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Rerefinement of *catena*-poly[[bis(2-pyrrolidone-κO)cobalt(II)]-di-μ-1,5-dicyanamido-$\kappa^4N^1:N^5$] in the centrosymmetric space group *C*2/*m*

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Key indicators

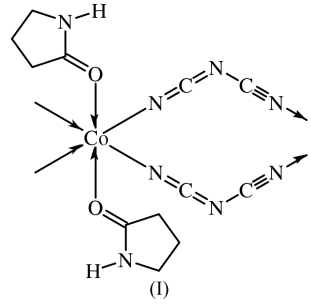
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.030
wR factor = 0.082
Data-to-parameter ratio = 14.0

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

The structure of the title compound, $[Co(C_2N_3)_2(C_4H_7NO)_2]_n$, which was reported in space group *Cm* [Sun *et al.* (2001). *Inorg. Chem. Commun.* **4**, 72–75], was rerefined in the centrosymmetric space group *C*2/*m* to reveal a close analogy with the structure of the Co–dicyanamide complex with *N*,*N*-dimethylformamide. The Co atom and the dicyanamide bridging ligand occupy special positions of symmetry 2/*m* and *m*, respectively.

Comment

The structure of the title compound, (I), which was reported in space group *Cm* (Sun *et al.*, 2001), was rerefined in the centrosymmetric space group *C*2/*m* to reveal a close analogy with the structure of the Co–dicyanamide complex with *N*,*N*-dimethylformamide (Tong *et al.*, 2003). A pair of L-shaped dicyanamido anions link the bis(2-pyrrolidone)cobalt(II) units into a linear chain running along the *b* axis of the crystal (Fig. 1). The Co atom and the dicyanamide bridging ligand occupy special positions of symmetry 2/*m* and *m*, respectively. Adjacent chains are linked by an N—H···N hydrogen bond [N···N = 3.072 (3) Å], giving rise to layers parallel to the *ab* plane of the crystal (Fig. 2). The same paper by Sun *et al.* (2001) also mentions the isostructural Mn complex. This structure has been rerefined in space group *C*2/*m* (Ng, 2003).



(I)

Experimental

The synthesis of the title compound is detailed in the report by Sun *et al.* (2001).

Crystal data

$[Co(C_2N_3)_2(C_4H_7NO)_2]$
M_r = 361.24
Monoclinic, *C*2/*m*
a = 15.420 (3) Å
b = 7.220 (1) Å
c = 6.950 (1) Å
β = 112.94 (3)°
V = 712.6 (2) Å^3
Z = 2
D_x = 1.684 Mg m^{-3}
Mo *K*α radiation
Cell parameters from 6994 reflections
θ = 4.1–28.5°
μ = 1.23 mm^{-1}
T = 298 (2) K
Block, pink
0.25 × 0.23 × 0.23 mm

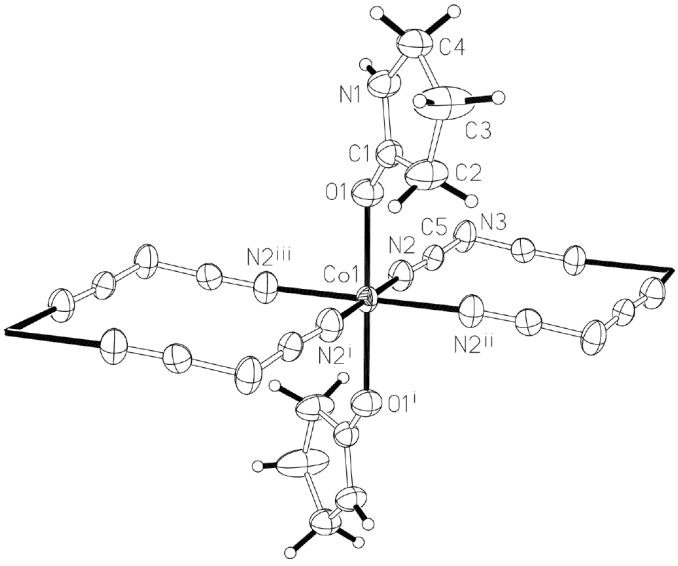


Figure 1
*ORTEP*II (Johnson, 1976) plot depicting a fragment of the structure. Displacement ellipsoids are drawn at the 50% probability level; H atoms are shown as small spheres of arbitrary radii. [Symmetry codes: (i) $1-x$, $1-y$, $1-z$; (ii) x, $1-y$, z; (iii) $1-x$, y, $1-z$.]

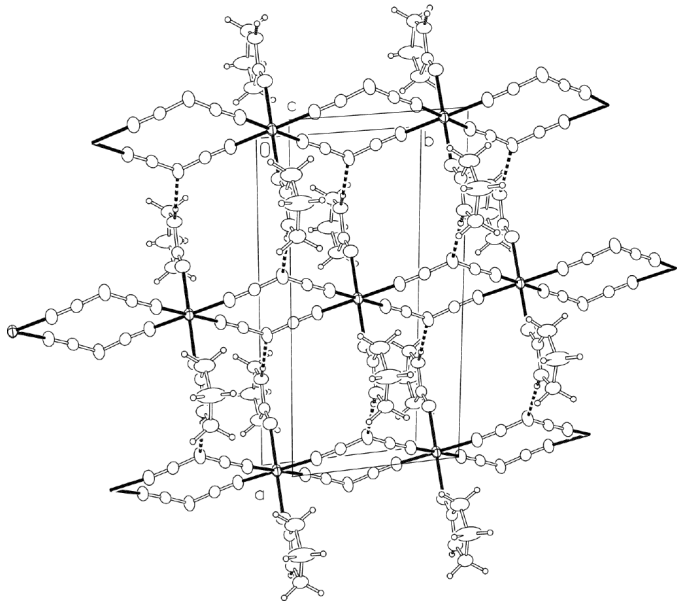


Figure 2
*ORTEP*II (Johnson, 1976) plot of the hydrogen-bonded layer structure.

Data collection

Nonius KappaCCD diffractometer	903 reflections with $I > 2\sigma(I)$
φ scans	$R_{int} = 0.033$
Absorption correction: multi-scan (Blessing, 1995)	$\theta_{max} = 28.5^\circ$
$T_{min} = 0.712$, $T_{max} = 0.754$	$h = -20 \rightarrow 20$
6996 measured reflections	$k = -9 \rightarrow 9$
949 independent reflections	$l = -9 \rightarrow 9$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0546P)^2 + 0.4762P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.030$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.082$	$\Delta\rho_{max} = 0.43$ e Å^{-3}
$S = 1.03$	$\Delta\rho_{min} = -0.41$ e Å^{-3}
949 reflections	
68 parameters	
H atoms treated by a mixture of independent and constrained refinement	

The diffraction measurements were those used in the original refinement (Sun *et al.*, 2001). The aliphatic H atoms were positioned geometrically (C—H = 0.97 Å) and were allowed to ride on their parent C atoms in the riding-model approximation; their displacement parameters were set to 1.2 times U_{eq} of the C atoms. The amide H atom was located and refined [N1—H1 = 0.83 (3) Å].

Data collection: *KappaCCD Software* (Nonius, 1998); cell refinement: *HKL SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* (Otwinowski & Minor, 1997) and *SCALEPACK*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

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