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Key indicators

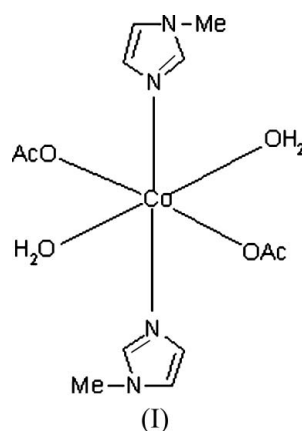
Single-crystal X-ray study
 $T = 100$ K
Mean $\sigma(\text{C}-\text{C}) = 0.002$ Å
 R factor = 0.033
 wR factor = 0.087
Data-to-parameter ratio = 11.4For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.Bis(acetato- κO)diaquabis(1-methylimidazole- κN^3)-cobalt(II)

The title complex, $[\text{Co}(\text{C}_2\text{H}_3\text{O}_2)_2(\text{C}_4\text{H}_6\text{N}_2)_2(\text{H}_2\text{O})_2]$, contains a Co centre with a slightly distorted octahedral coordination geometry. It is coordinated by two N atoms of two *N*-methylimidazole ligands, two O atoms of two acetate ligands and two O atoms of water molecules. The Co atom is located on a centre of inversion. The molecules are linked by O—H...O hydrogen bonds between the aqua ligands and neighbouring carboxylate groups. An intramolecular hydrogen bond between the uncoordinated carboxylate O atom and the water H atom is also observed.

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Comment

Cobalt complexes containing imidazole ligands and their derivatives often exhibit biological properties. Interest in the chemistry of transition metal complexes of imidazole and substituted imidazoles stems from attempts to model the binding site of the histidine residue in metalloproteins (Naumov *et al.*, 2000; Eilbeck *et al.*, 1967; Davis & Smith, 1971). Imidazole is a monodentate ligand and forms complexes with metal ions through its N atoms. Furthermore, the acetate anion is a versatile ligand in the synthesis of coordination compounds. It is well known that the incorporation of carboxylate groups into coordination compounds gives interesting supramolecular architectures (Puddephatt *et al.*, 2002). It therefore appeared to be interesting to study the conditions of the formation of acetate-containing cobalt(II) complexes with imidazole derivatives and to investigate the influence of steric properties on the magnetic behaviour as well as on the structure of the resulting species.



The crystal structure of the title complex, (I), is made up of neutral mononuclear $[\text{Co}(\text{C}_2\text{H}_3\text{O}_2)_2(\text{C}_4\text{H}_6\text{N}_2)_2(\text{H}_2\text{O})_2]$ units. The carboxylate ligands each bond in a monodentate fashion and the Co^{II} atom lies on a centre of symmetry. Fig. 1 shows

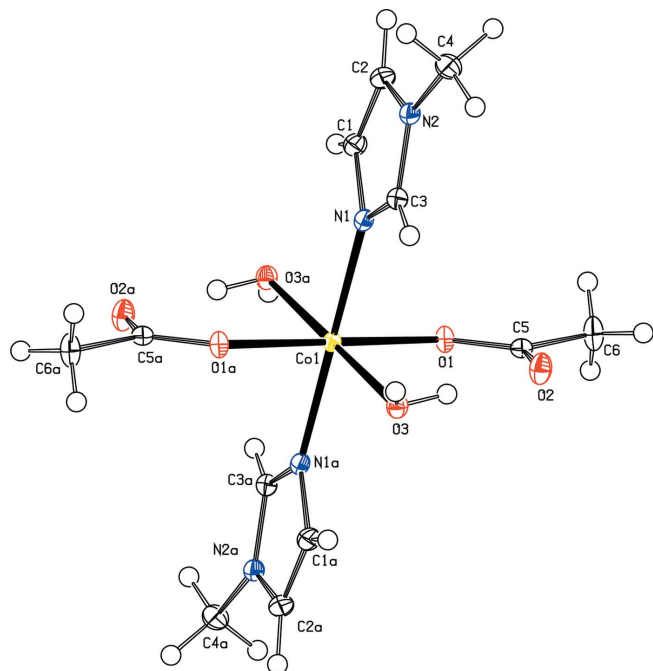


Figure 1
Molecular structure of (I). Displacement ellipsoids are drawn at the 50% probability level. [Symmetry code : (a) $-x + 1, -y, -z$]

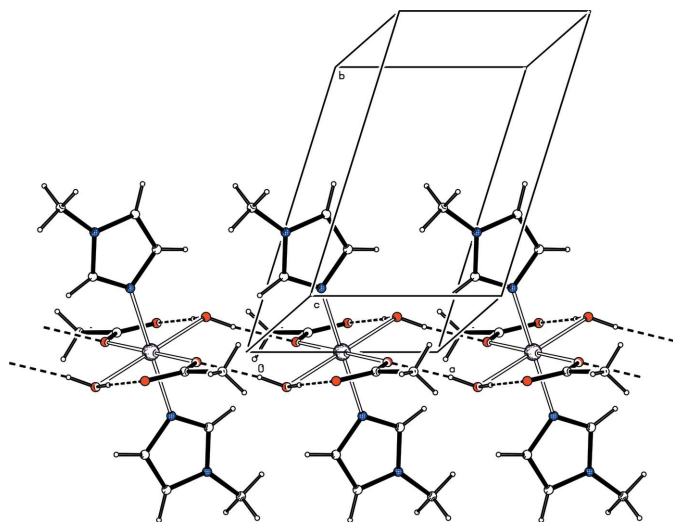


Figure 2
A packing diagram for (I) with a view on to the ab plane. Hydrogen bonds are indicated by dashed lines.

the molecular structure of (I). Each Co^{II} atom in (I) is coordinated by two O atoms from different acetate ligands, two *N*-methylimidazole N atoms and two water molecules, resulting in an octahedral N_4O_2 donor set. All the ligands show a *trans* arrangement of two equivalent donor atoms around the cobalt(II) ion.

The molecular packing of (I) is shown in Fig. 2. It is interesting to note that one H atom of the water molecule forms an intramolecular hydrogen bond with the neighbouring carboxylate group (Table 2). The other water H atom forms an intermolecular hydrogen bond with an adjacent molecule (Fig. 2).

Experimental

Cobalt diacetate tetrahydrate (1.2 mmol, 0.30 g) was dissolved in warm dried ethanol. Upon complete dissolution the reaction mixture was added dropwise to an *N*-methylimidazole (2.4 mmol, 1.04 g) solution in ethanol at room temperature with continuous stirring at 300 K. After stirring at this temperature for 24 h, the mixture was filtered and the resulting red–purple solution was allowed to evaporate slowly at room temperature over three months to give violet prisms of (I) suitable for X-ray diffraction. The crystals were found to be stable to air and X-ray exposure. Analysis calculated for $\text{C}_{12}\text{H}_{22}\text{CoN}_4\text{O}_6$: C 57.11, H 8.79, N 25.41%; found: C 57.30, H 9.09, N 25.08%.

Crystal data

$[\text{Co}(\text{C}_2\text{H}_3\text{O}_2)_2(\text{C}_4\text{H}_6\text{N}_2)(\text{H}_2\text{O})_2]$
 $M_r = 377.27$
 Triclinic, $P\bar{1}$
 $a = 5.5832$ (7) Å
 $b = 8.7122$ (7) Å
 $c = 8.9572$ (8) Å
 $\alpha = 76.301$ (7)°
 $\beta = 77.956$ (9)°
 $\gamma = 72.629$ (9)°

$V = 399.50$ (7) Å³
 $Z = 1$
 $D_x = 1.568$ Mg m⁻³
 Mo $K\alpha$ radiation
 $\mu = 1.11$ mm⁻¹
 $T = 100$ (2) K
 Prism, violet
 $0.50 \times 0.28 \times 0.20$ mm

Data collection

Oxford Diffraction Xcalibur diffractometer with Sapphire CCD detector
 ω scans
 Absorption correction: analytical (*CrysAlis RED*; Oxford Diffraction, 2004)
 $T_{\text{min}} = 0.586$, $T_{\text{max}} = 0.833$

2608 measured reflections
 1581 independent reflections
 1530 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.047$
 $\theta_{\text{max}} = 26.4^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.033$
 $wR(F^2) = 0.087$
 $S = 1.09$
 1581 reflections
 139 parameters
 Only H-atom coordinates refined

$w = 1/[\sigma^2(F_o^2) + (0.0568P)^2 + 0.1552P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.038$
 $\Delta\rho_{\text{max}} = 0.77$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.77$ e Å⁻³

Table 1

Selected bond lengths (Å).

Co1—O1	2.1220 (12)	Co1—O3	2.1702 (13)
Co1—N1	2.1273 (15)		

Table 2

Hydrogen-bond geometry (Å, °).

$D\text{—H}\cdots A$	$D\text{—H}$	$\text{H}\cdots A$	$D\cdots A$	$D\text{—H}\cdots A$
O3—H3A \cdots O1 ⁱ	0.847 (9)	1.963 (11)	2.7987 (18)	169 (2)
O3—H3B \cdots O2	0.847 (9)	1.773 (9)	2.6080 (18)	168 (2)

Symmetry code: (i) $x - 1, y, z$.

All H atoms were located in a difference Fourier map and their coordinates were refined [$\text{C—H} = 0.88$ (3)– 0.97 (3) Å]. Their

displacement parameters were constrained, with $U_{\text{iso}}(\text{H})$ values set at $1.2U_{\text{eq}}$ of the parent atom.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2003); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2004); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003) and *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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