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Poly[(μ_3-3,5-diisopropyl-4*H*-1,2,4-triazolato-κ^3N:N':N'')silver(I)]

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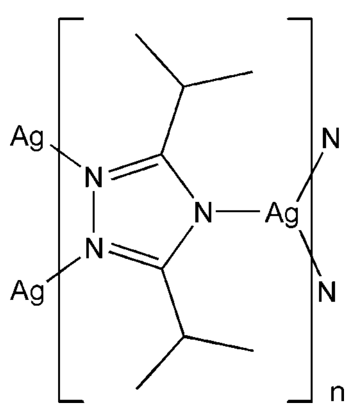
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.007 Å; R factor = 0.017; wR factor = 0.045; data-to-parameter ratio = 14.6.

In the polymeric title compound, $[Ag(C_8H_{14}N_3)]_n$, the Ag^I cation is coordinated by three N atoms from three 3,5-diisopropyl-1,2,4-triazolate anions in a T-shaped geometry. The Ag^I cation deviates from the coordination plane by 0.014 (1) Å and the N—Ag—N bond angles are 96.85 (11), 97.72 (10) and 165.39 (12)°. The triazolate anion bridges three Ag^I cations, forming a three-dimensional polymeric network.

Related literature

For the synthesis, see: Yang *et al.* (2009). For related structures, see: Yang *et al.* (2007); Ling *et al.* (2012).



Experimental

Crystal data

$[Ag(C_8H_{14}N_3)]$
M_r = 260.09
Orthorhombic, $Fdd2$
a = 20.853 (7) Å
b = 14.099 (5) Å
c = 14.364 (5) Å
V = 4223 (2) Å^3
Z = 16
Mo $K\alpha$ radiation
μ = 1.86 mm^{-1}
T = 296 K
0.20 × 0.15 × 0.10 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.707, T_{max} = 0.836
6151 measured reflections
1646 independent reflections
1626 reflections with $I > 2\sigma(I)$
R_{int} = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.017
$wR(F^2)$ = 0.045
S = 1.08
1646 reflections
113 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}
Absolute structure: Flack (1983), 645 Friedel pairs
Absolute structure parameter: −0.02 (4)

Table 1
Selected bond lengths (Å).

Ag1—N1	2.135 (2)	Ag1—N3^{ii}	2.504 (3)
Ag1—N2^{i}	2.131 (3)		

Symmetry codes: (i) $x-\frac{1}{4}, -y+\frac{1}{4}, z-\frac{1}{4}$; (ii) $-x+\frac{1}{4}, y-\frac{1}{4}, z-\frac{1}{4}$.

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supporting information for this paper is available from the IUCr electronic archives (Reference: XU5742).

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supplementary materials

Acta Cryst. (2014). E**70**, m189 [doi:10.1107/S1600536814008083]

Poly[(μ_3-3,5-diisopropyl-4*H*-1,2,4-triazolato-κ^3N:N':N'')silver(I)]

Guo-Gen Cui, Xiao-Xi Yang, Jian-Ping Yang and Xiang Jiang

1. Comment

The asymmetric unit of (I) contains one Ag(I) cation and one 3,5-diisopropyl-1,2,4-triazolate (diptrz) ligand. The coordination environment of the Ag (I) cation can be viewed as a "T" geometry, surrounded by three N atoms from three diptrz ligands (Fig. 1). The Ag1—N1 and Ag1—N2^{i} bond distances are 2.135 (3) and 2.131 (3) Å, respectively, agreement with those of Ag—N bond distances in reported 1,2,4-triazole-based silver compounds (Ling *et al.*, 2012). The Ag1—N3^{ii} bond distance is 2.504 (4) Å, agreeing well with those observed in 4-amino-3,5-diisopropyl-1,2,4-triazolate-based (4-NH_2-3,5-iPr_2-tz) silver compounds (Yang *et al.*, 2007). The diptrz ligand bridges neighboring three Ag(I) ions in a μ_3-N^1,N^2,N^4 fashion. The distance between Ag1^{iii} and Ag1^{iv} (bridged by diptrz in $\mu_{1,2}$-mode) is 3.3186 (11) Å, which is less than the sum of the van der Waals radii for the Ag atoms (3.44 Å). The infinite connection of Ag—N results the formation of three-dimensional compound (I) (Fig. 2).

2. Experimental

3,5-Diisopropyl-1*H*-1,2,4-triazole (Hdiptrz) was prepared according to the previous report (Yang *et al.*, 2009). Hdiptrz (0.046 g, 0.3 mmol) was dissolved in the mixture solution of acetonitrile (5 ml) and distilled water (5 ml). Then, silver acetate (0.075 g, 0.45 mmol) was added to the mixture. The mixture was stirred at room temperature for 10 min, and the white emulsion was obtained. The mixture was then transferred into a 15 ml Teflon-lined Parr bomb and heated at 413 K for 3 days. Then the reaction was cooled down to room temperature and block colourless crystals of (I) were obtained in 36% yield (based on Hdiptrz) by filtration.

3. Refinement

All H atoms were generated geometrically and allowed to ride on their parent atoms in riding-model approximations, with C—H = 0.96 Å and U_{iso}(H) = 1.2U_{eq}(C) for methyl H atoms, and C—H = 0.98 Å and U_{iso}(H) = 1.2U_{eq}(C) for methine H atoms.

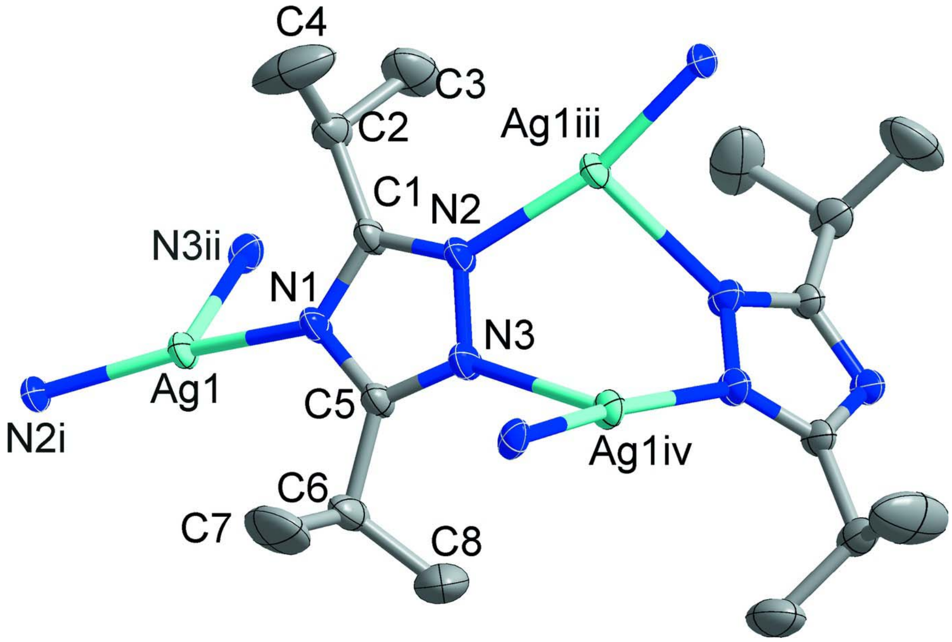

Figure 1

The coordination environment of the Ag[I] cation in (I), showing the atom-labelling number. Displacement ellipsoids are drawn at the 30% probability level (Hydrogen atoms are omitted for clarity). [Symmetry codes: (i) 1.25 - *x*, -0.25 + *y*, -0.25 + *z*; (ii) -0.25 + *x*, 0.25 - *y*, -0.25 + *z*; (iii) 1.25 - *x*, 0.25 + *y*, 0.25 + *z*; (iv) 0.25 + *x*, 0.25 - *y*, 0.25 + *z*.]

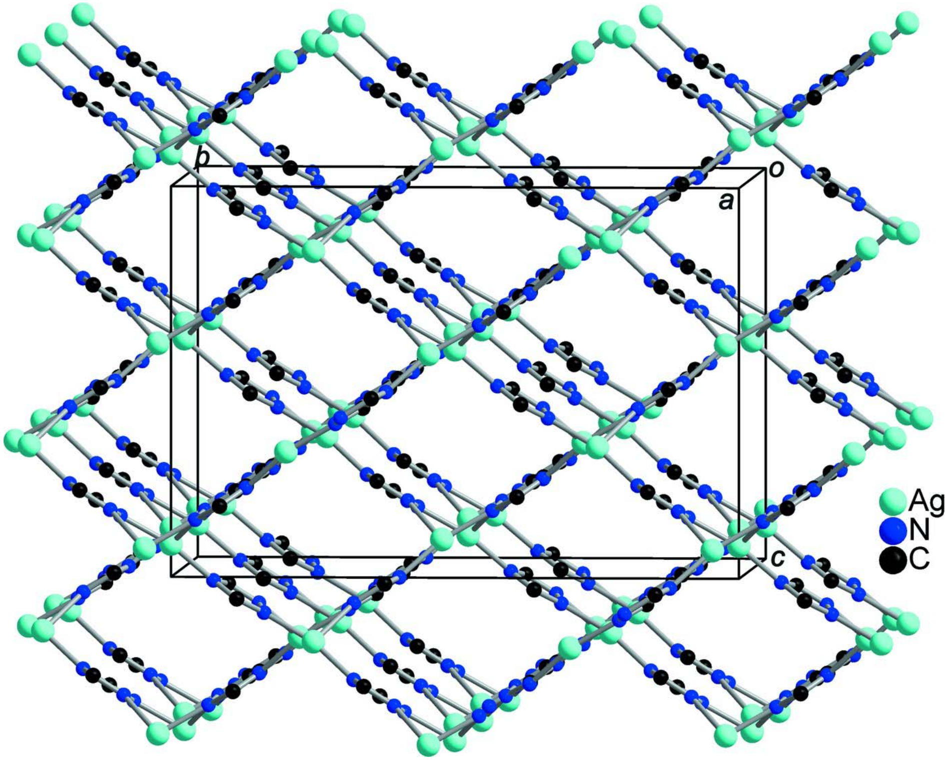

Figure 2

A view of the structure of (I), showing the three-dimensional network viewed along the *a* axis (the isopropyl groups are omitted for clarity).

Poly[(μ_3-3,5-diisopropyl-4*H*-1,2,4-triazolato-κ^3N:N':N'')silver(I)]

Crystal data

[$Ag(C_8H_{14}N_3)$]	D_x = 1.636 Mg m^{-3}
M_r = 260.09	Mo $K\alpha$ radiation, λ = 0.71073 Å
Orthorhombic, *Fdd*2	Cell parameters from 6779 reflections
a = 20.853 (7) Å	θ = 2.9–30.8°
b = 14.099 (5) Å	μ = 1.86 mm^{-1}
c = 14.364 (5) Å	*T* = 296 K
V = 4223 (2) Å^3	Block, colorless
Z = 16	0.20 × 0.15 × 0.10 mm
F(000) = 2080	

Data collection

Bruker APEXII CCD diffractometer	6151 measured reflections
Radiation source: fine-focus sealed tube	1646 independent reflections
Graphite monochromator	1626 reflections with $I > 2\sigma(I)$
φ and ω scans	R_{int} = 0.018
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)	θ_{max} = 25.2°, θ_{min} = 3.5°
T_{min} = 0.707, T_{max} = 0.836	h = −22→24
	k = −16→16
	l = −15→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.017$
$wR(F^2) = 0.045$
$S = 1.08$
1646 reflections
113 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0255P)^2 + 5.9277P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.35$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ e Å^{-3}
Absolute structure: Flack (1983), 645 Friedel pairs
Absolute structure parameter: −0.02 (4)

Special details

Experimental. Analysis calculated (found) for $Ag(C_8N_3H_{14})$ (%): C, 36.94 (36.82); H, 5.43 (5.71); N, 16.16 (16.23)%. IR spectrum for (I) (KBr,, cm^{-1}): 2962(*s*), 2925(*s*), 2871(*m*), 1498(*s*), 1466(*s*), 1435(*m*), 1380(*m*), 1361(*m*), 1301 (*m*), 1271(*m*), 1168(*m*), 1111(w), 1089(*m*), 1042(*m*), 774(w).

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ag1	0.017808 (10)	0.114711 (15)	0.64610 (4)	0.04068 (9)
N1	0.09085 (12)	0.1578 (2)	0.7413 (2)	0.0404 (6)
N2	0.18000 (12)	0.1560 (2)	0.8229 (2)	0.0422 (6)
N3	0.16637 (12)	0.25041 (19)	0.8030 (2)	0.0455 (7)
C1	0.13441 (15)	0.1034 (2)	0.7855 (3)	0.0409 (8)
C2	0.12967 (17)	−0.0027 (3)	0.7926 (3)	0.0569 (11)
H2	0.0971	−0.0231	0.7477	0.068*
C3	0.1906 (3)	−0.0505 (3)	0.7667 (5)	0.0918 (18)
H3A	0.2247	−0.0270	0.8052	0.138*
H3B	0.2002	−0.0376	0.7026	0.138*
H3C	0.1862	−0.1176	0.7755	0.138*
C4	0.1069 (4)	−0.0329 (4)	0.8876 (7)	0.141 (3)
H4A	0.1046	−0.1009	0.8902	0.211*
H4B	0.0652	−0.0066	0.8992	0.211*
H4C	0.1364	−0.0106	0.9340	0.211*
C5	0.11257 (13)	0.2480 (2)	0.7535 (2)	0.0394 (7)
C6	0.07883 (18)	0.3347 (3)	0.7186 (3)	0.0560 (9)
H6	0.0590	0.3188	0.6587	0.067*
C7	0.0254 (3)	0.3612 (5)	0.7860 (7)	0.120 (3)
H7A	0.0016	0.3053	0.8024	0.180*
H7B	−0.0028	0.4063	0.7570	0.180*

H7C	0.0436	0.3886	0.8412	0.180*
C8	0.1231 (3)	0.4168 (4)	0.7028 (6)	0.120 (3)
H8A	0.1429	0.4344	0.7606	0.180*
H8B	0.0992	0.4696	0.6788	0.180*
H8C	0.1557	0.3990	0.6588	0.180*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.03118 (11)	0.04062 (12)	0.05024 (14)	−0.00108 (8)	−0.01624 (8)	−0.00135 (12)
N1	0.0305 (12)	0.0401 (14)	0.0505 (16)	0.0034 (11)	−0.0191 (12)	−0.0062 (13)
N2	0.0315 (12)	0.0409 (15)	0.0542 (17)	0.0038 (11)	−0.0152 (11)	−0.0026 (13)
N3	0.0370 (13)	0.0367 (14)	0.0629 (19)	0.0008 (11)	−0.0149 (13)	−0.0033 (13)
C1	0.0341 (16)	0.0395 (16)	0.049 (2)	0.0037 (13)	−0.0117 (14)	−0.0069 (15)
C2	0.0544 (19)	0.0364 (19)	0.080 (3)	0.0010 (18)	−0.024 (2)	−0.003 (2)
C3	0.092 (3)	0.054 (3)	0.129 (5)	0.021 (2)	−0.020 (3)	−0.029 (3)
C4	0.200 (7)	0.059 (3)	0.164 (7)	0.006 (4)	0.085 (7)	0.027 (5)
C5	0.0344 (16)	0.0379 (17)	0.0458 (19)	0.0037 (15)	−0.0113 (12)	−0.0059 (16)
C6	0.051 (2)	0.047 (2)	0.070 (3)	0.0063 (17)	−0.0288 (18)	0.0000 (19)
C7	0.104 (5)	0.092 (4)	0.164 (8)	0.060 (4)	0.018 (5)	0.017 (5)
C8	0.096 (4)	0.077 (4)	0.188 (8)	−0.004 (3)	−0.019 (4)	0.064 (5)

Geometric parameters (Å, º)

Ag1—N1	2.135 (2)	C3—H3B	0.9600
Ag1—N2^{i}	2.131 (3)	C3—H3C	0.9600
Ag1—N3^{ii}	2.504 (3)	C4—H4A	0.9600
Ag1—Ag1^{iii}	3.3187 (11)	C4—H4B	0.9600
N1—C1	1.349 (4)	C4—H4C	0.9600
N1—C5	1.361 (4)	C5—C6	1.497 (5)
N2—C1	1.320 (4)	C6—C8	1.498 (7)
N2—N3	1.391 (4)	C6—C7	1.523 (9)
N2—Ag1^{iv}	2.131 (3)	C6—H6	0.9800
N3—C5	1.329 (4)	C7—H7A	0.9600
N3—Ag1^{v}	2.504 (3)	C7—H7B	0.9600
C1—C2	1.502 (5)	C7—H7C	0.9600
C2—C3	1.485 (6)	C8—H8A	0.9600
C2—C4	1.507 (9)	C8—H8B	0.9600
C2—H2	0.9800	C8—H8C	0.9600
C3—H3A	0.9600		
N2^{i}—Ag1—N1	165.39 (12)	H3B—C3—H3C	109.5
N2^{i}—Ag1—N3^{ii}	96.85 (11)	C2—C4—H4A	109.5
N1—Ag1—N3^{ii}	97.72 (10)	C2—C4—H4B	109.5
N2^{i}—Ag1—Ag1^{iii}	70.99 (8)	H4A—C4—H4B	109.5
N1—Ag1—Ag1^{iii}	115.93 (8)	C2—C4—H4C	109.5
N3^{ii}—Ag1—Ag1^{iii}	59.70 (6)	H4A—C4—H4C	109.5
C1—N1—C5	104.3 (2)	H4B—C4—H4C	109.5
C1—N1—Ag1	128.3 (2)	N3—C5—N1	111.9 (3)
C5—N1—Ag1	125.9 (2)	N3—C5—C6	123.8 (3)

C1—N2—N3	107.9 (2)	N1—C5—C6	124.3 (3)
C1—N2—Ag1^{iv}	138.0 (2)	C5—C6—C8	113.0 (4)
N3—N2—Ag1^{iv}	114.09 (19)	C5—C6—C7	109.3 (4)
C5—N3—N2	105.0 (3)	C8—C6—C7	111.0 (5)
C5—N3—Ag1^{v}	139.9 (2)	C5—C6—H6	107.8
N2—N3—Ag1^{v}	113.20 (19)	C8—C6—H6	107.8
N2—C1—N1	110.9 (3)	C7—C6—H6	107.8
N2—C1—C2	125.4 (3)	C6—C7—H7A	109.5
N1—C1—C2	123.7 (3)	C6—C7—H7B	109.5
C3—C2—C1	112.2 (3)	H7A—C7—H7B	109.5
C3—C2—C4	111.6 (5)	C6—C7—H7C	109.5
C1—C2—C4	111.3 (4)	H7A—C7—H7C	109.5
C3—C2—H2	107.1	H7B—C7—H7C	109.5
C1—C2—H2	107.1	C6—C8—H8A	109.5
C4—C2—H2	107.1	C6—C8—H8B	109.5
C2—C3—H3A	109.5	H8A—C8—H8B	109.5
C2—C3—H3B	109.5	C6—C8—H8C	109.5
H3A—C3—H3B	109.5	H8A—C8—H8C	109.5
C2—C3—H3C	109.5	H8B—C8—H8C	109.5
H3A—C3—H3C	109.5		

Symmetry codes: (i) $x-1/4$, $-y+1/4$, $z-1/4$; (ii) $-x+1/4$, $y-1/4$, $z-1/4$; (iii) $-x$, $-y$, z; (iv) $x+1/4$, $-y+1/4$, $z+1/4$; (v) $-x+1/4$, $y+1/4$, $z+1/4$.