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Tris(ethylenediamine-κ^2N,N')cadmium(II) bis(1,2-dicyanoethylenedithiolato-κ^2S,S')cuprate(II)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.034
wR factor = 0.095
Data-to-parameter ratio = 16.1

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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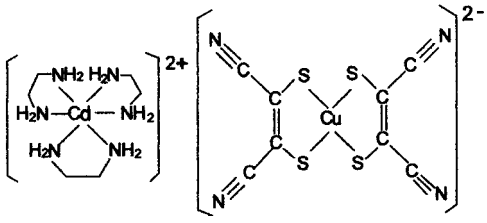
In the title complex, $[Cd(C_2H_8N_2)_3][Cu(C_4N_2S_2)_2]$, the Cd^{II} atom has a distorted octahedral geometry. The Cu^{II} atom is in a distorted square-planar geometry. Both ions lie on twofold rotation axes. They are not connected covalently.

Comment

Our previous paper reports a copper(II) complex with 2,3-dimercaptobutenedinitrile and ethylenediamine ligands (Fu *et al.*, 2004). As a subsequent part of our research on this series of complexes, we report here the crystal structure of the title compound, (I), which has the same anion as the previously reported complex.



(I)

The title compound consists of discrete $[Cd(C_2H_8N_2)_3]^{2+}$ cations and $[Cu(C_4N_2S_2)_2]^{2-}$ anions. The Cd^{II} atom in the cation is in a distorted octahedral geometry, coordinated by six N atoms of three ethylenediamine ligands (*L*1). A crystallographic twofold rotation axis in the cation passes through the Cd atom and the centre of the C7—C7^{i} bond [symmetry code: (i) $1-x, y, \frac{3}{2}-z$]. In the sixfold coordination, there are three unique Cd—N distances (Table 1). The Cu^{II} atom in the anion is coordinated by four S atoms of two 2,3-dimercaptobutenedinitrile ligands (*L*2), in a distorted square-planar geometry, and also lies on a twofold rotation axis, unlike the anion in the corresponding $[Cd(en)_3]^{2-}$ salt, which has inversion symmetry (Fu *et al.*, 2004). The Cu—S bond lengths are divided into two pairs (Table 1). All the amine N atoms in *L*1, and the nitrile N atom and mercapto S atom in *L*2, participate in intermolecular N—H···N and N—H···S hydrogen bonds, forming a three-dimensional hydrogen-bond network (Fig. 2 and Table 2).

Experimental

To a solution of $C_4H_2N_2S_2$ (1 mmol), NaOH (2 mmol) and $C_2H_8N_2$ (1.5 mmol) in ethanol (20 ml) was added an ethanol solution (10 ml) of $CuSO_4\cdot5H_2O$ (0.5 mmol) and $Cd(NO_3)_2\cdot6H_2O$ (0.5 mmol). The reaction mixture was stirred for 3 h at 313 K and part of the solvent was removed in a rotary vacuum evaporator. The resulting solution was filtered and left in air for about 6 d. Large blue crystals of (I)

were obtained. Elemental analysis found: C 26.38, H 3.72, N 22.01, S 20.05%; calculated for $C_{14}H_{24}CdCuN_{10}S_4$: C 26.41, H 3.80, N 22.08, S 20.15%.

Crystal data

$[Cd(C_2H_8N_2)_3][Cu(C_4N_2S_2)_2]$	D_x = 1.691 Mg m^{-3}
M_r = 636.61	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 3045 reflections
a = 13.490 (3) Å	θ = 2.3–25.0°
b = 12.103 (2) Å	μ = 2.06 mm^{-1}
c = 15.620 (3) Å	T = 293 (2) K
β = 101.331 (3)°	Plate, blue
V = 2500.7 (9) Å^3	0.50 × 0.50 × 0.10 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	2206 independent reflections
φ and ω scans	1828 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	R_{int} = 0.033
T_{min} = 0.426, T_{max} = 0.821	θ_{max} = 25.0°
6440 measured reflections	$h = -15 \rightarrow 16$
	$k = -14 \rightarrow 14$
	$l = -18 \rightarrow 12$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.034	$w = 1/[\sigma^2(F_o^2) + (0.062P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.095	$(\Delta/\sigma)_{max} < 0.001$
S = 1.00	$\Delta\rho_{max}$ = 1.20 e Å^{-3}
2206 reflections	$\Delta\rho_{min}$ = −0.37 e Å^{-3}
137 parameters	

Table 1
Selected geometric parameters (Å, °).

Cd1—N3	2.358 (3)	Cu1—S1	2.2559 (11)
Cd1—N5	2.382 (4)	Cu1—S2	2.2682 (12)
Cd1—N4	2.395 (3)		
N3^i—Cd1—N3	148.20 (19)	N5—Cd1—N4	85.97 (13)
N3^i—Cd1—N5	113.58 (15)	N4^i—Cd1—N4	115.99 (18)
N3—Cd1—N5	92.31 (15)	S1—Cu1—S1^i	154.45 (7)
N5—Cd1—N5^i	73.02 (19)	S1—Cu1—S2	93.81 (4)
N3—Cd1—N4^i	88.17 (11)	S1^i—Cu1—S2	92.24 (4)
N5—Cd1—N4^i	157.27 (13)	S2^i—Cu1—S2	152.36 (8)
N3—Cd1—N4	75.02 (12)		

Symmetry code: (i) $1-x, y, \frac{3}{2}-z$.

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3A···N2^{ii}	0.90	2.52	3.343 (6)	152
N3—H3B···N1^{iii}	0.90	2.36	3.235 (6)	166
N4—H4A···S1^{iv}	0.90	2.84	3.698 (4)	161
N4—H4B···N2^{v}	0.90	2.56	3.162 (5)	125
N4—H4B···S1^{vi}	0.90	2.87	3.643 (4)	145
N5—H5A···S1^{iv}	0.90	2.67	3.563 (4)	172
N5—H5B···N1^{iii}	0.90	2.70	3.572 (6)	164

Symmetry codes: (ii) $x, 1-y, z-\frac{1}{2}$; (iii) $\frac{1}{2}-x, \frac{1}{2}-y, 1-z$; (iv) $\frac{1}{2}-x, \frac{1}{2}+y, \frac{3}{2}-z$; (v) $1-x, 1-y, 2-z$; (vi) $x, 1+y, z$.

All H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H = 0.97 Å and U_{iso}(H) = 1.2U_{eq}(C), or with N—H = 0.90 Å and U_{iso}(H) = 1.2U_{eq}(N). The highest electron-density peak is 0.85 Å from Cd1.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

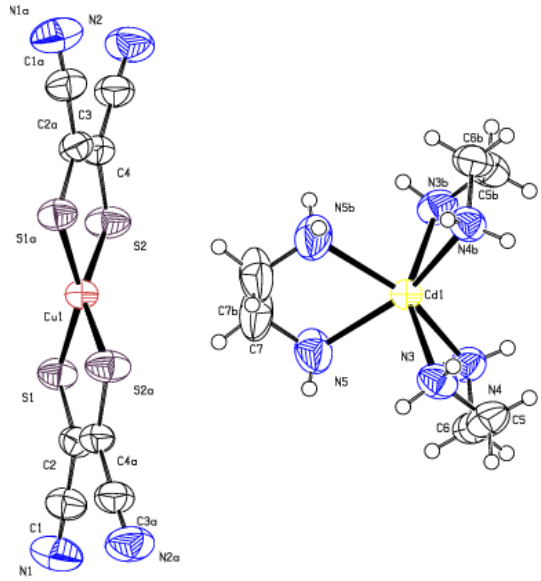


Figure 1
The structure of the title compound (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme. Suffixes a and b both correspond to symmetry code (i) in Table 1.

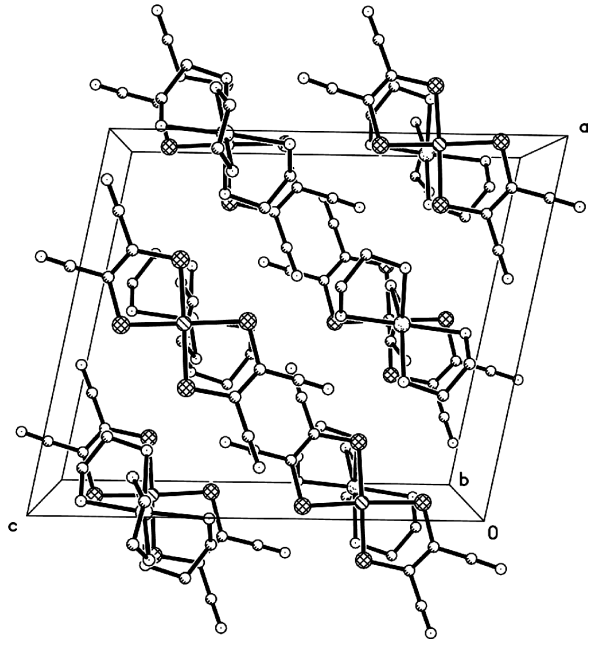


Figure 2
Crystal packing of (I), showing the N···N and N···S hydrogen-bond interactions as dashed lines. H atoms have been omitted for clarity.

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