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Bis(cyanido-κC)(ethane-1,2-diamine-$\kappa^2 N,N'$)silver(II)

Saeed Ahmad,[a]* Muhammad Monim-ul-Mehboob,[a] Muhammad Hanif,[a] Muhammad Altaf[b] and Helen Stoeckli-Evans[b]‡

[a]Department of Chemistry, University of Engineering and Technology, Lahore, Pakistan, and [b]Institute of Microtechnology, University of Neuchâtel, Rue Emile-Argand 11, CH-2009 Neuchâtel, Switzerland
Correspondence e-mail: saeed_a786@hotmail.com

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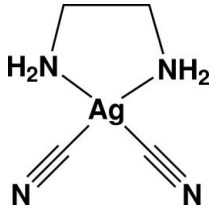
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.003 Å; R factor = 0.016; wR factor = 0.042; data-to-parameter ratio = 22.8.

The title compound, $[Ag(CN)_2(C_2H_8N_2)]$, was obtained from the reaction of ethane-1,2-diamine (en) with $K[Ag(CN)_2]$. The compound crystallizes as an inversion twin, the ratio of the twin components being 0.72 (4):0.28 (4). The Ag^{II} atom is in a slightly disorted square-planar environment. The chelate ring has an envelope conformation. The Ag^{II}—N(en) bond lengths are 2.071 (2) and 2.078 (2) Å. In the crystal structure, symmetry-related molecules are linked by N—H···N hydrogen bonds to form a three-dimensional network.

Related literature

For related literature, see: Pretsch & Hartl (2005); Wang *et al.* (2002); Po *et al.* (1991).



Experimental

Crystal data

$[Ag(CN)_2(C_2H_8N_2)]$
M_r = 220.01
Orthorhombic, $P2_12_12_1$
a = 6.9140 (8) Å
b = 9.3481 (11) Å
c = 11.0289 (11) Å
V = 712.83 (14) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.74 mm^{-1}
T = 173 (2) K
0.50 × 0.20 × 0.10 mm

Data collection

Stoe IPDS II diffractometer
Absorption correction: multi-scan (*MULABS* in *PLATON*; Spek, 2003)
T_{min} = 0.539, T_{max} = 0.760
6842 measured reflections
1913 independent reflections
1889 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.016
$wR(F^2)$ = 0.042
S = 1.08
1913 reflections
84 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.51 e Å^{-3}
Absolute structure: Flack (1983), with 784 Friedel pairs
Flack parameter: 0.28 (4)

Table 1
Selected geometric parameters (Å, °).

Ag1—N1	2.078 (2)	Ag1—C3	1.960 (2)
Ag1—N2	2.071 (2)	Ag1—C4	1.965 (3)
N1—Ag1—N2	83.14 (8)	N2—Ag1—C4	93.84 (9)
N1—Ag1—C3	94.12 (9)	C3—Ag1—C4	88.78 (10)
N1—Ag1—C4	175.20 (10)	Ag1—N1—C1	107.03 (15)
N2—Ag1—C3	176.69 (10)	Ag1—N2—C2	109.18 (14)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1NA···N4^{i}	0.92	2.27	3.099 (3)	150
N1—H1NB···N4^{ii}	0.92	2.18	3.097 (3)	172
N2—H2NA···N3^{iii}	0.92	2.10	3.002 (3)	167
N2—H2NB···N3^{i}	0.92	2.16	3.042 (3)	161

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

Data collection: *X-AREA* (Stoe & Cie, 2005); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2005); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); 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: LH2497).

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‡ Additional correspondence author, e-mail helen.stoeckli-evans@unine.ch.

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supplementary materials

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Bis(cyanido-κC)(ethane-1,2-diamine-$\kappa^2 N,N'$)silver(II)

S. Ahmad, M. Monim-ul-Mehboob, M. Hanif, M. Altaf and H. Stoeckli-Evans

Comment

The molecular stucture of the title compound is shown in Fig. 1. The compound crystallized in the chiral space group $P2_12_12_1$ as an inversion twin; the refined BASF value is 0.28 (4).

The Ag^{II} atom has an almost perfect square planar environement (Table 1). The five-membered chelate ring has an envelope conformation with atom C1 at the flap.

The Ag^{II}—N(en) bond distances of 2.071 (2) and 2.078 (2) Å are significantly shorter than the same distances observed in some silver(II) 1,4,8,11-tetramethyl-1,4,8,11-tetraazacyclotetradecane macrocyclic complexes; 2.185 (5) to 2.195 (6) Å (Wang *et al.*, 2002) and 2.194 (3) to 2.196 (3) Å (Po *et al.*, 1991). In the corresponding silver(I) complex, [Ag(CN)en)], prepared solvothermally, the Ag^{I}—N(en) distances are 2.283 (6) and 2.355 (6) Å (Pretsch & Hartl, 2005).

In the crystal structure symmetry related molecules are linked by N—H···N(CN) hydrogen bonds to form a three-dimensional network (Fig. 2).

Experimental

The title compound was prepared by the addition of ethane-1,2-diamine in methanol to an equimolar amount of $K[Ag(CN)_2]$ in water. The solution was stirred for 15 min then filtered and allowed to evaporate slowly in air. Colourless crystals appeared along with some black deposits on the walls of the vessel, which suggested disproportionation of silver(I) to give silver(II) and silver(0).

Refinement

The H-atoms were included in calculated positions and treated as riding atoms: N—H = 0.92 Å and C—H = 0.99 Å, with U_{iso}(H) = 1.2U_{eq}(N or C).

Figures

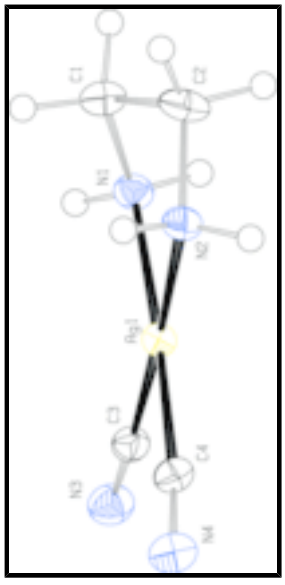

Fig. 1. The molecular sturcture showing the atomic numbering scheme and displacement parameters drawn at the 50% probabilty level.

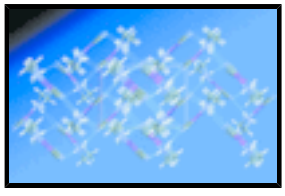

Fig. 2. The crystal packing viewed along the *c* axis. Intermolecular N—H···N hydrogen bonds are shown as dotted lines.

Bis(cyanido-κ*C*)(ethane-1,2-diamine-κ^2*N*,*N*$'$)silver(II)

Crystal data

$[Ag(CN)_2(C_2H_8N_2)]$	F_{000} = 428
M_r = 220.01	D_x = 2.050 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2ac 2ab	Cell parameters from 6960 reflections
a = 6.9140 (8) Å	θ = 1.8–28.7°
b = 9.3481 (11) Å	μ = 2.74 mm^{-1}
c = 11.0289 (11) Å	*T* = 173 (2) K
V = 712.83 (14) Å^3	Needle, colourless
Z = 4	0.50 × 0.20 × 0.10 mm

Data collection

Stoe IPDS II diffractometer	1913 independent reflections
Radiation source: fine-focus sealed tube	1889 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.022
T = 173(2) K	θ_{max} = 29.1°

φ and ω scans	θ_{min} = 2.9º
Absorption correction: multi-scan (MULABS in PLATON; Spek, 2003)	h = −9→9
T_{min} = 0.539, T_{max} = 0.760	k = −12→12
6842 measured reflections	l = −14→15

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0247P)^2 + 0.4752P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.016	$(\Delta/\sigma)_{max}$ = 0.001
$wR(F^2)$ = 0.042	$\Delta\rho_{max}$ = 0.46 e Å^{-3}
S = 1.08	$\Delta\rho_{min}$ = −0.51 e Å^{-3}
1913 reflections	Extinction correction: SHELXL 97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
84 parameters	Extinction coefficient: 0.0269 (10)
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), with 784 Friedel pairs (99.7%)
Secondary atom site location: difference Fourier map	Flack parameter: 0.28 (4)
Hydrogen site location: inferred from neighbouring sites	

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

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	0.31636 (2)	0.86283 (2)	0.26335 (1)	0.0170 (1)
N1	0.1329 (3)	0.7590 (2)	0.3838 (2)	0.0200 (6)
N2	0.1723 (3)	0.7398 (2)	0.13599 (18)	0.0198 (5)
N3	0.5059 (3)	1.0508 (2)	0.4625 (2)	0.0265 (6)
N4	0.5486 (4)	1.0323 (3)	0.0698 (2)	0.0269 (6)
C1	−0.0334 (4)	0.7046 (3)	0.3122 (2)	0.0247 (6)
C2	0.0448 (4)	0.6364 (3)	0.1993 (2)	0.0268 (6)
C3	0.4387 (4)	0.9800 (2)	0.3892 (2)	0.0196 (6)
C4	0.4706 (4)	0.9651 (3)	0.1414 (2)	0.0204 (6)
H1NA	0.19650	0.68450	0.42100	0.0240*
H1A	−0.12130	0.78440	0.29080	0.0300*

H1B	−0.10710	0.63360	0.36010	0.0300*
H1NB	0.09080	0.82150	0.44250	0.0240*
H2A	0.11910	0.54940	0.22070	0.0320*
H2B	−0.06310	0.60800	0.14550	0.0320*
H2NA	0.09970	0.79770	0.08630	0.0240*
H2NB	0.26030	0.69130	0.08880	0.0240*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.0170 (1)	0.0154 (1)	0.0187 (1)	−0.0005 (1)	0.0004 (1)	0.0002 (1)
N1	0.0218 (10)	0.0187 (9)	0.0195 (10)	−0.0020 (7)	0.0021 (7)	0.0031 (8)
N2	0.0204 (9)	0.0184 (9)	0.0207 (9)	−0.0039 (9)	−0.0009 (9)	−0.0017 (7)
N3	0.0250 (11)	0.0283 (11)	0.0261 (11)	−0.0039 (8)	−0.0002 (8)	−0.0037 (9)
N4	0.0252 (10)	0.0304 (11)	0.0252 (11)	−0.0051 (10)	0.0005 (9)	0.0003 (9)
C1	0.0223 (10)	0.0255 (11)	0.0264 (12)	−0.0071 (9)	0.0016 (9)	0.0010 (10)
C2	0.0318 (11)	0.0209 (9)	0.0278 (11)	−0.0119 (11)	0.0012 (10)	−0.0019 (11)
C3	0.0182 (10)	0.0195 (10)	0.0210 (11)	−0.0009 (9)	0.0016 (9)	0.0028 (9)
C4	0.0173 (10)	0.0228 (10)	0.0212 (11)	−0.0023 (9)	−0.0005 (9)	−0.0006 (9)

Geometric parameters (Å, °)

Ag1—N1	2.078 (2)	N1—H1NB	0.9200
Ag1—N2	2.071 (2)	N2—H2NA	0.9200
Ag1—C3	1.960 (2)	N2—H2NB	0.9200
Ag1—C4	1.965 (3)	C1—C2	1.500 (3)
N1—C1	1.485 (3)	C1—H1A	0.9900
N2—C2	1.483 (3)	C1—H1B	0.9900
N3—C3	1.143 (3)	C2—H2A	0.9900
N4—C4	1.144 (4)	C2—H2B	0.9900
N1—H1NA	0.9200		
N1—Ag1—N2	83.14 (8)	C2—N2—H2NA	110.00
N1—Ag1—C3	94.12 (9)	C2—N2—H2NB	110.00
N1—Ag1—C4	175.20 (10)	N1—C1—C2	107.9 (2)
N2—Ag1—C3	176.69 (10)	N2—C2—C1	109.2 (2)
N2—Ag1—C4	93.84 (9)	Ag1—C3—N3	178.2 (2)
C3—Ag1—C4	88.78 (10)	Ag1—C4—N4	174.6 (3)
Ag1—N1—C1	107.03 (15)	N1—C1—H1A	110.00
Ag1—N2—C2	109.18 (14)	N1—C1—H1B	110.00
C1—N1—H1NB	110.00	C2—C1—H1A	110.00
H1NA—N1—H1NB	109.00	C2—C1—H1B	110.00
Ag1—N1—H1NB	110.00	H1A—C1—H1B	108.00
C1—N1—H1NA	110.00	N2—C2—H2A	110.00
Ag1—N1—H1NA	110.00	N2—C2—H2B	110.00
Ag1—N2—H2NA	110.00	C1—C2—H2A	110.00
Ag1—N2—H2NB	110.00	C1—C2—H2B	110.00
H2NA—N2—H2NB	108.00	H2A—C2—H2B	108.00
N2—Ag1—N1—C1	−20.61 (15)	Ag1—N1—C1—C2	45.1 (2)

C3—Ag1—N1—C1	157.53 (16)	Ag1—N2—C2—C1	34.7 (2)
N1—Ag1—N2—C2	−7.65 (16)	N1—C1—C2—N2	−53.5 (3)
C4—Ag1—N2—C2	176.10 (17)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1NA···N4^{i}	0.92	2.27	3.099 (3)	150
N1—H1NB···N4^{ii}	0.92	2.18	3.097 (3)	172
N2—H2NA···N3^{iii}	0.92	2.10	3.002 (3)	167
N2—H2NB···N3^{i}	0.92	2.16	3.042 (3)	161

Symmetry codes: (i) −*x*+1, *y*−1/2, −*z*+1/2; (ii) −*x*+1/2, −*y*+2, *z*+1/2; (iii) −*x*+1/2, −*y*+2, *z*−1/2.

Fig. 1

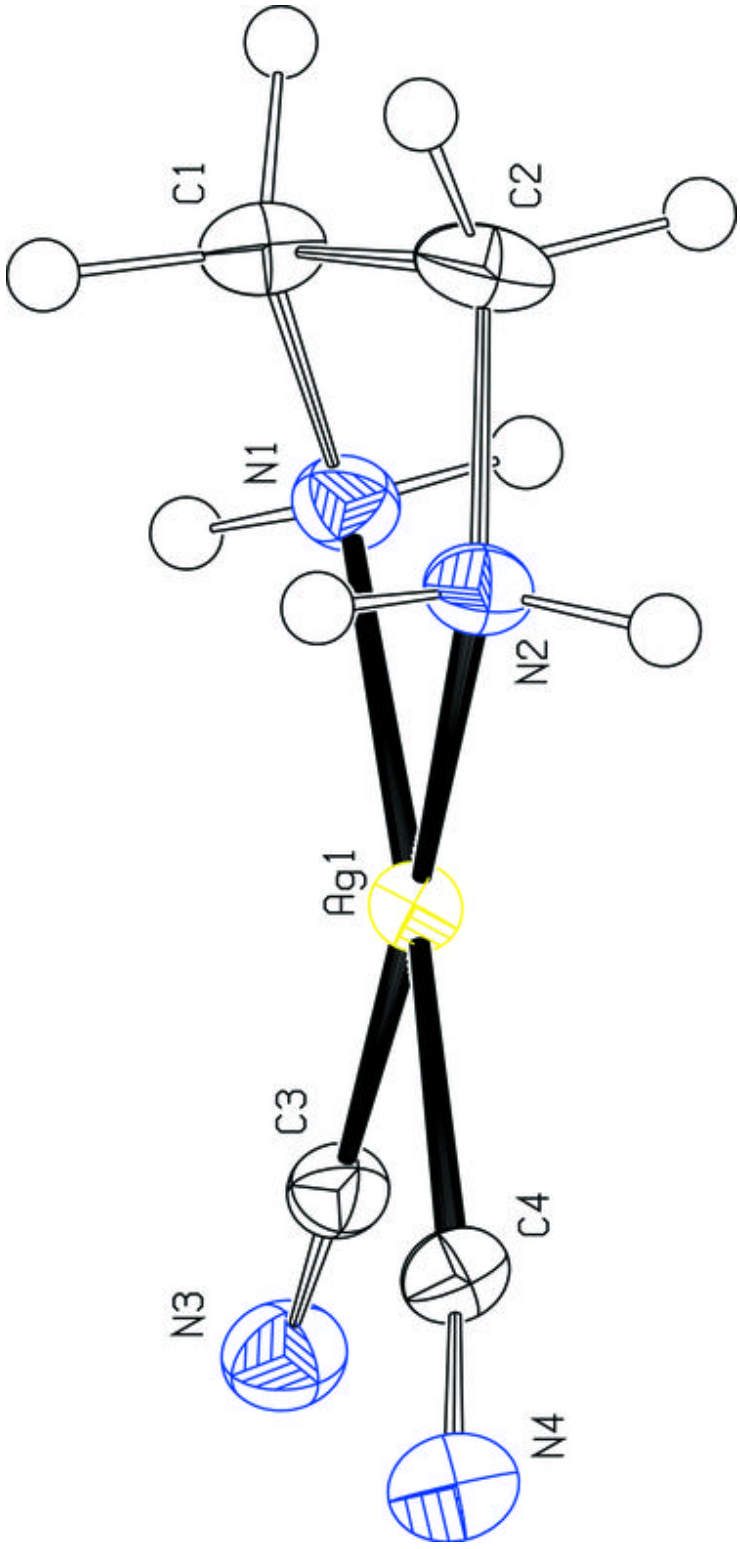

Fig. 2