5	N3—N2—Ag1	127.7 (2)
N3—C8—C7	110.1 (4)	C8—N3—N2	107.7 (3)
N3—C8—H8	125.0	C8—N3—Ag2	131.3 (3)
C7—C8—H8	125.0	N2—N3—Ag2	120.5 (2)
N4—C9—C10	124.1 (4)	C9—N4—C13	117.7 (3)
N4—C9—H9	118.0	C9—N4—Ag2	132.2 (3)
C10—C9—H9	118.0	C13—N4—Ag2	110.0 (2)
C9—C10—C11	117.8 (4)	C14—N5—N6	109.3 (3)
C9—C10—H10	121.1	C14—N5—Ag2	120.9 (2)
C11—C10—H10	121.1	N6—N5—Ag2	129.8 (2)
C10—C11—C12	119.3 (4)	C16—N6—N5	107.5 (3)
C10—C11—H11	120.3	C16—N6—Ag3 ⁱ	130.4 (3)
C12—C11—H11	120.3	N5—N6—Ag3 ⁱ	121.5 (2)
C11—C12—C13	119.6 (4)	C17—N7—C21	118.1 (4)
C11—C12—H12	120.2	C17—N7—Ag3	131.7 (3)
C13—C12—H12	120.2	C21—N7—Ag3	109.7 (2)
N4—C13—C12	121.5 (4)	C22—N8—N9 ⁱ	108.6 (3)

N4—C13—C14	116.9 (3)	C22—N8—Ag3	122.8 (2)
C12—C13—C14	121.6 (4)	N9 ⁱ —N8—Ag3	128.0 (2)
N5—C14—C15	108.0 (3)	C24—N9—N8 ⁱ	107.5 (3)
N5—C14—C13	120.8 (3)	C24—N9—Ag1	130.9 (3)
C15—C14—C13	131.2 (3)	N8 ⁱ —N9—Ag1	119.9 (2)
N3—Ag2—Ag3—N6 ⁱ	61.47 (13)	Ag1—N2—N3—C8	-177.3 (3)
N5—Ag2—Ag3—N6 ⁱ	-105.85 (11)	C6—N2—N3—Ag2	172.3 (2)
N4—Ag2—Ag3—N6 ⁱ	-177.98 (11)	Ag1—N2—N3—Ag2	-4.7 (4)
N3—Ag2—Ag3—N8	-126.29 (13)	N5—Ag2—N3—C8	169.4 (5)
N5—Ag2—Ag3—N8	66.39 (12)	N4—Ag2—N3—C8	-12.9 (4)
N4—Ag2—Ag3—N8	-5.75 (11)	Ag3—Ag2—N3—C8	83.1 (4)
N3—Ag2—Ag3—N7	-62.14 (12)	N5—Ag2—N3—N2	-1.2 (8)
N5—Ag2—Ag3—N7	130.54 (12)	N4—Ag2—N3—N2	176.5 (2)
N4—Ag2—Ag3—N7	58.41 (11)	Ag3—Ag2—N3—N2	-87.5 (3)
N1—C1—C2—C3	-0.7 (7)	C10—C9—N4—C13	0.3 (6)
C1—C2—C3—C4	1.0 (6)	C10—C9—N4—Ag2	-175.4 (3)
C2—C3—C4—C5	-0.3 (6)	C12—C13—N4—C9	-1.5 (5)
C3—C4—C5—N1	-0.8 (6)	C14—C13—N4—C9	-179.9 (3)
C3—C4—C5—C6	178.1 (3)	C12—C13—N4—Ag2	175.0 (3)
N1—C5—C6—N2	2.6 (5)	C14—C13—N4—Ag2	-3.3 (4)
C4—C5—C6—N2	-176.3 (3)	N3—Ag2—N4—C9	-0.4 (4)
N1—C5—C6—C7	-179.7 (4)	N5—Ag2—N4—C9	179.1 (4)
C4—C5—C6—C7	1.3 (6)	Ag3—Ag2—N4—C9	-111.7 (3)
N2—C6—C7—C8	-0.5 (5)	N3—Ag2—N4—C13	-176.3 (2)
C5—C6—C7—C8	-178.4 (4)	N5—Ag2—N4—C13	3.2 (2)
C6—C7—C8—N3	0.3 (5)	Ag3—Ag2—N4—C13	72.4 (2)
N4—C9—C10—C11	0.4 (6)	C15—C14—N5—N6	-0.5 (4)
C9—C10—C11—C12	0.2 (6)	C13—C14—N5—N6	-179.9 (3)
C10—C11—C12—C13	-1.4 (6)	C15—C14—N5—Ag2	-178.6 (2)
C11—C12—C13—N4	2.1 (6)	C13—C14—N5—Ag2	2.0 (4)
C11—C12—C13—C14	-179.6 (4)	N3—Ag2—N5—C14	175.2 (5)
N4—C13—C14—N5	1.4 (5)	N4—Ag2—N5—C14	-2.7 (2)
C12—C13—C14—N5	-177.0 (3)	Ag3—Ag2—N5—C14	-93.9 (3)
N4—C13—C14—C15	-177.9 (4)	N3—Ag2—N5—N6	-2.5 (8)
C12—C13—C14—C15	3.8 (6)	N4—Ag2—N5—N6	179.6 (3)
N5—C14—C15—C16	0.2 (4)	Ag3—Ag2—N5—N6	88.4 (3)
C13—C14—C15—C16	179.5 (4)	C15—C16—N6—N5	-0.5 (4)
C14—C15—C16—N6	0.2 (5)	C15—C16—N6—Ag3 ⁱ	170.5 (3)
N7—C17—C18—C19	-1.8 (8)	C14—N5—N6—C16	0.6 (4)
C17—C18—C19—C20	1.7 (8)	Ag2—N5—N6—C16	178.5 (2)
C18—C19—C20—C21	-0.6 (7)	C14—N5—N6—Ag3 ⁱ	-171.4 (2)
C19—C20—C21—N7	-0.5 (6)	Ag2—N5—N6—Ag3 ⁱ	6.5 (4)
C19—C20—C21—C22	179.9 (4)	C18—C17—N7—C21	0.7 (7)
N7—C21—C22—N8	1.1 (5)	C18—C17—N7—Ag3	-170.4 (4)
C20—C21—C22—N8	-179.3 (4)	C20—C21—N7—C17	0.5 (6)
N7—C21—C22—C23	-179.0 (4)	C22—C21—N7—C17	-179.9 (3)
C20—C21—C22—C23	0.6 (6)	C20—C21—N7—Ag3	173.5 (3)

supplementary materials

N8—C22—C23—C24 ⁱ	−0.1 (4)	C22—C21—N7—Ag3	−7.0 (4)
C21—C22—C23—C24 ⁱ	−180.0 (4)	N6 ⁱ —Ag3—N7—C17	−9.6 (4)
C4—C5—N1—C1	1.1 (6)	N8—Ag3—N7—C17	179.4 (4)
C6—C5—N1—C1	−177.8 (3)	Ag2—Ag3—N7—C17	62.5 (4)
C4—C5—N1—Ag1	178.7 (3)	N6 ⁱ —Ag3—N7—C21	178.7 (2)
C6—C5—N1—Ag1	−0.3 (4)	N8—Ag3—N7—C21	7.8 (2)
C2—C1—N1—C5	−0.4 (6)	Ag2—Ag3—N7—C21	−109.1 (2)
C2—C1—N1—Ag1	−177.2 (3)	C23—C22—N8—N9 ⁱ	−0.2 (4)
N9—Ag1—N1—C5	−174.8 (2)	C21—C22—N8—N9 ⁱ	179.7 (3)
N2—Ag1—N1—C5	−1.2 (2)	C23—C22—N8—Ag3	−172.4 (2)
N9—Ag1—N1—C1	2.2 (4)	C21—C22—N8—Ag3	7.5 (5)
N2—Ag1—N1—C1	175.8 (4)	N6 ⁱ —Ag3—N8—C22	−152.0 (5)
C7—C6—N2—N3	0.5 (4)	N7—Ag3—N8—C22	−7.9 (3)
C5—C6—N2—N3	178.7 (3)	Ag2—Ag3—N8—C22	63.2 (3)
C7—C6—N2—Ag1	177.7 (3)	N6 ⁱ —Ag3—N8—N9 ⁱ	37.4 (7)
C5—C6—N2—Ag1	−4.2 (5)	N7—Ag3—N8—N9 ⁱ	−178.5 (3)
N1—Ag1—N2—C6	2.8 (3)	Ag2—Ag3—N8—N9 ⁱ	−107.4 (3)
N1—Ag1—N2—N3	179.4 (3)	C23 ⁱ —C24—N9—N8 ⁱ	0.4 (4)
C7—C8—N3—N2	0.0 (5)	C23 ⁱ —C24—N9—Ag1	−164.0 (3)
C7—C8—N3—Ag2	−171.5 (3)	N1—Ag1—N9—C24	−5.3 (4)
C6—N2—N3—C8	−0.3 (4)	N1—Ag1—N9—N8 ⁱ	−168.1 (2)

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

Fig. 1

