Crystal structure of diaquabis(hydrogen 2-ethyl-4,5-imidazole-dicarboxylato-*N*,*O*)cobalt(II), $Co(H_2O)_2(C_7H_6N_2O_4)_2$

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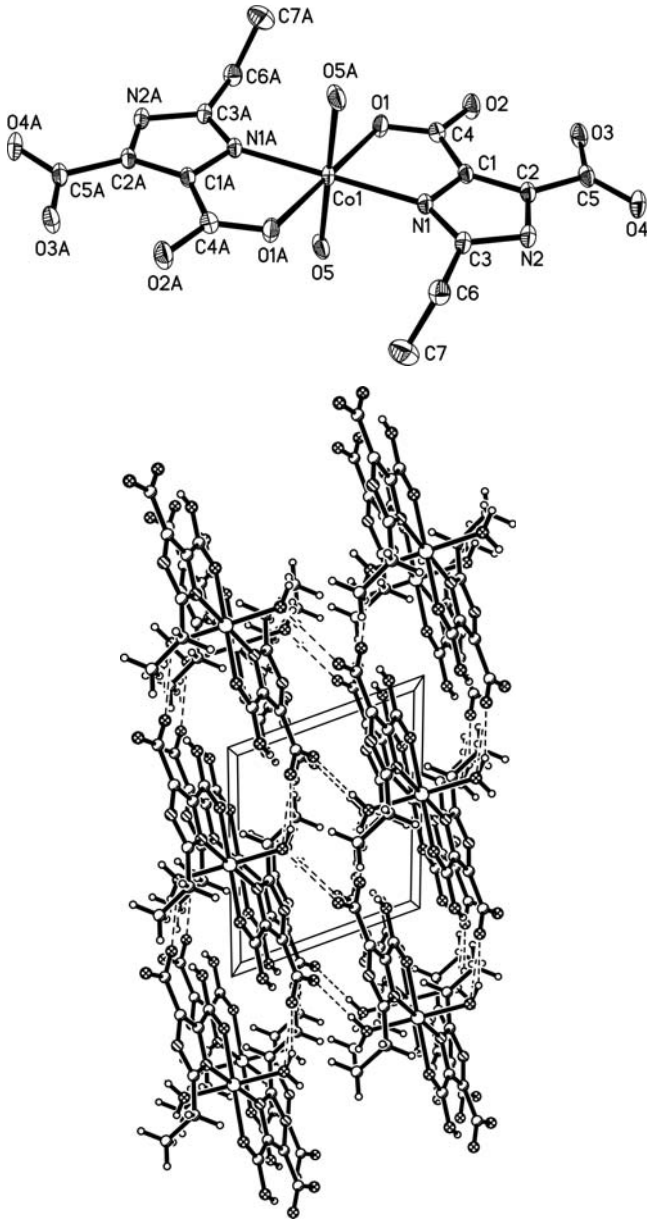

Abstract

$C_{14}H_{16}CoN_4O_{10}$, triclinic, $P\bar{1}$ (no. 2), a = 7.166(2) Å, b = 8.904(2) Å, c = 9.356(2) Å, α = 65.992(2)°, β = 88.404(2)°, γ = 70.914(2)°, V = 511.5 Å^3, Z = 1, $R_{gt}(F)$ = 0.029, $wR_{ref}(F^2)$ = 0.086, T = 293 K.

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Source of material

2-Ethyl-4,5-imidazoledicarboxylic acid (0.055 g, 0.3 mmol), $Co(CH_3CH_2COO) \cdot 4H_2O$ (0.050 g, 0.2 mmol) and NaOH (0.004 g, 0.5 mmol) were added to water (10 ml) in a Teflon-lined stainless steel reactor. The mixture was heated at 403 K for 4 d and then slowly cooled down to room temperature. Pink block-shaped crystals of the title compound were obtained.

Discussion

The design and synthesis of supramolecular polymeric networks, especially those constructed by hydrogen bonding and intermolecular weak interactions are a field of rapid growth due to their special physical properties and potential application in functional materials [1-4]. 2-Ethyl-4,5-imidazoledicarboxylate acid attracted our attention because (a) it has two carboxyl groups which may be completely or partially deprotonated, inducing rich coordination modes and allowing interesting structures with higher dimensions; (b) it can act not only as a hydrogen bond acceptor but also as a hydrogen bond donor, depending upon the degree of deprotonation [5,6].

In the title crystal structur, there are two hydrogen 2-ethyl-4,5-imidazoledicarboxylate, two water molecules and a colbat(II) cation. The Co(II) atom is six-coordinated by two nitrogen atoms, two carboxylate oxygen atoms from two hydrogen 2-ethyl-4,5-imidazoledicarboxylate (d(Co—N) = 2.125(2) Å and the d(Co—O) = 2.1646 Å) and two oxygen atoms from two coordinating water molecule (d(Co—O) = 2.064(1) Å), forming a distorted octahedral coordination (figure, top). The bond angles are in the range from 78.22(6)° to 180.0°.

There are hydrogen bonds in the crystal structure: intramolecular hydrogen bond between the two carboxylate groups (d(O2–H2···O3) = 2.482(2) Å, ∠O2–H2···O3 = 177.5°); intermolecular hydrogen bonds between a coordinating water molecule and oxygen atoms of the carboxylate groups: O5–H1W···O4 (d(O5···O4) = 2.723(2) Å, ∠O5–H1W···O4 =161.1°) and O5–H2W···O3 (d(O5···O3) = 2.771(2)Å, ∠O5–H2W···O3 = 158.1°). These hydrogen bonds interlink the moleculars into a 3D framework (figure, bottom).

Table 1. Data collection and handling.

Crystal:	pink block, size 0.10 × 0.12 × 0.35 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	8.96 cm^{-1}
Diffractometer, scan mode:	Bruker SMART CCD, φ/ω
$2\theta_{max}$:	50.98°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	3922, 1897
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1745
$N(param)_{refined}$:	135
Programs:	SHELXS-97, SHELXL-97 [7]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	*x*	*y*	*z*	U_{iso}
H(2)	2*i*	0.2194	–0.1021	1.1675	0.063
H(1W)	2*i*	0.3593	0.3923	1.0849	0.064
H(2W)	2*i*	0.3188	0.5556	1.0838	0.064
H(6A)	2*i*	0.0523	0.6156	0.5786	0.041
H(6B)	2*i*	0.2074	0.5076	0.5036	0.041
H(7A)	2*i*	0.3106	0.6320	0.7126	0.078
H(7B)	2*i*	0.3278	0.7087	0.5313	0.078
H(7C)	2*i*	0.4680	0.5194	0.6427	0.078

Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Co(1)	1*c*	0	½	0	0.0278(2)	0.0181(2)	0.0291(2)	–0.0038(1)	0.0033(1)	–0.0141(2)
N(1)	2*i*	0.1364(2)	0.3495(2)	0.8737(2)	0.0272(8)	0.0190(7)	0.0299(8)	–0.0049(6)	0.0031(6)	–0.0128(6)
N(2)	2*i*	0.2746(2)	0.2021(2)	0.7337(2)	0.0303(8)	0.0255(8)	0.0337(9)	–0.0046(7)	0.0030(7)	–0.0185(7)
O(1)	2*i*	0.0570(2)	0.2354(2)	1.1764(2)	0.0419(8)	0.0242(7)	0.0327(7)	–0.0068(6)	0.0094(6)	–0.0160(6)
O(2)	2*i*	0.1714(3)	–0.0447(2)	1.2177(2)	0.064(1)	0.0221(7)	0.0372(8)	–0.0113(7)	0.0129(7)	–0.0123(6)
O(3)	2*i*	0.3196(2)	–0.2111(2)	1.0601(2)	0.0513(9)	0.0209(7)	0.0464(9)	–0.0085(6)	0.0052(7)	–0.0167(6)
O(4)	2*i*	0.4346(2)	–0.1637(2)	0.8271(2)	0.0448(8)	0.0286(7)	0.0511(9)	–0.0006(6)	0.0040(7)	–0.0267(7)
O(5)	2*i*	0.2753(2)	0.4842(2)	1.0780(2)	0.0321(7)	0.0264(7)	0.073(1)	–0.0040(6)	–0.0046(7)	–0.0282(7)
C(1)	2*i*	0.1808(3)	0.1729(2)	0.9650(2)	0.0245(8)	0.0189(8)	0.031(1)	–0.0050(7)	0.0011(7)	–0.0130(7)
C(2)	2*i*	0.2667(3)	0.0803(2)	0.8793(2)	0.0257(9)	0.0216(9)	0.033(1)	–0.0044(7)	–0.0003(7)	–0.0153(8)
C(3)	2*i*	0.1946(3)	0.3638(2)	0.7340(2)	0.0260(9)	0.0237(9)	0.030(1)	–0.0034(7)	0.0012(7)	–0.0155(8)
C(4)	2*i*	0.1326(3)	0.1197(2)	1.1288(2)	0.0316(9)	0.0238(9)	0.029(1)	–0.0087(7)	0.0024(8)	–0.0121(8)
C(5)	2*i*	0.3463(3)	–0.1119(2)	0.9230(3)	0.0275(9)	0.0223(9)	0.043(1)	–0.0026(7)	–0.0033(8)	–0.0189(8)
C(6)	2*i*	0.1846(3)	0.5297(3)	0.5970(2)	0.040(1)	0.028(1)	0.029(1)	–0.0079(8)	0.0015(8)	–0.0107(8)
C(7)	2*i*	0.3368(4)	0.6044(3)	0.6233(3)	0.067(2)	0.050(1)	0.044(1)	–0.034(1)	0.007(1)	–0.013(1)

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