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A two-dimensional cobalt(II) coordination polymer: poly[chloro(μ-imidazole-1,3-diyldiacetato-$\kappa^4O:O':O'':O'''$)cobalt(II)]

Xian-Fa Zhang, Shan Gao,* Li-Hua Huo and Hui Zhao

Laboratory of Functional Materials, School of Chemistry and Materials Science, Heilongjiang University, Harbin 150080, People's Republic of China

Correspondence e-mail: shangao67@yahoo.com

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In the title coordination polymer, $[Co(IDA)Cl]_n$ (IDA^- is the imidazolyl-1,3-diyldiacetate anion, $C_7H_7N_2O_4$), each Co^{2+} cation has an octahedral geometry, defined by four O atoms from four different IDA^- anions and two Cl^- anions. The IDA^- anion serves as a bridging ligand to link the Co^{2+} cations into a two-dimensional layer structure. The Co atom lies on a centre of symmetry. The Cl atom and one CH group of the imidazole ring lie on twofold rotation axes.

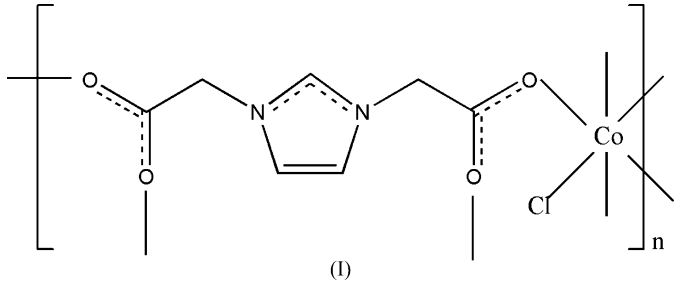
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 Å
R factor = 0.028
wR factor = 0.072
Data-to-parameter ratio = 14.8

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

Comment

1,3-Bis(carboxymethyl)imidazole represents the first member of a new class of *N*-heterocyclic amino acids. The deprotonated monoanion is, interestingly, a zwitterionic aminoacetate anion having two $-CH_2CO_2^-$ arms which can each bind to a metal centre. Its metal derivatives have been reported only very recently and are so far limited to the barium, caesium, calcium, strontium, cobalt and zinc derivatives (Fei, Ang *et al.*, 2006; Fei, Geldbach *et al.*, 2005, 2006; Fei, Zhao *et al.*, 2005); the interest in these compounds arises from the nature of the water aggregates. Recently, we reported the structure of a two-dimensional Cd^{II} polymer, namely $[Cd(IDA)_2]_n$ (where IDA^- is the imidazolyl-1,3-diyldiacetate anion, $C_7H_7N_2O_4$) (Zhang *et al.*, 2006), in which each IDA^- ligand acts in a bis-bidentate chelating mode to connect the Cd^{II} atoms, forming a two-dimensional layer structure. In our further efforts to investigate the behaviour of the IDA^- ligand, we have synthesized the title Co^{II} polymer $[Co(IDA)Cl]_n$, (I), and report its structure here.



(I)

As shown in Fig. 1, the asymmetric unit of (I) comprises half of a Co^{2+} cation, half of an IDA^- anion and half of a coordinated Cl^- anion. The Co atom lies on a centre of symmetry. The Cl atom and atoms C3, H3 of the imidazole ring lie on twofold rotation axes. Each Co^{2+} cation has an octahedral coordination geometry, defined by four O atoms from four IDA^- ligands and two Cl^- anions (Table 1). The equatorial plane is defined by atoms O2, $O2^{ii}$, $O1^{i}$ and $O1^{iii}$ [symmetry

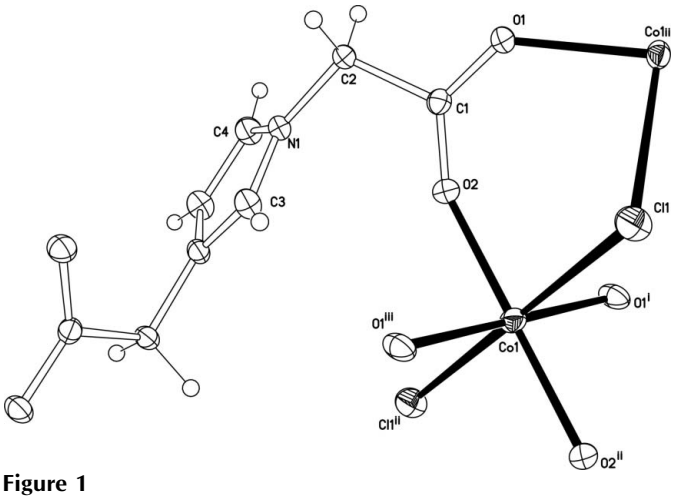


Figure 1
Part of the polymeric structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry codes: (i) $-x$, y, $-z+\frac{1}{2}$; (ii) $-x$, $-y+1$, $-z+1$; (iii) x, $-y+1$, $z+\frac{1}{2}$].

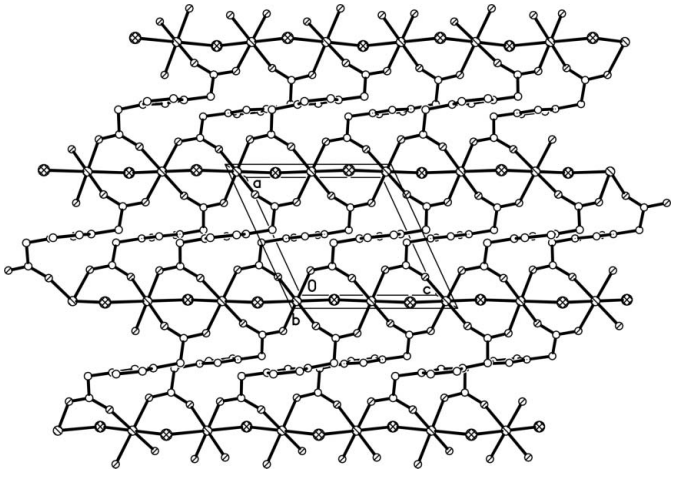


Figure 2
A packing diagram for (I). H atoms have been omitted for clarity.

codes: (i) $-x$, y, $-z+\frac{1}{2}$; (ii) $-x$, $-y+1$, $-z+1$; (iii) x, $-y+1$, $z+\frac{1}{2}$]. Atoms Cl1 and Cl1^{ii} occupy the axial sites.

The C—O bonds (Table 1) in the carboxylate group indicate an even delocalization of the bonding. In addition, each Cl^- anion bridges two Co^{2+} cations, forming a one-dimensional chain structure. The IDA^- anion, as a tetradentate bridging ligand, links the chains into a two-dimensional layer structure (Fig. 2).

Experimental

1,3-Bis(carboxymethyl)imidazole was synthesized according to the literature method of Kratochvíl *et al.* (1988). Cobalt dichloride (1.30 g, 10 mmol) and 1,3-bis(carboxymethyl)imidazole (1.84 g, 10 mmol) were dissolved in a 1:1 ethanol–water solution (25 ml). The mixture was sealed in a 50 ml Teflon-lined stainless steel bomb. The bomb was heated at 393 K for 3 d, and then cooled to room temperature to yield pink crystals of the title compound.

Crystal data

$[Co(C_7H_7N_2O_4)Cl]$	$Z = 4$
$M_r = 277.53$	$D_x = 1.999$ Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
$a = 7.7105$ (15) Å	$\mu = 2.14$ mm^{-1}
$b = 16.322$ (3) Å	$T = 295$ (2) K
$c = 8.0745$ (16) Å	Prism, pink
$\beta = 114.85$ (3)°	0.30 × 0.26 × 0.16 mm
$V = 922.1$ (4) Å^3	

Data collection

Rigaku R-AXIS RAPID IP diffractometer	4407 measured reflections
ω scans	1052 independent reflections
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	919 reflections with $I > 2\sigma(I)$
$T_{min} = 0.535$, $T_{max} = 0.715$	$R_{int} = 0.036$
	$\theta_{max} = 27.4°$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0341P)^2 + 0.88P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.028$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.072$	$\Delta\rho_{max} = 0.53$ e Å^{-3}
$S = 1.07$	$\Delta\rho_{min} = -0.39$ e Å^{-3}
1052 reflections	
71 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Co1—O2	2.0426 (15)	O1—C1	1.254 (2)
Co1—O1^{i}	2.0726 (16)	O2—C1	1.245 (2)
Co1—Cl1	2.6290 (7)		
Cl1^{ii}—Co1—Cl1	180.0		

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

H atoms were positioned geometrically, with C—H = 0.93 and 0.97 Å for aromatic and methylene H, respectively, and constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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