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#### Key indicators

Single-crystal X-ray study  
T = 295 K  
Mean  $\sigma(\text{C}-\text{C}) = 0.009 \text{ \AA}$   
R factor = 0.068  
wR factor = 0.160  
Data-to-parameter ratio = 12.9

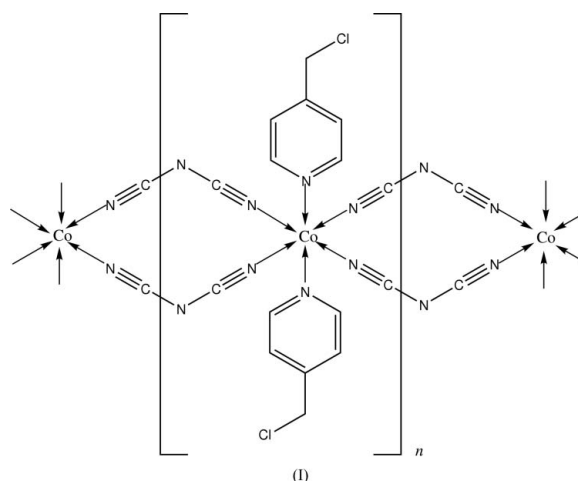
For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

## catena-Poly[[bis(4-chloromethylpyridine- $\kappa\text{N}$ )-cobalt(II)]-di- $\mu$ -dicyanamido- $\kappa^2\text{N}^1:\kappa^2\text{N}^5$ ]

The title compound,  $[\text{Co}(\text{C}_2\text{N}_3)(\text{C}_6\text{H}_6\text{ClN})_2]_n$ , is a polymeric cobalt(II) complex with the metal ion located on an inversion centre. The  $\text{Co}^{\text{II}}$  ion is six-coordinated by two N atoms of two 4-chloromethylpyridine ligands and four N atoms from four dicyanamide ligands, forming a slightly distorted octahedral configuration. In the crystal structure, neighbouring Co atoms are linked together by double dicyanamide bridges to form a polymeric cobalt(II) complex.

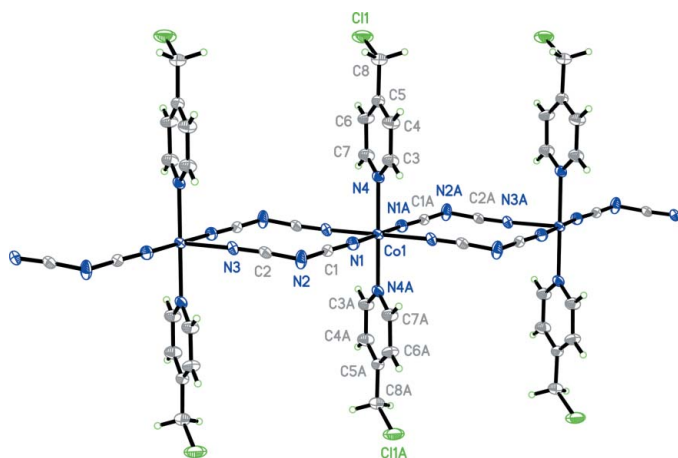
#### Comment

To date, the dicyanamide ligand has frequently been used to bridge polynuclear transition metal complexes in the study of multidimensional molecule-based magnetic materials and other areas. Many such compounds have been reported. Most of them are focused on low-oxidation state systems, such as  $M^{\text{I}}$  (Britton, 1990; Batten *et al.*, 2000; Bessler *et al.*, 2000) and  $M^{\text{II}}$  (Manson *et al.*, 1998; Claramunt *et al.*, 2000; Dasna, *et al.*, 2000; Jensen *et al.*, 2000; Sun, Gao, Ma, Niu & Wang, 2000; Triki *et al.*, 2001; Shi *et al.*, 2002) ( $M^{\text{I}} = \text{Cu}$  or  $\text{Ag}$ ;  $M^{\text{II}} = \text{Cd}$ ,  $\text{Cu}$ ,  $\text{Co}$ ,  $\text{Ni}$ ,  $\text{Zn}$ ,  $\text{Mn}$  or  $\text{Fe}$ ). Cobalt complexes have been synthesized previously but the different kinds of interactions observed for  $\text{Co}^{\text{II}}$  are still not clear and deserve the attention of magnetochemists (Marshall *et al.*, 2000; Sun, Gao, Ma, Niu & Wang, 2000; Sun, Gao, Ma & Wang, 2000; Jäger *et al.*, 2001; Jensen *et al.*, 2001). Here, we report the structure of the title  $\text{Co}^{\text{II}}$  compound, (I).



The structure of (I) is illustrated in Fig. 1, and selected bond distances and angles are given in Table 1. The  $\text{Co}^{\text{II}}$  ion, which lies on an inversion centre, is in an octahedral geometry and is six-coordinated by six N atoms, from four dicyanamide ligands and two 4-chloromethylpyridine ligands in a *trans* arrange-

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**Figure 1**  
Part of the polymeric structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (A)  $1 - x, 1 - y, 1 - z$ .]

ment. The resulting coordination geometry is very close to that expected for an ideal octahedral complex.

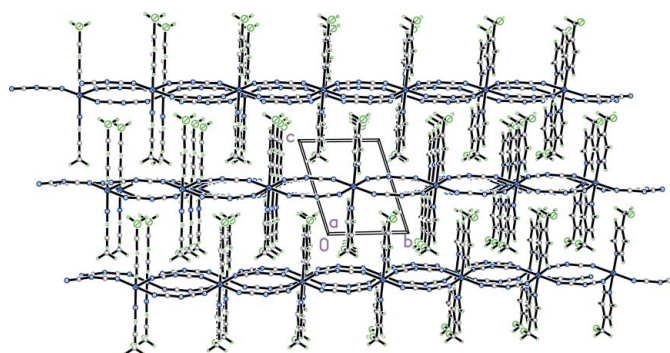
In the crystal structure, the  $\text{Co}^{\text{II}}$  ions are bridged to form a one-dimensional chain along the [010] axis by dicyanamide ligands, through single end-to-end coordination, *i.e.* the dicyanamide ligand acts as a bidentate bridging ligand by coordinating to adjacent  $\text{Co}^{\text{II}}$  centres through its two terminal nitrile N atoms. No significant contacts are observed between adjacent chains in the crystal structure. Neighbouring benzene rings of the 4-chloromethylpyridine ligands along a chain do not display  $\pi$ - $\pi$  interactions, the distance between the centroids of the rings being 7.4810 (9) Å (Fig. 2).

## Experimental

All chemicals were of reagent grade quality, obtained from commercial sources and used without further purification. A mixture of  $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$  (120 mg, 0.504 mmol) and 4-chloromethylpyridine (90 mg, 0.549 mmol) was dissolved in methanol (10 ml) with stirring. To this solution was added an aqueous solution (5 ml) of dicyanamide (90 mg, 1.01 mmol), with stirring. The solution was refluxed for 30 min and then filtered. After allowing the filtrate to evaporate in air for 24 h, well shaped red needles of (I) were obtained (70% yield). Analysis, found: C 43.85, H 2.61, N 26.09%; calculated for  $\text{C}_{16}\text{H}_{12}\text{Cl}_2\text{CoN}_8$ : C 43.03, H 2.69, N, 25.10%.

### Crystal data

$[\text{Co}(\text{C}_2\text{N}_3)(\text{C}_6\text{H}_6\text{ClN})_2]$	$Z = 1$
$M_r = 446.17$	$D_x = 1.624 \text{ Mg m}^{-3}$
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 7.2910(9) \text{ \AA}$	Cell parameters from 668 reflections
$b = 7.4810(9) \text{ \AA}$	$\theta = 2.3\text{--}25.1^\circ$
$c = 9.0070(13) \text{ \AA}$	$\mu = 1.25 \text{ mm}^{-1}$
$\alpha = 104.444(2)^\circ$	$T = 295(2) \text{ K}$
$\beta = 96.971(2)^\circ$	Needle, red
$\gamma = 102.618(2)^\circ$	$0.44 \times 0.14 \times 0.10 \text{ mm}$
$V = 456.15(10) \text{ \AA}^3$	



**Figure 2**  
The crystal packing of (I), viewed along the [100] axis.

### Data collection

Bruker APEX area-detector diffractometer	1601 independent reflections
$\varphi$ and $\omega$ scans	1368 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Bruker, 2002)	$R_{\text{int}} = 0.040$
$T_{\text{min}} = 0.805, T_{\text{max}} = 0.885$	$\theta_{\text{max}} = 25.2^\circ$
2408 measured reflections	$h = -8 \rightarrow 6$
	$k = -8 \rightarrow 8$
	$l = -9 \rightarrow 10$

### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0336P)^2 + 2.6609P]$
$R[F^2 > 2\sigma(F^2)] = 0.068$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.160$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.09$	$\Delta\rho_{\text{max}} = 0.49 \text{ e \AA}^{-3}$
1601 reflections	$\Delta\rho_{\text{min}} = -0.78 \text{ e \AA}^{-3}$
124 parameters	
H-atom parameters constrained	

**Table 1**

Selected geometric parameters (Å, °).

$\text{Co1}-\text{N3}^{\text{i}}$	2.121 (5)	$\text{Co1}-\text{N4}$	2.154 (4)
$\text{Co1}-\text{N1}$	2.129 (5)		
$\text{N3}^{\text{i}}-\text{Co1}-\text{N1}$	92.10 (19)	$\text{N3}^{\text{ii}}-\text{Co1}-\text{N4}$	88.90 (18)
$\text{N3}^{\text{ii}}-\text{Co1}-\text{N1}$	87.90 (19)		

Symmetry codes: (i)  $x, y - 1, z$ ; (ii)  $-x + 1, -y + 2, -z + 1$ .

H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances constrained to 0.93 (aromatic CH) or 0.97 Å (methylene  $\text{CH}_2$ ) and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{carrier C atom})$ .

Data collection: SMART (Bruker, 2002); cell refinement: SAINT (Bruker, 2002); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 2002); software used to prepare material for publication: SHELXTL.

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