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Diaquabis(1*H*-imidazole-4,5-dicarboxylato-κN^3)-cobalt(II) *N*,*N*-dimethylformamide disolvate

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Key indicators

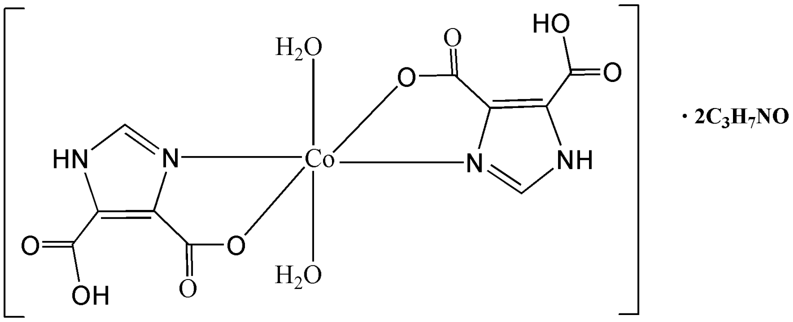
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.051
wR factor = 0.115
Data-to-parameter ratio = 11.7

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

In the title compound, $[Co(C_5H_3O_4)_2(H_2O)_2]\cdot 2C_3H_7NO$, the octahedrally coordinated Co^{II} atom lies on an inversion centre. The equatorial plane of the octahedron comprises two bidentate 1*H*-imidazole-4,5-dicarboxylate monoanions, coordinated through the N-3 atoms, and one carboxylate O atom, with two water molecules in the axial coordination sites. A one-dimensional chain structure is formed by intermolecular hydrogen bonds in the equatorial plane, between the uncoordinated N atom in the imidazole ring and an uncoordinated carboxyl O atom. The two O atoms of the coordinated water molecules in each chain are engaged in two hydrogen bonds with the uncoordinated carboxyl O atoms of two adjacent chains, forming a two-dimensional network structure.

Comment

N-Heterocyclic carboxylic acids, such as pyrazine-2,3-dicarboxylic acid, pyrazine-2-carboxylic acid, pyridine-3,5-dicarboxylic acid, pyridine-2,6-dicarboxylic acid, pyrazole-3,5-dicarboxylic acid and imidazole-4,5-dicarboxylic acid, are recognized as efficient N,O-donors, exhibiting diverse modes of coordination (Min *et al.*, 2001; Sanna *et al.*, 1998; Sengupta *et al.*, 2001; Tian *et al.*, 2003; Wang *et al.*, 2001; Xiang *et al.*, 2004). In this work, we have chosen 1*H*-imidazole-4,5-dicarboxylic acid as the building block to obtain the title compound, (I).



(I)

In (I), the Co^{II} atom lies on an inversion centre and has a slightly distorted octahedral environment (Fig. 1 and Table 1). The equatorial plane contains two bidentate 1*H*-imidazole-4,5-dicarboxylate monoanionic ligands [O1, $O1^i$, N1 and $N1^i$; symmetry code: (i) $2 - x$, $2 - y$, $2 - z$], forming five-membered chelate rings. Two coordinated water molecules (O6 and $O6^i$) occupy the apical sites. The coordinated carboxylate group and the free carboxylic acid residue are almost coplanar, with a mean deviation of 0.016 (3) Å.

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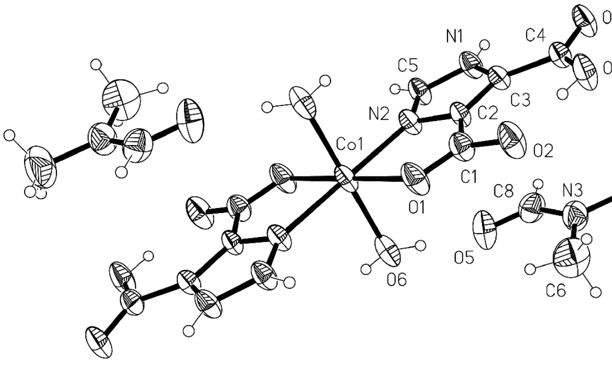

Figure 1
The coordination environment of the Co1 atom in (I), showing the atom numbering, with displacement ellipsoids drawn at the 50% probability level. Unlabelled atoms are related to labelled atoms by the symmetry code (2 − x, 2 − y, 2 − z).

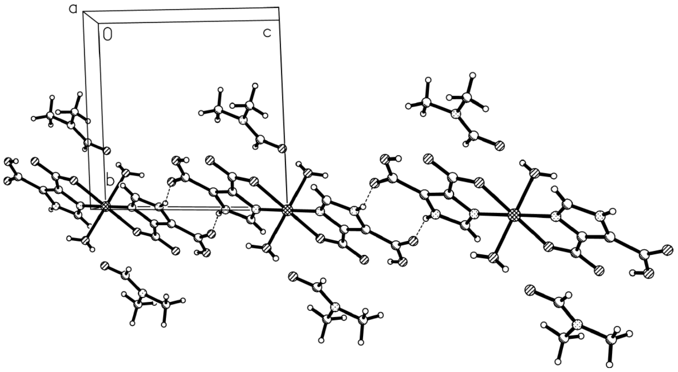

Figure 2
The one-dimensional chain structure formed by N—H···O hydrogen bonds (dashed lines).

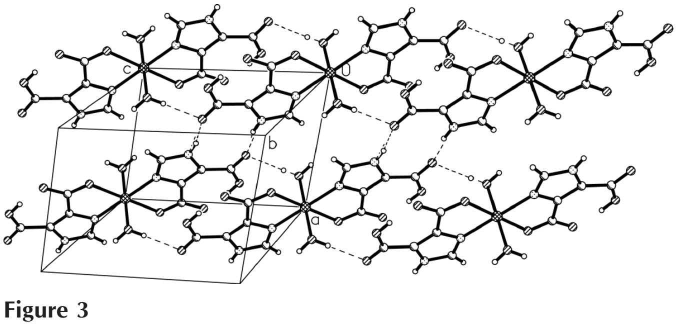

Figure 3
The two-dimensional network structure formed by N—H···O and O—H···O hydrogen bonds (dashed lines). For clarity, the *N*,*N*-dimethylformamide molecules have been omitted.

The uncoordinated N atom in the imidazole ring forms an intermolecular hydrogen bond with an uncoordinated carboxyl O atom, with a distance of 2.824 (4) Å, forming a one-dimensional chain structure (Fig. 2). The two O atoms of the coordinated water in each chain are also involved in hydrogen bonds, with the uncoordinated carboxyl O atoms of two adjacent chains, to yield a two-dimensional network structure (Fig. 3). There are also two other intermolecular hydrogen-bonding interactions between two O atoms of the coordinated water molecules and O atoms of two *N*,*N*-dimethylformamide solvent molecules.

Experimental

A solution (15 ml) of $CoCl_2\cdot 6H_2O$ (0.25 mmol) and imidazole-4,5-dicarboxylic acid (0.25 mmol) in *N*,*N*-dimethylformamide and water was added slowly to a solution of 1,10-phenanthroline (0.5 mmol) in methanol (5 ml). The mixture was left to stand at room temperature for about three weeks to afford red crystals of the title compound.

Crystal data

$[Co(C_5H_3O_4)_2(H_2O)_2]\cdot 2C_3H_7NO$
$M_r = 551.34$
Triclinic, $P\overline{1}$
$a = 6.9316\ (9)$ Å
$b = 9.1453\ (11)$ Å
$c = 9.3055\ (11)$ Å
$\alpha = 87.093\ (2)^\circ$
$\beta = 77.229\ (2)^\circ$
$\gamma = 87.885\ (2)^\circ$
$V = 574.36\ (12)$ Å^3

$Z = 1$
$D_x = 1.594$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 985 reflections
$\theta = 2.3$–23.3°
$\mu = 0.82$ mm^{-1}
$T = 298\ (2)$ K
Prism, red
0.21 × 0.12 × 0.08 mm

Data collection

Bruker APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min} = 0.847$, $T_{max} = 0.937$
4178 measured reflections

2039 independent reflections
1618 reflections with $I > 2\sigma(I)$
$R_{int} = 0.030$
$\theta_{max} = 25.2^\circ$
$h = -8 \rightarrow 8$
$k = -10 \rightarrow 10$
$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.115$
$S = 1.03$
2039 reflections
174 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.054P)^2 + 0.2338P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.40$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O6	2.069 (3)	Co1—O1	2.146 (2)
Co1—N2	2.100 (3)		
O6—Co1—N2	90.97 (11)	N2—Co1—O1	78.68 (9)
O6—Co1—O1	88.77 (11)		

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O6—H6*D*···O5^{ii}	0.813 (17)	1.86 (2)	2.661 (4)	167 (4)
O6—H6*E*···O4^{iii}	0.811 (17)	1.993 (18)	2.804 (3)	178 (4)
O3—H3*A*···O2	0.841 (19)	1.63 (2)	2.467 (3)	173 (4)
N1—H1*A*···O4^{iv}	0.841 (19)	2.02 (2)	2.824 (4)	160 (4)

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

H atoms attached to the C atoms were included in the refinement in calculated positions in the riding-model approximation [C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$]. The water H atoms were located and refined with distance restraints [O—H = 0.82 (2) Å and H···H =

1.39 (1) Å; U_{iso}(H) = 1.2U_{eq}(O)]. The H atom attached to the imidazole N atom was located and refined with restraints [N—H = 0.85 (2) Å; U_{iso}(H) = 1.2U_{eq}(N)].

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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