Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Tetraaquabis[4-(1*H*-imidazol-1-yl-κN^3)-benzoato]cobalt(II)

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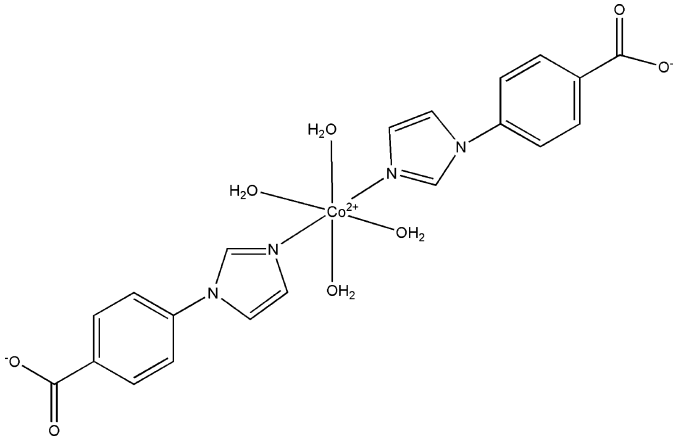
Received 23 February 2012; accepted 9 March 2012

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.002 Å; R factor = 0.032; wR factor = 0.092; data-to-parameter ratio = 12.3.

In the title compound, $[Co(C_{10}H_7N_2O_2)_2(H_2O)_4]$, the Co^{II} atom lies on an inversion centre and displays a slightly distorted octahedral geometry. The coordination sphere is defined by two mutually *trans* N atoms from two 4-(imidazol-1-yl)benzoate ligands and the O atoms from four water molecules. The crystal structure is stabilized by O—H···O hydrogen bonds.

Related literature

For our previous work on imidazole derivatives as ligands, see: Li, Song *et al.* (2011); Li, Ma *et al.* (2011); Fan *et al.* (2010); Li *et al.* (2010).



Experimental

Crystal data

$[Co(C_{10}H_7N_2O_2)_2(H_2O)_4]$
M_r = 505.35
Monoclinic, $P2_1/c$
a = 12.1976 (15) Å
b = 10.6555 (13) Å
c = 7.9602 (10) Å
β = 96.816 (2)°
V = 1027.3 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.89 mm^{-1}
T = 296 K
0.22 × 0.19 × 0.15 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.616, T_{max} = 0.744
7094 measured reflections
1850 independent reflections
1720 reflections with $I > 2\sigma(I)$
R_{int} = 0.048

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.092
S = 1.07
1850 reflections
151 parameters
6 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

Table 1
Selected bond lengths (Å).

Co1—O1*W*	2.1286 (13)	Co1—N2	2.1238 (15)
Co1—O2*W*	2.0644 (13)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2*W*—H3*W*···O2^{i}	0.84	1.88	2.6745 (17)	157
O2*W*—H4*W*···O2^{ii}	0.85	1.86	2.6964 (18)	170
O1*W*—H2*W*···O2^{i}	0.83	2.03	2.8287 (19)	163
O1*W*—H1*W*···O1^{iii}	0.83	1.87	2.7014 (18)	177

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

The work was supported by the National Marine Public Welfare Projects (grant No. 2000905021), the Guangdong Chinese Academy of Science comprehensive strategic cooperation project (grant No. 2009B091300121), the Guangdong Province Key Project in the Field of Social Development [grant No. A2009011–007(c)], the Science and Technology Department of Guangdong Province Project (grant No. 00087061110314018) and the Guangdong Natural Science Foundation (No. 925240880002).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ5202).

References

Bruker (2004). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.

Fan, R.-Z., Li, S.-J., Song, W.-D., Miao, D.-L. & Hu, S.-W. (2010). *Acta Cryst.* E**66**, m897–m898.

Li, S.-J., Ma, X.-T., Song, W.-D., Li, X.-F. & Liu, J.-H. (2011). *Acta Cryst.* E**67**, m295–m296.

Li, S.-J., Miao, D.-L., Song, W.-D., Li, S.-H. & Yan, J.-B. (2010). *Acta Cryst.* E**66**, m1096–m1097.

Li, S. J., Song, W. D., Miao, D. L., Hu, S. W., Ji, L. L. & Ma, D. Y. (2011). *Z. Anorg. Allg. Chem.* **637**, 1246–1252.

Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supplementary materials

Acta Cryst. (2012). E**68**, m486–m487 [doi:10.1107/S1600536812010562]

Tetraaquabis[4-(1*H*-imidazol-1-yl-κN^3)benzoato]cobalt(II)

Jian Guo, Shao-Wei Tong, Jian-She Liu, Wen-Dong Song and Jing-Bo An

Comment

During the past decade, considerable efforts have been devoted to design and construct new metal-organic frameworks due to their intriguing structural diversity and potential application in many areas. In recent years, our research group has shown great interest in the design and synthesis of interesting metal-organic complexes with imidazole derivatives such as 2-propyl-imidazole-4,5-dicarboxylic acid (Fan *et al.*, 2010; Li *et al.*, 2010) and 2-ethyl-1*H*-imidazole-4,5-dicarboxylic acid (Li, Song *et al.*, 2011; Li, Ma *et al.*, 2011). In this paper, we report the synthesis and structure of a new Co^{II} complex, $[Co(C_{10}H_7N_2O_2)_2(H_2O)_4]$.

As illustrated in Fig. 1, the title compound, consists of a Co^{II} cation, two deprotonated 4-(imidazol-1-yl)benzoic acid ligands and four coordinated water molecules. Each six coordinate Co^{II} ion, lies on an inversion center with the N atoms of the 4-(imidazol-1-yl)benzoic acid ligands mutually *trans* and the four water molecules in an equatorial plane. The Co–N distance is 2.1238 (15) Å and Co–O distances are 2.0643 (13) Å and 2.1287 (14) Å, respectively. It is interesting to note that in this molecule, the 4-(imidazol-1-yl)benzoic acid ligands coordinate to Co(II) *via* a nitrogen atom of the imidazole residue unlike several other complexes of dicarboxylic acid derivatives we have reported previously, which coordinate to metal atoms via the carboxylate group (Fan *et al.*, 2010; Li *et al.*, 2010; Li, Song *et al.*, 2011; Li, Ma *et al.*, 2011). In the crystal structure, molecules form a three-dimensional network through an extensive series of intermolecular O—H···O hydrogen bonds.

Experimental

A mixture of $Co(NO_3)_2.6H_2O$ (0.5 mmol, 0.15 g) and 4-(imidazol-1-yl)benzoic acid (1 mmol, 0.19 g) in 12 ml of H_2O was sealed in an autoclave equipped with a Teflon liner (20 ml) and then heated to 433 K for 4 days. After gradual cooling to room temperature, red crystals were obtained and collected by filtration with a yield of 31% based on Co.

Refinement

Carbon and nitrogen bound H atoms were placed at calculated positions and were treated as riding on the parent C or N atoms with C—H = 0.93 Å, N—H = 0.86 Å, and with U_{iso}(H) = 1.2 U_{eq}(C, N). H atoms of the water molecules were located in a difference Fourier map and refined as riding with an O—H distance restraint of 0.84 (1) Å and with U_{iso}(H) = 1.5 U_{eq}. The H···H distances within the water molecules were also restrained to 1.39 (1) Å.

Computing details

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008).

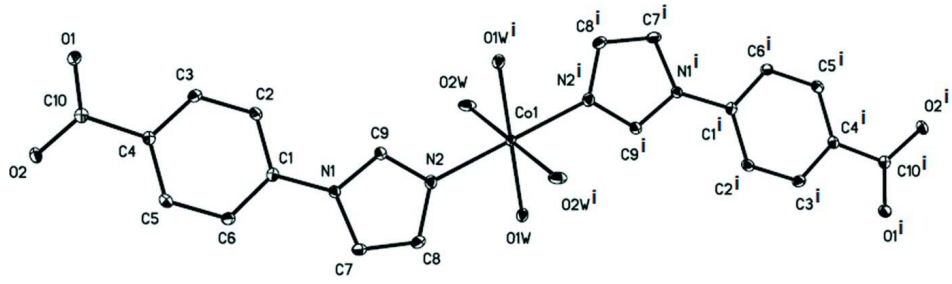


Figure 1

The structure of the title compound, showing the atomic numbering scheme. Non-H atoms are shown with 30% probability displacement ellipsoids (H atoms are omitted for clarity). [Symmetry code: i = 2 - *x*, 1 - *y*, 2 - *z*.]

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Crystal data

$[Co(C_{10}H_7N_2O_2)_2(H_2O)_4]$
M_r = 505.35
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 12.1976 (15) Å
b = 10.6555 (13) Å
c = 7.9602 (10) Å
β = 96.816 (2)°
V = 1027.3 (2) Å^3
Z = 2
$F(000)$ = 522
D_x = 1.634 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5837 reflections
θ = 2.8–27.9°
μ = 0.89 mm^{-1}
T = 296 K
Block, red
0.22 × 0.19 × 0.15 mm

Data collection

Bruker APEXII area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scan
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.616, T_{max} = 0.744
7094 measured reflections
1850 independent reflections
1720 reflections with $I > 2\sigma(I)$
R_{int} = 0.048
θ_{max} = 25.2°, θ_{min} = 1.7°
h = −14→14
k = −12→12
l = −9→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.092
S = 1.07
1850 reflections
151 parameters
6 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0491P)^2 + 0.4159P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.55457 (14)	0.61139 (17)	0.8770 (2)	0.0122 (4)
C2	0.52906 (16)	0.51963 (18)	0.7536 (2)	0.0159 (4)
H2	0.5827	0.4630	0.7282	0.019*
C3	0.42300 (17)	0.51351 (17)	0.6690 (3)	0.0158 (4)
H3	0.4066	0.4530	0.5855	0.019*
C4	0.34080 (14)	0.59535 (17)	0.7058 (2)	0.0122 (4)
C5	0.36592 (15)	0.68373 (17)	0.8335 (2)	0.0146 (4)
H5	0.3111	0.7374	0.8625	0.018*
C6	0.47249 (14)	0.69250 (17)	0.9181 (2)	0.0140 (4)
H6	0.4887	0.7526	1.0022	0.017*
C7	0.70472 (16)	0.70111 (19)	1.0893 (2)	0.0208 (4)
H7	0.6644	0.7599	1.1427	0.025*
C8	0.81424 (16)	0.67658 (18)	1.1233 (2)	0.0194 (4)
H8	0.8623	0.7168	1.2056	0.023*
C9	0.75273 (15)	0.55233 (18)	0.9212 (2)	0.0156 (4)
H9	0.7490	0.4911	0.8374	0.019*
C10	0.22864 (14)	0.59036 (17)	0.6021 (2)	0.0132 (4)
Co1	1.0000	0.5000	1.0000	0.01069 (15)
N1	0.66473 (12)	0.62083 (14)	0.95870 (17)	0.0124 (3)
N2	0.84354 (12)	0.58317 (15)	1.01756 (18)	0.0150 (3)
O1	0.22401 (10)	0.54154 (14)	0.45864 (16)	0.0187 (3)
O2	0.14737 (10)	0.63844 (12)	0.66430 (15)	0.0158 (3)
O1W	1.02638 (11)	0.52252 (13)	1.26744 (17)	0.0167 (3)
H1W	1.0866	0.5265	1.3281	0.025*
H2W	0.9794	0.4800	1.3089	0.025*
O2W	0.93348 (12)	0.32615 (13)	1.04136 (16)	0.0231 (3)
H4W	0.9150	0.2686	0.9701	0.035*
H3W	0.8941	0.3241	1.1211	0.035*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0122 (8)	0.0135 (9)	0.0108 (8)	−0.0007 (7)	0.0013 (6)	0.0028 (7)
C2	0.0131 (10)	0.0182 (9)	0.0161 (10)	0.0045 (7)	0.0010 (8)	−0.0030 (7)
C3	0.0163 (10)	0.0177 (10)	0.0130 (9)	0.0001 (7)	−0.0007 (8)	−0.0029 (7)
C4	0.0123 (9)	0.0147 (9)	0.0100 (8)	−0.0002 (7)	0.0023 (7)	0.0032 (7)
C5	0.0142 (9)	0.0144 (9)	0.0157 (9)	0.0027 (7)	0.0035 (7)	0.0003 (7)

C6	0.0153 (9)	0.0137 (9)	0.0132 (9)	−0.0011 (7)	0.0025 (7)	−0.0014 (6)
C7	0.0175 (10)	0.0228 (10)	0.0208 (10)	0.0045 (8)	−0.0025 (8)	−0.0110 (8)
C8	0.0170 (10)	0.0222 (10)	0.0179 (9)	0.0011 (8)	−0.0034 (7)	−0.0074 (8)
C9	0.0118 (9)	0.0203 (10)	0.0145 (9)	0.0017 (7)	0.0011 (7)	−0.0035 (7)
C10	0.0145 (9)	0.0132 (9)	0.0119 (9)	−0.0004 (7)	0.0020 (7)	0.0039 (7)
Co1	0.0086 (2)	0.0135 (2)	0.0097 (2)	−0.00079 (11)	0.00011 (15)	−0.00126 (11)
N1	0.0111 (7)	0.0148 (7)	0.0111 (7)	0.0016 (6)	0.0010 (6)	−0.0004 (6)
N2	0.0123 (8)	0.0189 (8)	0.0135 (7)	0.0005 (6)	0.0001 (6)	0.0004 (6)
O1	0.0144 (7)	0.0289 (8)	0.0124 (7)	0.0013 (6)	−0.0005 (5)	−0.0042 (6)
O2	0.0112 (6)	0.0231 (7)	0.0132 (6)	0.0029 (5)	0.0023 (5)	0.0021 (5)
O1W	0.0128 (7)	0.0254 (7)	0.0118 (6)	−0.0028 (5)	0.0006 (5)	−0.0006 (5)
O2W	0.0325 (8)	0.0198 (7)	0.0197 (7)	−0.0101 (6)	0.0145 (6)	−0.0077 (5)

Geometric parameters (Å, º)

C1—C6	1.391 (3)	C8—H8	0.9300
C1—C2	1.395 (3)	C9—N2	1.312 (2)
C1—N1	1.425 (2)	C9—N1	1.360 (2)
C2—C3	1.387 (3)	C9—H9	0.9300
C2—H2	0.9300	C10—O1	1.250 (2)
C3—C4	1.386 (3)	C10—O2	1.268 (2)
C3—H3	0.9300	Co1—O1W^{i}	2.1286 (13)
C4—C5	1.393 (3)	Co1—O1W	2.1286 (13)
C4—C10	1.513 (2)	Co1—O2W	2.0644 (13)
C5—C6	1.395 (2)	Co1—O2W^{i}	2.0644 (13)
C5—H5	0.9300	Co1—N2	2.1238 (15)
C6—H6	0.9300	Co1—N2^{i}	2.1238 (15)
C7—C8	1.357 (3)	O1W—H1W	0.8307
C7—N1	1.389 (2)	O1W—H2W	0.8296
C7—H7	0.9300	O2W—H4W	0.8479
C8—N2	1.378 (2)	O2W—H3W	0.8402
C6—C1—C2	119.67 (16)	O2—C10—C4	118.10 (15)
C6—C1—N1	120.96 (15)	O2W—Co1—O2W^{i}	180.0
C2—C1—N1	119.37 (16)	O2W—Co1—N2	89.47 (6)
C3—C2—C1	119.48 (17)	O2W^{i}—Co1—N2	90.53 (6)
C3—C2—H2	120.3	O2W—Co1—N2^{i}	90.53 (6)
C1—C2—H2	120.3	O2W^{i}—Co1—N2^{i}	89.47 (6)
C4—C3—C2	121.60 (17)	N2—Co1—N2^{i}	180.0
C4—C3—H3	119.2	O2W—Co1—O1W^{i}	92.45 (5)
C2—C3—H3	119.2	O2W^{i}—Co1—O1W^{i}	87.55 (5)
C3—C4—C5	118.53 (16)	N2—Co1—O1W^{i}	94.73 (5)
C3—C4—C10	119.50 (16)	N2^{i}—Co1—O1W^{i}	85.27 (5)
C5—C4—C10	121.91 (16)	O2W—Co1—O1W	87.55 (5)
C4—C5—C6	120.65 (16)	O2W^{i}—Co1—O1W	92.45 (5)
C4—C5—H5	119.7	N2—Co1—O1W	85.27 (5)
C6—C5—H5	119.7	N2^{i}—Co1—O1W	94.73 (5)
C1—C6—C5	120.01 (16)	O1W^{i}—Co1—O1W	180.0
C1—C6—H6	120.0	C9—N1—C7	106.18 (15)
C5—C6—H6	120.0	C9—N1—C1	125.99 (15)

C8—C7—N1	106.30 (16)	C7—N1—C1	127.83 (15)
C8—C7—H7	126.9	C9—N2—C8	106.02 (15)
N1—C7—H7	126.9	C9—N2—Co1	124.04 (13)
C7—C8—N2	109.76 (16)	C8—N2—Co1	129.94 (12)
C7—C8—H8	125.1	Co1—O1W—H1W	127.2
N2—C8—H8	125.1	Co1—O1W—H2W	107.9
N2—C9—N1	111.74 (16)	H1W—O1W—H2W	113.7
N2—C9—H9	124.1	Co1—O2W—H4W	128.4
N1—C9—H9	124.1	Co1—O2W—H3W	114.5
O1—C10—O2	124.93 (16)	H4W—O2W—H3W	110.8
O1—C10—C4	116.95 (15)		

Symmetry code: (i) −*x*+2, −*y*+1, −*z*+2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2*W*—H3*W*···O2^{ii}	0.84	1.88	2.6745 (17)	157
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O1*W*—H1*W*···O1^{iv}	0.83	1.87	2.7014 (18)	177

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