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Poly[bis[bis(ethylenediamine)copper(II)]-tetra-μ-cyano-[tetracyanomolybdate(IV)]]

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Key indicators

Single-crystal X-ray study
T = 291 K
Mean σ(C–C) = 0.004 Å
R factor = 0.026
wR factor = 0.059
Data-to-parameter ratio = 19.0

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

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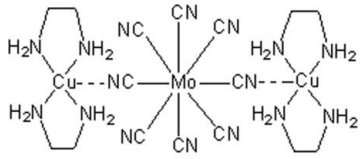
The title cyano-bridged heteronuclear coordination polymer, $[Cu_2Mo(CN)_8(C_2H_8N_2)_4]_n$, was synthesized by the reaction of $[CuL_2]^{2+}$ (L is ethylenediamine) and $[Mo(CN)_8]^{4-}$ in an aqueous solution. The structure is a three-dimensional polymer; the Cu sits on a position with twofold symmetry and the Mo sits on a position with $\bar{4}$ symmetry.

Comment

In recent decades there has been considerable interest in photomagnetic materials based on octacyanometalate precursors (Ohkoshi *et al.*, 2001; Arimoto *et al.*, 2003; Dei, 2005). Octacyanomolybdate(IV) ions, which act as good building blocks, have played an important role in realising bimetallic assemblies of photomagnetic materials. Recently, a photomagnetic high-spin molecule, $[Mo^{IV}(CN)_2(CN–Cu^{II}L)_6](ClO_4)_8$ [L = tris(2-aminoethyl)amine], was synthesized by treating potassium octacyanomolybdate(IV) with a mononuclear copper(II) complex, generated *in situ* from the tris(2-aminoethyl)amine terminal ligand L and Cu^{II} perchlorate (Herrera *et al.*, 2004). In the present study, L was replaced by ethylenediamine and the title polymer, (I), was obtained. The structure (Fig. 1) consists of $[Mo(CN)_8]^{4-}$ bonded to $[CuL_2]^{2+}$ centers by cyanide bridges in a ratio of 1:2 (Fig. 2).



(I)

Experimental

A solution of ethylenediamine (0.24 g, 4 mmol) in water (5 ml) was added to a solution of copper(II) chloride dihydrate (0.34 g, 2 mmol) in water (5 ml). The mixture was stirred for 2 min before the addition of potassium octacyanomolybdate(IV) (0.497 g, 1 mmol) dissolved in a minimum volume of water. After filtration, the solution was left to stand for several days, leading to the formation of blue needles (yield 75%). Crystals suitable for single-crystal X-ray diffraction were selected directly from the sample as prepared.

Crystal data

$[Cu_2Mo(CN)_8(C_2H_8N_2)_4]$
M_r = 671.60
Tetragonal, $P4_2/n$
a = 9.2676 (7) Å
c = 15.550 (2) Å
V = 1335.6 (2) Å^3
Z = 2
D_x = 1.670 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 2.08 mm^{-1}
T = 291 (2) K
Needle, blue
0.36 × 0.17 × 0.08 mm

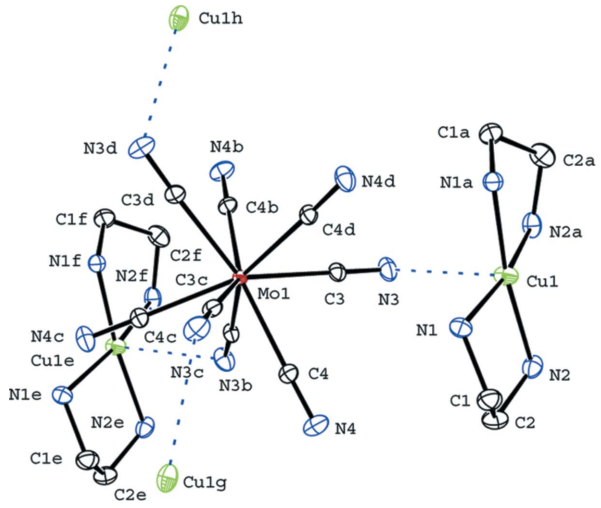


Figure 1
The structure (30% probability displacement ellipsoids) of the title compound. H atoms are not shown for clarity. The dashed lines represent weak bonds. [Symmetry codes: (a) x, y, z; (b) $-x+\frac{1}{2}, -y+\frac{1}{2}, z$; (c) $-y, x+\frac{1}{2}, z+\frac{1}{2}$; (d) $y+\frac{1}{2}, -x, z+\frac{1}{2}$; (e) $x-\frac{1}{2}, y-\frac{1}{2}, -z$; (f) $y, -x-\frac{1}{2}, -z-\frac{1}{2}$; (g) $-y-\frac{1}{2}, x, -z-\frac{1}{2}$.]

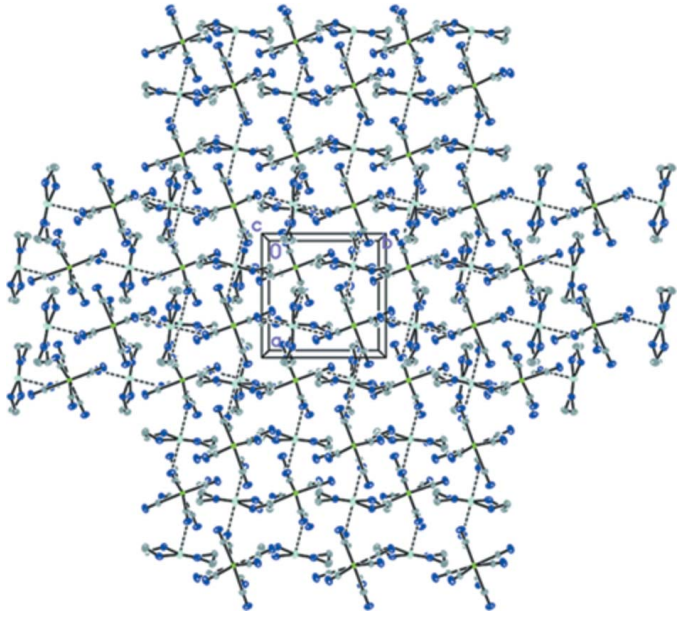


Figure 2
View, along the *c* axis, of the packing of the title compound.

Data collection

Bruker SMART APEX-II diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.524$, $T_{max} = 0.848$
5810 measured reflections
1524 independent reflections
1215 reflections with $I > 2\sigma(I)$
$R_{int} = 0.072$
$\theta_{max} = 27.5^{\circ}$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.027$
$wR(F^2) = 0.059$
$S = 0.96$
1524 reflections
80 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0203P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.52$ e Å^{-3}
$\Delta\rho_{min} = -0.50$ e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···N4^{i}	0.90	2.12	3.004 (3)	168
N2—H2A···N4^{ii}	0.90	2.36	3.150 (3)	147
N2—H2B···N3^{iii}	0.90	2.60	3.084 (3)	115

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

H atoms were placed in calculated positions (N—H = 0.90 Å and C—H = 0.97 Å) and refined as riding, with $U_{iso}(H) = 1.2U_{eq}(N)$ and $1.2U_{eq}(C)$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 1995); software used to prepare material for publication: *SHELXTL*.

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