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Poly[(μ_4-tetrazole-1-acetato-κ^4N^3:N^4:O:-O')silver(I)]

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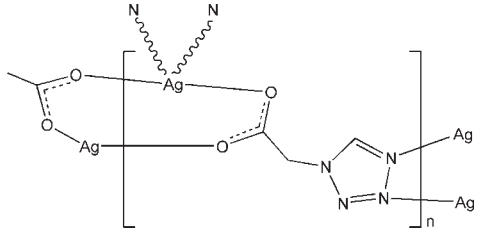
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.012 Å; R factor = 0.062; wR factor = 0.177; data-to-parameter ratio = 13.8.

In the title complex, $[Ag(C_3H_3N_4O_2)]_n$, the Ag^I atom is four-coordinated in a slightly distorted tetrahedral coordination geometry by two N atoms from two tetrazole-1-acetate (tza) ligands and two O atoms from the other two tza ligands. The tza ligand bridges two Ag atoms through the carboxylate O atoms and simultaneously binds to the other two Ag atoms through the tetrazole N atoms, forming a two-dimensional network parallel to (100).

Related literature

For the diverse coordination modes and potential applications of metal complexes with tetrazole derivatives, see: Stagni *et al.* (2006); Ye *et al.* (2006).



Experimental

Crystal data

$[Ag(C_3H_3N_4O_2)]$ M_r = 234.96
Triclinic, $P\overline{1}$
a = 5.1584 (10) Å
b = 7.7805 (16) Å
c = 7.8711 (16) Å
α = 109.40 (3)°
β = 98.87 (3)°
γ = 104.85 (3)°
V = 277.92 (14) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 3.56 mm^{-1}
T = 293 K
0.25 × 0.23 × 0.21 mm

Data collection

Rigaku/MSC Mercury CCD diffractometer
Absorption correction: multi-scan (*REQAB*; Jacobson, 1998)
T_{min} = 0.470, T_{max} = 0.522
2722 measured reflections
1267 independent reflections
1150 reflections with $I > 2\sigma(I)$
R_{int} = 0.056

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.062
$wR(F^2)$ = 0.177
S = 1.23
1267 reflections
92 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 2.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.97 e Å^{-3}

Table 1
Selected bond lengths (Å).

Ag1—O1	2.330 (7)	Ag1—N3^{ii}	2.494 (9)
Ag1—O2^{i}	2.282 (7)	Ag1—N4^{iii}	2.442 (8)

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

Data collection: *CrystalStructure* (Rigaku/MSC, 2002); cell refinement: *CrystalStructure*; data reduction: *CrystalStructure*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPII* (Johnson, 1976) and *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2270).

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supplementary materials

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Poly[(μ_4-tetrazole-1-acetato-$\kappa^4N^3:N^4:O:O'$)silver(I)]

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Comment

In recent years, organic ligands with a tetrazole functional group have been greatly used in coordination chemistry for construction of metal-organic frameworks due to their diverse coordination modes and potential applications in varied fields (Stagni *et al.*, 2006; Ye *et al.*, 2006). The reaction of tetrazole-1-acetic acid (Htza) with $AgNO_3$ in an alkaline aqueous solution yielded a new Ag^I coordination polymer, whose crystal structure is reported here.

In the title complex, the Ag^I atom is four-coordinated in a slightly distorted tetrahedral coordination geometry by two N atoms and two O atoms from four different tza ligands (Table 1), as illustrated in Fig. 1. The adjacent Ag^I atoms are co-bridged by tza liands. The tza ligand acts as a tetradentate ligand, bridging two Ag atoms through its carboxylate O atoms, while simultaneously binding to the other two Ag atoms through two N atoms of the tetrazole group, forming a two-dimensional network parallel to (1 0 0).

Experimental

A mixture of $AgNO_3$ (0.073 g, 0.5 mmol) and Htza (0.990 g, 0.5 mmol) in 15 ml of H_2O solution was sealed in an autoclave equipped with a Teflon liner (20 ml) and then heated at 373 K for 4 d. Crystals of the title compound were obtained by slow evaporation of the solvent at room temperature.

Refinement

H atoms were placed at calculated positions and treated as riding on the parent C atoms, with C—H = 0.93 (CH) and 0.97 (CH_2) Å and with U_{iso}(H) = 1.2U_{eq}(C). The highest residual electron density was found 1.40 Å from N4 and the deepest hole 1.12 Å from Ag1.

Figures

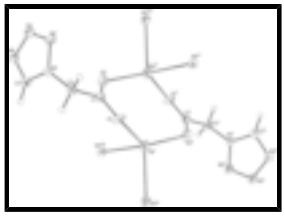


Fig. 1. The asymmetric unit of the title compound, with symmetrically related atoms to complete the Ag coordination. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry codes: (i) 1-x, -y, -z; (ii) x, -1+y, -1+z; (iii) 1-x, -y, 1-z; (iv) 1-x, 1-y, 1-z; (v) x, y, -1+z.]

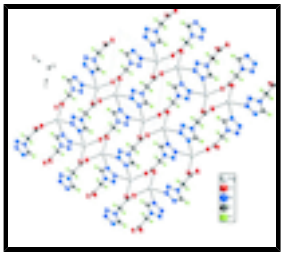


Fig. 2. A view of the layer structure of the title compound.

Poly[(μ$_4$-tetrazole-1-acetato- κ^4*N*^{3}:*N*^{4}:*O*:*O*')silver(I)]

Crystal data

[Ag($C_3H_3N_4O_2$)]	Z = 2
M_r = 234.96	F(000) = 224
Triclinic, $P\overline{1}$	D_x = 2.808 Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, λ = 0.71073 Å
a = 5.1584 (10) Å	Cell parameters from 3600 reflections
b = 7.7805 (16) Å	θ = 1.4–28°
c = 7.8711 (16) Å	μ = 3.56 mm^{-1}
α = 109.40 (3)°	T = 293 K
β = 98.87 (3)°	Block, blue
γ = 104.85 (3)°	0.25 × 0.23 × 0.21 mm
V = 277.92 (14) Å^3	

Data collection

Rigaku/MSC Mercury CCD diffractometer	1267 independent reflections
Radiation source: fine-focus sealed tube	1150 reflections with $I > 2\sigma(I)$
graphite	R_{int} = 0.056
ω scans	θ_{max} = 27.5°, θ_{min} = 3.2°
Absorption correction: multi-scan (REQAB; Jacobson, 1998)	h = −6→6
T_{min} = 0.470, T_{max} = 0.522	k = −9→10
2722 measured reflections	l = −10→9

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.062	H-atom parameters constrained
$wR(F^2)$ = 0.177	$w = 1/[\sigma^2(F_o^2) + (0.0519P)^2 + 3.2858P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.23	$(\Delta/\sigma)_{max} < 0.001$
1267 reflections	$\Delta\rho_{max}$ = 2.15 e Å^{-3}

92 parameters

0 restraints

Primary atom site location: structure-invariant direct methods

$\Delta\rho_{min} = -0.97$ e Å^{-3}

Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.052 (15)

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Ag1	0.61189 (17)	−0.19436 (12)	−0.05077 (10)	0.0387 (5)
O1	0.9281 (15)	0.0639 (10)	0.2082 (10)	0.0365 (16)
O2	0.6195 (14)	0.1949 (12)	0.3227 (10)	0.0360 (16)
N1	0.9120 (16)	0.3243 (11)	0.6770 (10)	0.0277 (16)
N2	0.872 (2)	0.4946 (12)	0.7248 (12)	0.0376 (19)
N3	0.7161 (19)	0.4973 (12)	0.8396 (12)	0.0363 (19)
N4	0.656 (2)	0.3322 (13)	0.8697 (12)	0.0351 (18)
C1	0.8444 (18)	0.1645 (13)	0.3374 (12)	0.0265 (17)
C2	1.0509 (18)	0.2615 (13)	0.5323 (12)	0.0267 (17)
H2A	1.1368	0.1710	0.5545	0.032*
H2B	1.1964	0.3719	0.5373	0.032*
C3	0.781 (2)	0.2254 (15)	0.7646 (14)	0.034 (2)
H3	0.7775	0.1022	0.7545	0.041*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.0430 (6)	0.0441 (6)	0.0259 (5)	0.0145 (4)	0.0071 (3)	0.0105 (3)
O1	0.033 (3)	0.031 (3)	0.034 (4)	0.013 (3)	0.010 (3)	−0.003 (3)
O2	0.028 (3)	0.055 (4)	0.029 (3)	0.020 (3)	0.008 (3)	0.016 (3)
N1	0.033 (4)	0.030 (4)	0.021 (3)	0.011 (3)	0.008 (3)	0.009 (3)
N2	0.051 (5)	0.027 (4)	0.033 (4)	0.013 (4)	0.017 (4)	0.008 (3)
N3	0.045 (5)	0.030 (4)	0.030 (4)	0.010 (4)	0.012 (4)	0.008 (3)
N4	0.048 (5)	0.034 (4)	0.030 (4)	0.020 (4)	0.017 (4)	0.014 (3)
C1	0.026 (4)	0.028 (4)	0.025 (4)	0.010 (3)	0.005 (3)	0.009 (3)
C2	0.023 (4)	0.032 (4)	0.022 (4)	0.010 (3)	0.003 (3)	0.007 (3)
C3	0.041 (5)	0.033 (5)	0.032 (5)	0.014 (4)	0.013 (4)	0.015 (4)

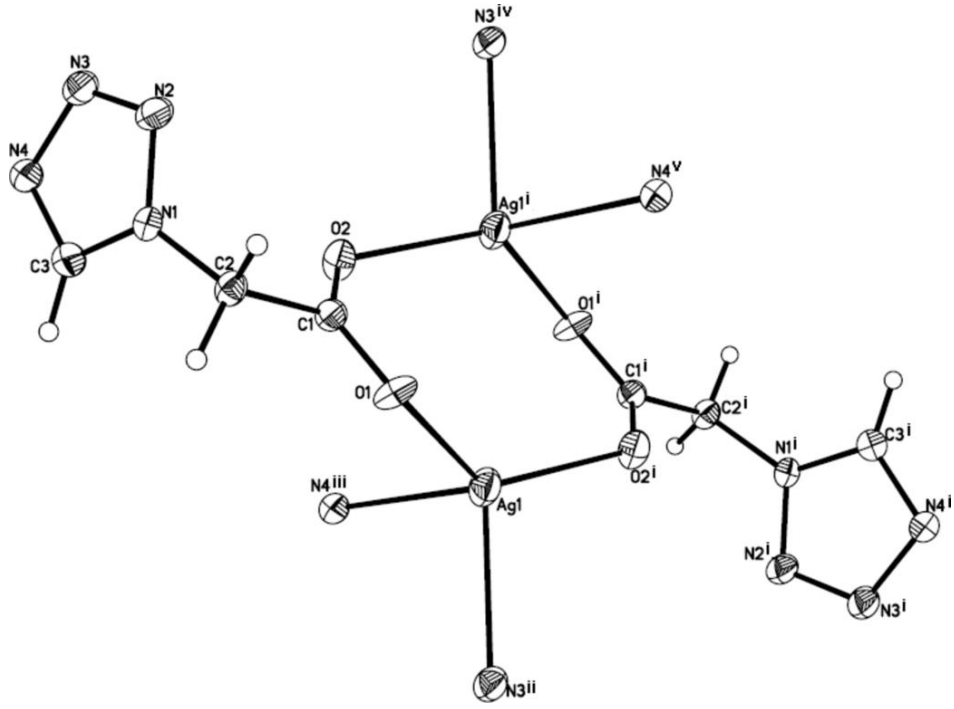
Geometric parameters (Å, °)

Ag1—O1	2.330 (7)	N1—C2	1.453 (11)
Ag1—O2^{i}	2.282 (7)	N2—N3	1.297 (12)
Ag1—N3^{ii}	2.494 (9)	N3—N4	1.350 (12)
Ag1—N4^{iii}	2.442 (8)	N4—C3	1.331 (13)
O1—C1	1.270 (11)	C1—C2	1.540 (12)
O2—C1	1.238 (11)	C2—H2A	0.9700
N1—C3	1.324 (12)	C2—H2B	0.9700
N1—N2	1.331 (12)	C3—H3	0.9300

O2^{i}—Ag1—O1	129.2 (3)	C3—N4—N3	105.1 (8)
O2^{i}—Ag1—N4^{iii}	118.7 (3)	C3—N4—Ag1^{iii}	117.8 (6)
O1—Ag1—N4^{iii}	95.0 (3)	N3—N4—Ag1^{iii}	137.0 (6)
O2^{i}—Ag1—N3^{ii}	102.2 (3)	O2—C1—O1	127.3 (9)
O1—Ag1—N3^{ii}	118.0 (3)	O2—C1—C2	117.2 (8)
N4^{iii}—Ag1—N3^{ii}	86.0 (3)	O1—C1—C2	115.5 (8)
C1—O1—Ag1	120.6 (6)	N1—C2—C1	111.1 (7)
C1—O2—Ag1^{i}	121.2 (6)	N1—C2—H2A	109
C3—N1—N2	109.2 (8)	C1—C2—H2A	109
C3—N1—C2	128.9 (8)	N1—C2—H2B	109
N2—N1—C2	121.4 (8)	C1—C2—H2B	109
N3—N2—N1	106.3 (8)	H2A—C2—H2B	108
N2—N3—N4	111.0 (8)	N1—C3—N4	108.4 (9)
N2—N3—Ag1^{iv}	112.1 (6)	N1—C3—H3	126
N4—N3—Ag1^{iv}	136.9 (6)	N4—C3—H3	126

Symmetry codes: (i) −*x*+1, −*y*, −*z*; (ii) *x*, *y*−1, *z*−1; (iii) −*x*+1, −*y*, −*z*+1; (iv) *x*, *y*+1, *z*+1.

Fig. 1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N4
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O2
C3
C2
C1
O1i
C1i
O1
C2i
N1i
C3i
N4iii
O2i
Ag1
N4i
N2i
N3i
N3ii

Fig. 2