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Diaquabis(5-carboxy-2-methyl-1*H*-imidazole-4-carboxylato-κ^2N^3,O^4)cobalt(II)

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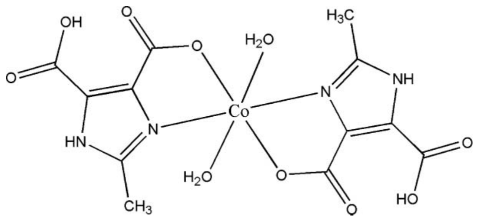
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.002 Å; R factor = 0.028; wR factor = 0.084; data-to-parameter ratio = 14.3.

The Co atom in the title compound, $[Co(C_6H_5N_2O_4)_2(H_2O)_2]$, is located on an inversion centre and exhibits a distorted octahedral geometry. It is *trans* coordinated by two *N*,*O*-bidentate 5-carboxy-2-methyl-1*H*-imidazole-4-carboxylate monoanionic ligands with two water molecules in the axial positions. Each ligand is stabilized by a strong, almost symmetrical, hydrogen bond. Intermolecular N—H⋯O hydrogen bonds link the molecules into layers, which are further linked into a three-dimensional supramolecular framework through O—H⋯O hydrogen-bonding interactions involving the water molecules.

Related literature

For related literature, see: Nie *et al.* (2007); Liu *et al.* (2004); Liu *et al.* (2006).



Experimental

Crystal data

$[Co(C_6H_5N_2O_4)_2(H_2O)_2]$
M_r = 433.20
Orthorhombic, *Pbca*
a = 6.8261 (8) Å
b = 13.9705 (16) Å
c = 16.7173 (19) Å
V = 1594.2 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.14 mm^{-1}
T = 291 (2) K
0.38 × 0.18 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.673, T_{max} = 0.839
10909 measured reflections
1825 independent reflections
1459 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.084
S = 1.08
1825 reflections
128 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
O3—H3⋯O2	1.19 (2)	1.28 (2)	2.4619 (18)	168 (2)
O5—H1*W*⋯O2^{i}	0.82	1.98	2.7920 (18)	171
O5—H2*W*⋯O1^{ii}	0.84	1.95	2.7789 (17)	172
N2—H2⋯O3^{iii}	0.86	2.13	2.9564 (18)	162

Symmetry codes: (i) $-x+\frac{3}{2}, -y+1, z-\frac{1}{2}$; (ii) $x+\frac{1}{2}, y, -z+\frac{3}{2}$; (iii) $-x+1, y-\frac{1}{2}, -z+\frac{3}{2}$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2222).

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supplementary materials

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Diaquabis(5-carboxy-2-methyl-1*H*-imidazole-4-carboxylato-κ^2N^3,O^4)cobalt(II)

C.-B. Liu, **X.-L. Nie** and **H.-L. Wen**

Comment

Recently, our group (Nie *et al.*, 2007) described the structure of diaquabis [2-methyl-1*H*-imidazole-4,5-dicarboxylato(1-)]cadmium (II) as a three-dimensional network of [Cd(H_2MIA)$_2$(H_2O)$_2$] molecules held together by hydrogen-bonding interactions. The present centrosymmetric Co complex is similiar to the Cd complex, but there are some differences in their structures.

The molecule of (I) is a discrete neutral monomer, in which the asymmetric unit contains one-half of the [Co(H_2MIA)$_2$(H_2O)$_2$] formula unit. The Co atom lies on a crystallographic inversion center and has a slightly distorted octahedral geometry. Two coordinated water molecules occupy the apical positions. The equatorial plane contains two bidentate 2-methyl-1*H*-imidazole-4,5-dicarboxylic acid monoanionic ligands which display a strong intramolecular O—H···O symmetrical hydrogen bond with a short O···O distance of 2.462 (2) Å (Fig. 1; Table 1). Similar strong intramolecular hydrogen bondings has been already reported with this ligand (Liu *et al.*, 2004; Liu *et al.*, 2006).

Owing to the location of the Co on an inversion center, the two chelate rings are coplanar, with a mean deviation 0.042 (2) Å, whereas in the Cd complex, the two chelate rings are shifted with a distance between the two planes of 0.5615 Å.. In the Cd complex, N—H···O hydrogen bonds link the molecules into chains which are further linked to a three-dimensional supramolecular framework *via* O—H···O hydrogen bonds whereas in the title complex, N—H···O hydrogen bonds (Table 1) link the molecules into a two-dimensional layers (Fig. 2). These layers are further linked through O—H···O (Table 1) involving the coordinated water O atoms and two carboxy O atoms to form a three-dimensional supramolecular framework. The Cd complex crystallizes in Monoclinic, space group P 2_1/c whereas the Co complex belongs to the orthorhombic, Pbca space group.

Experimental

Preparation of [Co(H_2MIA)$_2$(H_2O)$_2$]: A heavy-walled prex tube containing a mixture of Co(OAc)$_2$·6H_2O (0.0285 g, 0.1 mmol), 2-methyl −1*H*-imidazole-4,5-dicarboxylic acid (0.034 g, 0.2 mmol), 0.65 mol/*L* NaOH solutions (0.3 ml) and H_2O (2 ml) was frozen in liquid N_2, sealed under vacuum and placed inside an oven at 150 °C. The red single crystals (I) suitable for X-ray analysis were then obtained after heating of 3 d. Yield: 0.026 g, 60%. Analysis, calculated for C12H14CoN4O10 (433.20): C 33.27, H 3.26, N 12.93%; found: C 33.12, H 3.36, N 12.90%.

Refinement

All H atoms attached to C atoms and N atom were fixed geometrically and treated as riding with C—H = 0.93 Å (aromatic) or 0.96 Å (methyl) and N—H = 0.86 Å with $U_{\rm iso}$(H) = $xU_{\rm eq}$(C or N) where x=1.2 for C(aromatic) or N and 1.5 for methyl group.. H atoms of water molecule were located in difference Fourier maps and included in the subsequent refinement using restraints (O—H= 0.85 (1)Å and H···H= 1.39 (2) Å) with $U_{\rm iso}$(H) = 1.5$U_{\rm eq}$(O)·In the final stage of refinement they coordinates were fixed.

Figures

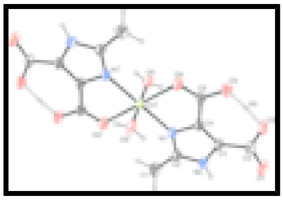

Fig. 1. Molecular view of the Co(II) complex (I) with the atom-labelling scheme. Ellipsoids are drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii. [Symmetry code: (i) 1 − *x*, 1 − *y*, 1 − *z*]

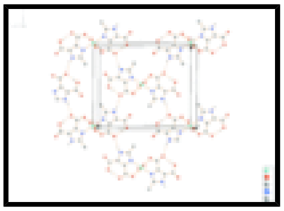

Fig. 2. Partial packing view of (I), showing a two-dimensional sheet viewed down the *a* axis. H-bonds are shown as dashed lines.

Diaqua(5-carboxy-2-methyl-1*H*-imidazole-4-carboxylato-\ κ^2N^3,O^4)cobalt(II)

Crystal data

[$Co(C_6H_5N_2O_4)_2(H_2O)_2$]

M_r = 433.20

Orthorhombic, *Pbca*

Hall symbol: -P 2ac 2ab

a = 6.8261 (8) Å

b = 13.9705 (16) Å

c = 16.7173 (19) Å

V = 1594.2 (3) Å^3

Z = 4

F_{000} = 884

D_x = 1.805 Mg m^{-3}

Mo *K*α radiation
λ = 0.71073 Å

Cell parameters from 3494 reflections

θ = 2.9–28.1°

μ = 1.14 mm^{-1}

T = 291 (2) K

Block, red

0.38 × 0.18 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

T = 291(2) K

φ and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{\rm min}$ = 0.673, $T_{\rm max}$ = 0.839

10909 measured reflections

1825 independent reflections

1459 reflections with $I > 2\sigma(I)$

$R_{\rm int}$ = 0.025

$\theta_{\rm max}$ = 27.5°

$\theta_{\rm min}$ = 2.9°

h = −8→8

k = −17→18

l = −20→21

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.028$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.084$	$w = 1/[\sigma^2(F_o^2) + (0.0453P)^2 + 0.4264P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.08$	$(\Delta/\sigma)_{max} < 0.001$
1825 reflections	$\Delta\rho_{max} = 0.33$ e Å^{-3}
128 parameters	$\Delta\rho_{min} = -0.33$ e Å^{-3}
3 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Co1	0.5000	0.5000	0.5000	0.02327 (13)
O1	0.4610 (2)	0.37350 (9)	0.87496 (7)	0.0384 (3)
O2	0.5322 (2)	0.52489 (10)	0.84444 (8)	0.0353 (3)
O3	0.5701 (2)	0.62758 (8)	0.72576 (7)	0.0354 (3)
H3	0.545 (3)	0.5850 (17)	0.7866 (15)	0.053*
O4	0.5556 (2)	0.60690 (8)	0.59313 (7)	0.0321 (3)
O5	0.7904 (2)	0.46448 (11)	0.49466 (6)	0.0356 (3)
H1W	0.8536	0.4646	0.4530	0.053*
H2W	0.8482	0.4340	0.5309	0.053*
N1	0.47986 (19)	0.41778 (10)	0.60525 (8)	0.0234 (3)
N2	0.4548 (2)	0.32451 (10)	0.71031 (8)	0.0273 (3)
H2	0.4385	0.2738	0.7387	0.033*
C1	0.4181 (4)	0.24506 (13)	0.57651 (11)	0.0446 (5)
H1A	0.4148	0.2657	0.5218	0.067*
H1B	0.2958	0.2152	0.5900	0.067*
H1C	0.5228	0.2000	0.5837	0.067*

C2	0.4504 (3)	0.32885 (12)	0.62924 (10)	0.0269 (4)
C3	0.4899 (2)	0.41492 (12)	0.73939 (10)	0.0232 (3)
C4	0.5065 (2)	0.47207 (13)	0.67325 (10)	0.0228 (3)
C5	0.4943 (2)	0.43642 (13)	0.82581 (10)	0.0268 (4)
C6	0.5460 (2)	0.57575 (12)	0.66241 (10)	0.0248 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0353 (2)	0.0211 (2)	0.0134 (2)	−0.00068 (12)	−0.00038 (11)	0.00064 (11)
O1	0.0641 (9)	0.0341 (7)	0.0171 (6)	0.0043 (6)	0.0036 (6)	0.0033 (5)
O2	0.0582 (9)	0.0314 (7)	0.0163 (6)	0.0004 (6)	−0.0036 (5)	−0.0031 (5)
O3	0.0631 (9)	0.0227 (6)	0.0205 (6)	−0.0040 (6)	−0.0022 (6)	−0.0050 (5)
O4	0.0538 (8)	0.0232 (6)	0.0194 (6)	−0.0038 (6)	−0.0007 (5)	0.0001 (5)
O5	0.0367 (7)	0.0506 (8)	0.0195 (6)	0.0070 (7)	0.0023 (5)	0.0063 (5)
N1	0.0350 (7)	0.0204 (7)	0.0148 (7)	−0.0014 (5)	−0.0013 (5)	−0.0008 (5)
N2	0.0412 (8)	0.0223 (7)	0.0186 (7)	−0.0018 (6)	0.0003 (6)	0.0027 (5)
C1	0.0819 (15)	0.0254 (9)	0.0265 (10)	−0.0102 (10)	−0.0024 (10)	−0.0040 (7)
C2	0.0389 (9)	0.0228 (8)	0.0189 (8)	−0.0005 (7)	−0.0004 (7)	−0.0001 (6)
C3	0.0296 (8)	0.0220 (8)	0.0180 (8)	0.0015 (6)	−0.0002 (6)	−0.0005 (6)
C4	0.0304 (8)	0.0215 (8)	0.0166 (8)	0.0004 (6)	−0.0004 (6)	−0.0015 (6)
C5	0.0328 (9)	0.0292 (10)	0.0185 (9)	0.0053 (6)	−0.0004 (6)	−0.0004 (7)
C6	0.0344 (8)	0.0216 (8)	0.0186 (8)	0.0010 (6)	−0.0007 (6)	−0.0019 (6)

Geometric parameters (Å, °)

Co1—O5	2.0453 (14)	O5—H2W	0.8386
Co1—O5$^{\rm i}$	2.0453 (14)	N1—C2	1.321 (2)
Co1—N1$^{\rm i}$	2.1057 (14)	N1—C4	1.379 (2)
Co1—N1	2.1057 (14)	N2—C2	1.357 (2)
Co1—O4$^{\rm i}$	2.1904 (12)	N2—C3	1.374 (2)
Co1—O4	2.1904 (12)	N2—H2	0.8600
O1—C5	1.225 (2)	C1—C2	1.482 (2)
O2—C5	1.301 (2)	C1—H1A	0.9600
O2—H3	1.28 (2)	C1—H1B	0.9600
O3—C6	1.2933 (19)	C1—H1C	0.9600
O3—H3	1.19 (2)	C3—C4	1.368 (2)
O4—C6	1.239 (2)	C3—C5	1.476 (2)
O5—H1W	0.8190	C4—C6	1.485 (2)
O5—Co1—O5$^{\rm i}$	180.0	C2—N2—C3	108.42 (14)
O5—Co1—N1$^{\rm i}$	91.87 (5)	C2—N2—H2	125.8
O5$^{\rm i}$—Co1—N1$^{\rm i}$	88.13 (5)	C3—N2—H2	125.8
O5—Co1—N1	88.13 (5)	C2—C1—H1A	109.5
O5$^{\rm i}$—Co1—N1	91.87 (5)	C2—C1—H1B	109.5
N1$^{\rm i}$—Co1—N1	180.0	H1A—C1—H1B	109.5
O5—Co1—O4$^{\rm i}$	88.36 (5)	C2—C1—H1C	109.5
O5$^{\rm i}$—Co1—O4$^{\rm i}$	91.64 (5)	H1A—C1—H1C	109.5

N1^{i}—Co1—O4^{i}	77.84 (5)	H1B—C1—H1C	109.5
N1—Co1—O4^{i}	102.16 (5)	N1—C2—N2	110.00 (15)
O5—Co1—O4	91.64 (5)	N1—C2—C1	125.79 (15)
O5^{i}—Co1—O4	88.36 (5)	N2—C2—C1	124.21 (16)
N1^{i}—Co1—O4	102.16 (5)	C4—C3—N2	105.35 (14)
N1—Co1—O4	77.84 (5)	C4—C3—C5	132.11 (17)
O4^{i}—Co1—O4	180.000 (1)	N2—C3—C5	122.46 (16)
C5—O2—H3	117.1 (11)	C3—C4—N1	109.54 (15)
C6—O3—H3	113.7 (11)	C3—C4—C6	133.06 (15)
C6—O4—Co1	114.58 (10)	N1—C4—C6	117.40 (14)
Co1—O5—H1W	123.2	O1—C5—O2	123.94 (16)
Co1—O5—H2W	123.2	O1—C5—C3	120.47 (16)
H1W—O5—H2W	111.5	O2—C5—C3	115.58 (15)
C2—N1—C4	106.68 (14)	O4—C6—O3	124.21 (15)
C2—N1—Co1	140.96 (12)	O4—C6—C4	117.79 (14)
C4—N1—Co1	112.35 (11)	O3—C6—C4	118.00 (14)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···O2	1.19 (2)	1.28 (2)	2.4619 (18)	168 (2)
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O5—H2W···O1^{iii}	0.84	1.95	2.7789 (17)	172
N2—H2···O3^{iv}	0.86	2.13	2.9564 (18)	162

Symmetry codes: (ii) $-x+3/2, -y+1, z-1/2$; (iii) $x+1/2, y, -z+3/2$; (iv) $-x+1, y-1/2, -z+3/2$.

Fig. 1

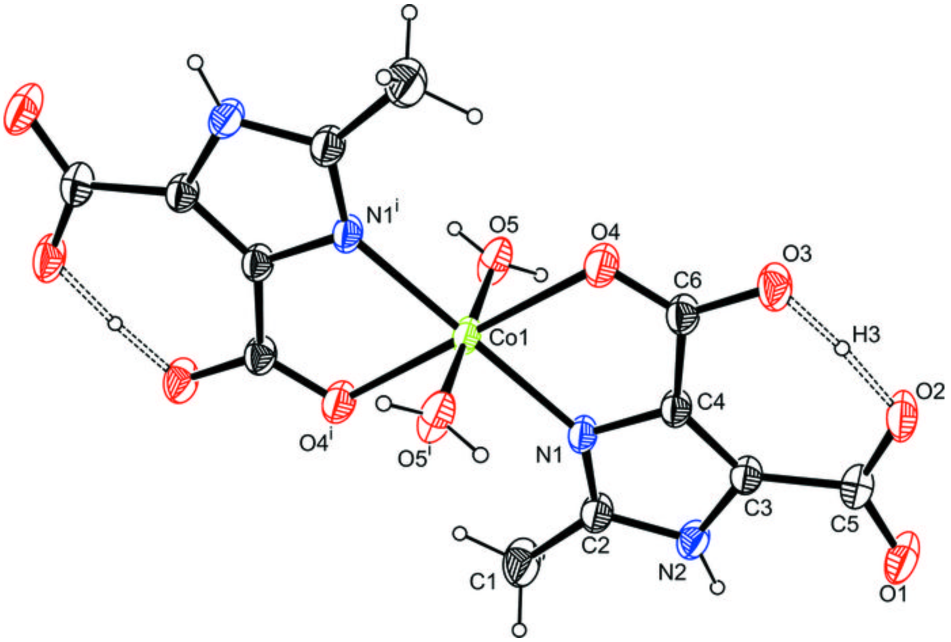

Fig. 2