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Key indicators

Single-crystal X-ray study
 T = 295 K
 Mean $\sigma(C-C) = 0.008 \text{ \AA}$
 H-atom completeness 96%
 Disorder in solvent or counterion
 R factor = 0.072
 wR factor = 0.201
 Data-to-parameter ratio = 14.4

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

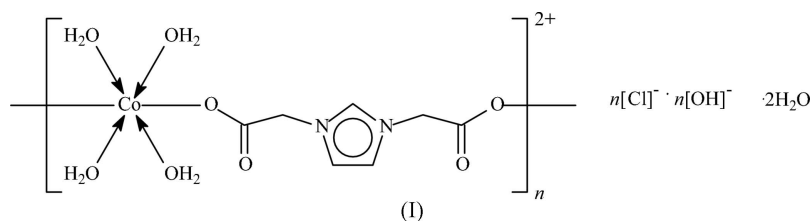
catena-Poly[[[tetraaquacobalt(III)]- μ -1*H*-imidazole-1,3-diylacetato- κ^2 O:O'] chloride hydroxide dihydrate]

In the crystal structure of the title compound, $[\text{Co}(\text{C}_7\text{H}_7\text{N}_2\text{O}_4)(\text{H}_2\text{O})_4]\text{Cl}(\text{OH})\cdot 2\text{H}_2\text{O}$, the cations form a polycationic chain that propagates along the *b* axis of the monoclinic unit cell. The Co^{III} atom and two coordinated water molecules lie on special positions of site symmetry *m*. The $\text{C}_7\text{H}_7\text{N}_2\text{O}_4$ anion displays crystallographic mirror symmetry. The chloride and hydroxide anions are disordered and they interact, along with the uncoordinated water molecule, with the polycationic chain to form a three-dimensional, hydrogen-bonded network.

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Comment

A previous study documents the structure of the cadmium(II) derivative of 1,3-bis(carboxymethyl)imidazole; the zwitterionic organic ligand when deprotonated is another zwitterion that exists as a negatively charged monoanion. This meatl carboxylate is an anhydrous compound whose metal center shows square-prismatic coordination as it is chelated by four different carboxylate $-\text{CO}_2$ portions of the monoanion (Zhang *et al.*, 2006). A similar synthesis with cobalt(II) chloride yields the covalently bonded cobalt(III) mono(carboxylate), but the metal undergoes oxidation to the trivalent state; the 2+ charge of the (imidazolyl-1,3-diylacetato)cobalt(III) species is balanced by a chloride anion and a hydroxide anion. The formula unit is completed by four coordinated water and two uncoordinated water molecules (I) (Fig. 1). The Co^{III} atom and two coordinated water molecules lie on special positions of site symmetry *m*. The $\text{C}_7\text{H}_7\text{N}_2\text{O}_4$ anion displays crystallographic mirror symmetry. The cobalt(III) atom is linked to the carboxylate groups of two anions that are *cis* to each other in the octahedral geometry. The monoanions link the water-coordinated metal atoms into a linear chain that runs along the *b* axis of the monoclinic unit cell. The uncoordinated water molecules and the chloride and hydroxide anions interact with the polycationic chain (Table 2), forming a three-dimensional network.



Experimental

Cobalt dichloride (1.30 g, 10 mmol) was added to 1,3-bis(carboxymethyl)imidazole (1.84 g, 10 mmol) dissolved in a 1:1 mixture of

ethanol and water (20 ml). The mixture was placed in a 50 ml Teflon-lined stainless steel bomb which was heated at 393 K for 72 h. The bomb was cooled to room temperature, and the pink prismatic crystals that separated were picked out by hand.

Crystal data

[Co(C ₇ H ₇ N ₂ O ₄)(H ₂ O) ₄]- Cl(OH)·2H ₂ O	$V = 800.2(9) \text{ \AA}^3$
$M_r = 402.63$	$Z = 2$
Monoclinic, $P2_1/m$	$D_x = 1.671 \text{ Mg m}^{-3}$
$a = 5.245(4) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 11.744(7) \text{ \AA}$	$\mu = 1.29 \text{ mm}^{-1}$
$c = 13.030(7) \text{ \AA}$	$T = 295(2) \text{ K}$
$\beta = 94.45(3)^\circ$	Prism, pink
	$0.34 \times 0.24 \times 0.18 \text{ mm}$

Data collection

Rigaku R-Axis RAPID IP diffractometer	7919 measured reflections
ω scan	1920 independent reflections
Absorption correction: multi-scan (<i>ABSCOR</i> ; Higashi, 1995)	1506 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.393$, $T_{\max} = 0.801$	$R_{\text{int}} = 0.075$
	$\theta_{\text{max}} = 27.5^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.079P)^2 + 3.1848P]$
$R[F^2 > 2\sigma(F^2)] = 0.072$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.201$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.13$	$\Delta\rho_{\text{max}} = 0.84 \text{ e \AA}^{-3}$
1920 reflections	$\Delta\rho_{\text{min}} = -0.69 \text{ e \AA}^{-3}$
133 parameters	
H atoms treated by a mixture of independent and constrained refinement	

Table 1

Selected geometric parameters (\AA , $^\circ$).

Co1—O1	2.115 (4)	Co1—O2w	2.088 (6)
Co1—O1w	2.048 (6)	Co1—O3w	2.139 (4)
O1—Co1—O1 ⁱ	95.4 (2)	O1w—Co1—O2w	175.3 (3)
O1—Co1—O1w	91.7 (2)	O1w—Co1—O3w	91.3 (2)
O1—Co1—O2w	85.1 (2)	O2w—Co1—O3w	92.2 (2)
O1—Co1—O3w	174.2 (2)	O3w—Co1—O3w ⁱ	85.4 (2)
O1—Co1—O3w ⁱ	89.6 (2)		

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

Table 2

Hydrogen-bond geometry (\AA , $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1w—H1w1 \cdots O4w	0.85 (1)	1.92 (3)	2.731 (8)	160 (7)
O3w—H3w2 \cdots O1 ⁱⁱ	0.85 (1)	2.11 (3)	2.881 (6)	150 (5)
O3w—H3w1 \cdots O2 ⁱ	0.85 (1)	1.92 (3)	2.700 (5)	152 (6)
O4w—H4w1 \cdots Cl1	0.85 (1)	2.15 (5)	2.945 (8)	156 (10)
O4w—H4w2 \cdots O3 ⁱⁱⁱ	0.85 (1)	2.17 (6)	2.91 (2)	145 (10)

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

The chloride and hydroxide ions are disordered with partial occupancies of 0.46 (1) and 0.54 (1), respectively. The occupancies of

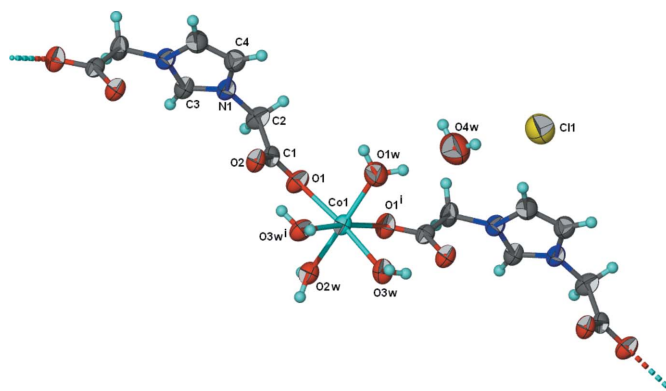


Figure 1

Part of the polycationic chain structure in (I), along with the ordered uncoordinated water molecule and the disordered chloride anion. The disordered hydroxide ion is not shown. Displacement ellipsoids are drawn at the 70% probability level and H atoms as spheres of arbitrary radii. [Symmetry code: (i) $x, \frac{1}{2} - y, z$.]

the disordered atoms Cl1 and O3 were later fixed at 0.50 each. If the two ions are excluded, the *SQUEEZE* procedure in *PLATON* (Spek, 2003) estimates the presence of 31 electrons in two 60 \AA^3 voids. The 15.5 electron count is in agreement with a mixed chloride/hydroxide species.

C-bound H atoms were positioned geometrically ($C-H = 0.93$ or 0.97 \AA) and were included in the riding-model approximation, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. Water H atoms were located in a difference Fourier map and were refined with distance restraints of $O-H = 0.85(1) \text{ \AA}$ and $H\cdots H = 1.39(1) \text{ \AA}$, and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{O})$. The H atom on the hydroxide ion could not be placed in any chemically sensible position.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MS, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2006).

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