

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

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

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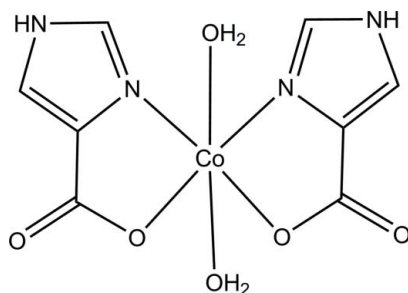
Received 18 December 2012; accepted 4 January 2013

Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(C-C) = 0.003$ Å; R factor = 0.027; wR factor = 0.063; data-to-parameter ratio = 12.2.

The title compound, $[Co(C_4H_3N_2O_2)_2(H_2O)_2]$, contains a Co^{II} cation on a twofold rotation axis, exhibiting a distorted octahedral coordination geometry. The equatorial plane is formed by two N,O -bidentate 1*H*-imidazole-4-carboxylate ligands and the axial positions are occupied by water molecules. The crystal packing consists of a three-dimensional network stabilized by $O-H\cdots O$ and $N-H\cdots O$ hydrogen bonds, together with weak $\pi-\pi$ interactions [centroid-centroid distance = $3.577(2)$ Å] between the imidazole rings.

Related literature

For the isostructural zinc(II) and cadmium(II) complexes, see: Yin *et al.* (2009); Shuai *et al.* (2011). For related homoleptic compounds, see: Kondo *et al.* (2003); Gryz *et al.* (2007); Zheng *et al.* (2011).



Experimental

Crystal data

$[Co(C_4H_3N_2O_2)_2(H_2O)_2]$
 $M_r = 317.13$
Orthorhombic, *Pccn*
 $a = 7.1236(16)$ Å
 $b = 11.6305(2)$ Å
 $c = 13.5496(4)$ Å

$V = 1122.6(3)$ Å³
 $Z = 4$
Mo $K\alpha$ radiation
 $\mu = 1.56$ mm⁻¹
 $T = 100$ K
 $0.09 \times 0.04 \times 0.03$ mm

Data collection

Agilent SuperNova (single source at offset) diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)
 $T_{min} = 0.947$, $T_{max} = 1.000$

2396 measured reflections
1162 independent reflections
1025 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.018$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.027$
 $wR(F^2) = 0.063$
 $S = 1.08$
1162 reflections
95 parameters
2 restraints

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{max} = 0.32$ e Å⁻³
 $\Delta\rho_{min} = -0.25$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Co1—N3	2.0763 (17)	Co1—O1	2.1774 (14)
Co1—O1W	2.1074 (15)		
N3—Co1—N3 ⁱ	97.39 (9)	N3—Co1—O1	78.47 (6)
N3—Co1—O1W	98.62 (6)	O1W—Co1—O1	83.04 (6)

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1 \cdots O2 ⁱⁱ	0.88	1.89	2.766 (2)	172
O1W—H1WA \cdots O2 ⁱⁱⁱ	0.86 (2)	1.91 (2)	2.760 (2)	171 (3)
O1W—H1WB \cdots O2 ^{iv}	0.85 (2)	1.98 (2)	2.812 (2)	167 (2)

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

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SUPERFLIP* (Palatinus & Chapuis, 2007); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

This work was financially supported by Eusko Jaurlaritz/Gobierno Vasco (grant Nos. IT477-10 and S-PE11UN062) and the Universidad de País Vasco UPV/EHU (grant No. UFI11/53). BA and AP thank EJ/GV for their predoctoral fellowships.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZJ2099).

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supplementary materials

Acta Cryst. (2013). E69, m94 [doi:10.1107/S1600536813000330]

Diaquabis(1*H*-imidazole-4-carboxylato- κ^2 N³,O)cobalt(II)

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Comment

The title compound, [Co(C₄H₃N₂O₂)₂(H₂O)₂] crystallizes in the orthorhombic crystal system, space group Pccn, and it is isostructural with the zinc and cadmium complexes previously reported by Yin *et al.* (2009) and Shuai *et al.* (2011). As expected, the Co—O and Co—N distances (Table 1) are similar to those of the Zn^{II} analogue and shorter than those of the Cd^{II} derivative. Table 2 summarizes the geometrical parameters of the O—H \cdots O and N—H \cdots O hydrogen bonding interactions. The centroid-to-centroid distance between interacting imidazole rings is 3.577 (2) Å.

Experimental

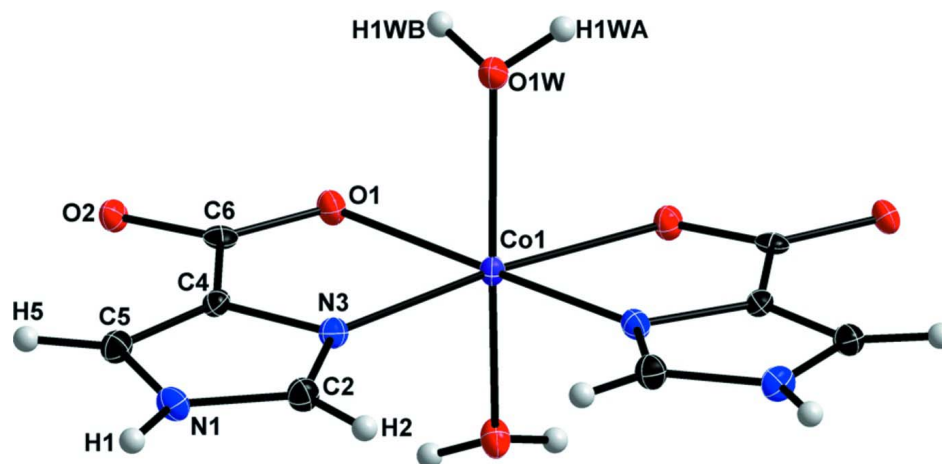
To a solution of CoCl₂·6H₂O (12 mg, 0.05 mmol) in 15 ml of water 4-imidazole carboxylic acid (6 mg, 0.05 mmol) was added and the resulting solution was stirred for 30 min at room temperature. Prismatic red crystals were obtained by slow evaporation after several days. IR (cm⁻¹): 3148 (*s*), 2934 (*s*), 1685 (*m*), 1588 (*vs*), 1555 (*vs*), 1528 (*s*), 1462 (*s*), 1406 (*vs*), 1333 (*m*), 1234 (*s*), 1177 (*m*), 1101 (*m*), 1005 (*m*), 930 (*m*), 845 (*m*), 820 (*m*), 791 (*m*), 731 (*w*), 658 (*s*), 610 (*m*), 492 (*m*).

Refinement

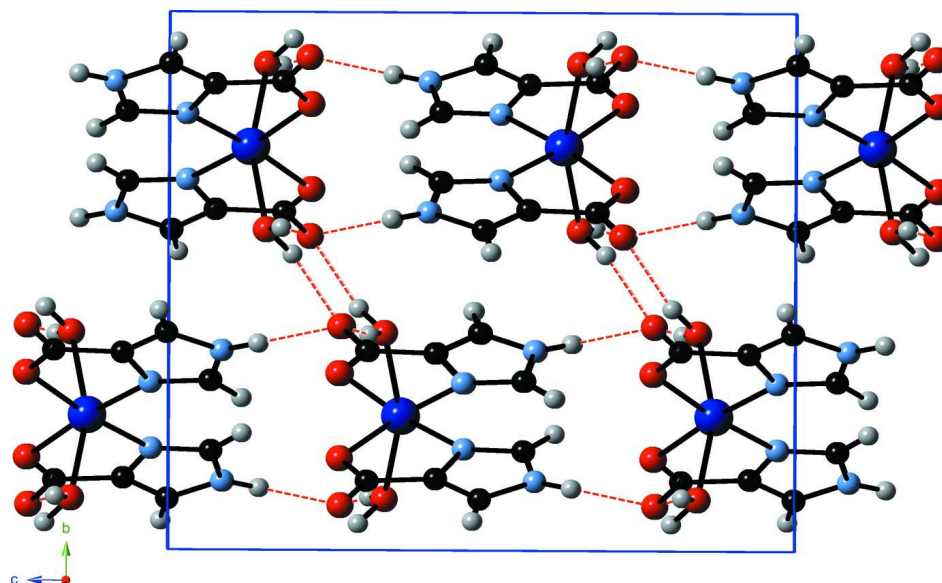
All atoms except H were refined anisotropically. H atoms of the water molecule were located in a Fourier difference map and refined isotropically with O—H bond lengths restrained to 0.84 (2) Å. All imidazole H atoms were positioned geometrically and refined using a riding model with C—H = 0.93 Å, N—H = 0.86 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C,N})$.

Computing details

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO* (Agilent, 2011); data reduction: *CrysAlis PRO* (Agilent, 2011); program(s) used to solve structure: SUPERFLIP (Palatinus & Chapuis, 2007); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).


Figure 1

Molecular structure of $[\text{Co}(\text{C}_4\text{H}_3\text{N}_2\text{O}_2)_2(\text{H}_2\text{O})_2]$ showing atom labelling for the asymmetric unit and 50% probability displacement ellipsoids.


Figure 2

View of the crystal packing along the crystallographic a axis (hydrogen bonds represented as dashed lines).

(I)

Crystal data

$[\text{Co}(\text{C}_4\text{H}_3\text{N}_2\text{O}_2)_2(\text{H}_2\text{O})_2]$

$M_r = 317.13$

Orthorhombic, $Pccn$

Hall symbol: $-P\ 2ab\ 2ac$

$a = 7.1236\ (16)\ \text{\AA}$

$b = 11.6305\ (2)\ \text{\AA}$

$c = 13.5496\ (4)\ \text{\AA}$

$V = 1122.6\ (3)\ \text{\AA}^3$

$Z = 4$

$F(000) = 644$

$D_x = 1.876\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 1055 reflections

$\theta = 1.8\text{--}28.1^\circ$

$\mu = 1.56\ \text{mm}^{-1}$

$T = 100\ \text{K}$

Prism, red

$0.09 \times 0.04 \times 0.03\ \text{mm}$

Data collection

Agilent SuperNova (single source at offset) diffractometer	$T_{\min} = 0.947$, $T_{\max} = 1.000$ 2396 measured reflections
Radiation source: SuperNova (Mo) X-ray Source	1162 independent reflections 1025 reflections with $I > 2\sigma(I)$
Mirror monochromator	$R_{\text{int}} = 0.018$
Detector resolution: 16.2439 pixels mm^{-1}	$\theta_{\max} = 26.5^\circ$, $\theta_{\min} = 3.0^\circ$
ω scans	$h = -8 \rightarrow 7$
Absorption correction: multi-scan (CrysAlis PRO; Agilent, 2011)	$k = -10 \rightarrow 14$ $l = -5 \rightarrow 17$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.027$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.063$	$w = 1/[\sigma^2(F_o^2) + (0.0201P)^2 + 1.0008P]$
$S = 1.08$	where $P = (F_o^2 + 2F_c^2)/3$
1162 reflections	$(\Delta/\sigma)_{\max} < 0.001$
95 parameters	$\Delta\rho_{\max} = 0.32 \text{ e } \text{\AA}^{-3}$
2 restraints	$\Delta\rho_{\min} = -0.25 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	

Special details

Experimental. CrysAlisPro, Agilent Technologies, Version 1.171.35.19 (release 27-10-2011 CrysAlis171 .NET) (compiled Oct 27 2011,15:02:11). Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	0.75	0.25	0.13009 (3)	0.00874 (13)
O1W	0.8972 (2)	0.09575 (13)	0.15593 (11)	0.0140 (3)
O1	0.54278 (18)	0.17114 (12)	0.22690 (10)	0.0120 (3)
O2	0.26134 (18)	0.08371 (12)	0.22474 (10)	0.0113 (3)
N3	0.5553 (2)	0.18870 (15)	0.02894 (12)	0.0107 (4)
N1	0.3584 (2)	0.12877 (15)	-0.08496 (13)	0.0125 (4)
H1	0.3094	0.1157	-0.1435	0.015*
C4	0.4058 (3)	0.13338 (17)	0.07356 (15)	0.0098 (4)
C6	0.4028 (3)	0.12899 (16)	0.18291 (15)	0.0096 (4)
C5	0.2836 (3)	0.09571 (18)	0.00325 (15)	0.0118 (4)
H5	0.1697	0.0549	0.0136	0.014*
C2	0.5204 (3)	0.18489 (18)	-0.06678 (15)	0.0123 (4)
H2	0.5989	0.2173	-0.1162	0.015*
H1WA	1.007 (3)	0.099 (3)	0.180 (2)	0.047 (9)*

H1WB	0.847 (4)	0.050 (2)	0.1974 (17)	0.039 (9)*
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Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0080 (2)	0.0098 (2)	0.0084 (2)	-0.00165 (15)	0	0
O1W	0.0110 (8)	0.0146 (8)	0.0163 (8)	-0.0018 (6)	-0.0014 (7)	0.0039 (7)
O1	0.0102 (7)	0.0140 (7)	0.0116 (7)	-0.0016 (6)	-0.0011 (6)	-0.0008 (6)
O2	0.0087 (7)	0.0137 (7)	0.0116 (7)	-0.0007 (6)	0.0021 (6)	0.0019 (6)
N3	0.0095 (8)	0.0111 (9)	0.0115 (8)	-0.0003 (7)	0.0013 (7)	0.0009 (7)
N1	0.0130 (9)	0.0151 (9)	0.0094 (8)	-0.0007 (7)	-0.0031 (7)	-0.0005 (7)
C4	0.0101 (10)	0.0072 (10)	0.0120 (10)	0.0000 (8)	0.0007 (8)	0.0006 (8)
C6	0.0105 (10)	0.0071 (9)	0.0113 (10)	0.0041 (8)	0.0009 (8)	0.0000 (8)
C5	0.0122 (10)	0.0113 (10)	0.0118 (9)	-0.0007 (8)	0.0012 (9)	0.0001 (9)
C2	0.0121 (10)	0.0137 (11)	0.0111 (10)	-0.0008 (8)	0.0005 (8)	0.0009 (9)

Geometric parameters (\AA , $^\circ$)

Co1—N3	2.0763 (17)	N3—C2	1.321 (3)
Co1—N3 ⁱ	2.0763 (17)	N3—C4	1.383 (2)
Co1—O1W ⁱ	2.1074 (15)	N1—C2	1.349 (3)
Co1—O1W	2.1074 (15)	N1—C5	1.364 (3)
Co1—O1 ⁱ	2.1774 (14)	N1—H1	0.88
Co1—O1	2.1774 (14)	C4—C5	1.363 (3)
O1W—H1WA	0.849 (17)	C4—C6	1.483 (3)
O1W—H1WB	0.853 (17)	C5—H5	0.95
O1—C6	1.261 (2)	C2—H2	0.95
O2—C6	1.271 (2)		
N3—Co1—N3 ⁱ	97.39 (9)	C2—N3—C4	105.60 (17)
N3—Co1—O1W ⁱ	93.98 (6)	C2—N3—Co1	141.72 (15)
N3 ⁱ —Co1—O1W ⁱ	98.62 (6)	C4—N3—Co1	112.67 (13)
N3—Co1—O1W	98.62 (6)	C2—N1—C5	108.11 (17)
N3 ⁱ —Co1—O1W	93.98 (6)	C2—N1—H1	125.9
O1W ⁱ —Co1—O1W	160.87 (9)	C5—N1—H1	125.9
N3—Co1—O1 ⁱ	174.42 (6)	C5—C4—N3	109.62 (18)
N3 ⁱ —Co1—O1 ⁱ	78.47 (6)	C5—C4—C6	132.70 (18)
O1W ⁱ —Co1—O1 ⁱ	83.04 (6)	N3—C4—C6	117.64 (17)
O1W—Co1—O1 ⁱ	85.47 (6)	O1—C6—O2	125.27 (18)
N3—Co1—O1	78.47 (6)	O1—C6—C4	116.60 (17)
N3 ⁱ —Co1—O1	174.42 (6)	O2—C6—C4	118.13 (17)
O1W ⁱ —Co1—O1	85.47 (6)	C4—C5—N1	105.79 (17)
O1W—Co1—O1	83.04 (6)	C4—C5—H5	127.1
O1 ⁱ —Co1—O1	105.91 (7)	N1—C5—H5	127.1
Co1—O1W—H1WA	119 (2)	N3—C2—N1	110.87 (18)
Co1—O1W—H1WB	115.7 (19)	N3—C2—H2	124.6
H1WA—O1W—H1WB	100 (3)	N1—C2—H2	124.6
C6—O1—Co1	114.52 (12)		
N3—Co1—O1—C6	-1.93 (13)	Co1—N3—C4—C5	179.84 (13)

N3 ⁱ —Co1—O1—C6	-44.3 (6)	C2—N3—C4—C6	-177.35 (18)
O1W ⁱ —Co1—O1—C6	93.08 (13)	Co1—N3—C4—C6	1.8 (2)
O1W—Co1—O1—C6	-102.24 (13)	Co1—O1—C6—O2	-176.57 (15)
O1 ⁱ —Co1—O1—C6	174.51 (15)	Co1—O1—C6—C4	3.4 (2)
N3 ⁱ —Co1—N3—C2	-5.2 (2)	C5—C4—C6—O1	178.9 (2)
O1W ⁱ —Co1—N3—C2	94.1 (2)	N3—C4—C6—O1	-3.6 (3)
O1W—Co1—N3—C2	-100.4 (2)	C5—C4—C6—O2	-1.1 (3)
O1 ⁱ —Co1—N3—C2	36.6 (7)	N3—C4—C6—O2	176.37 (17)
O1—Co1—N3—C2	178.6 (2)	N3—C4—C5—N1	-0.3 (2)
N3 ⁱ —Co1—N3—C4	176.15 (16)	C6—C4—C5—N1	177.4 (2)
O1W ⁱ —Co1—N3—C4	-84.61 (14)	C2—N1—C5—C4	-0.2 (2)
O1W—Co1—N3—C4	80.96 (14)	C4—N3—C2—N1	-0.8 (2)
O1 ⁱ —Co1—N3—C4	-142.1 (6)	Co1—N3—C2—N1	-179.56 (16)
O1—Co1—N3—C4	-0.06 (13)	C5—N1—C2—N3	0.7 (2)
C2—N3—C4—C5	0.7 (2)		

Symmetry code: (i) $-x+3/2, -y+1/2, z$.

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N1—H1...O2 ⁱⁱ	0.88	1.89	2.766 (2)	172
O1W—H1WA...O2 ⁱⁱⁱ	0.86 (2)	1.91 (2)	2.760 (2)	171 (3)
O1W—H1WB...O2 ^{iv}	0.85 (2)	1.98 (2)	2.812 (2)	167 (2)

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