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Hexakis(1*H*-imidazole-κN^3)cobalt(II) bis(3,5-dinitrobenzoate) dihydrate

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.002 Å
R factor = 0.034
wR factor = 0.084
Data-to-parameter ratio = 16.1

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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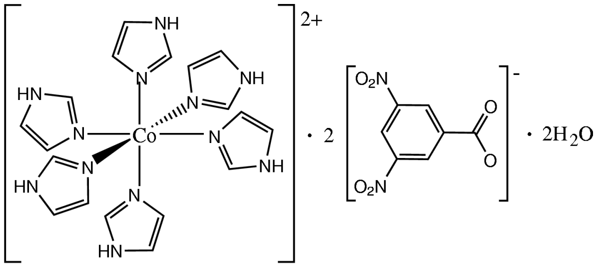
The structure of the title compound, $[Co(C_3H_4N_2)_6](C_7H_3N_2O_6)_2\cdot 2H_2O$, consists of Co^{II}-containing complex cations, dinitrobenzoate anions and water molecules. The Co atom is located on an inversion centre and assumes an octahedral coordination geometry. The dinitrobenzoate anions link with the complex cation *via* N—H···O hydrogen bonds.

Comment

As part of our investigations into aromatic π–π stacking, a series of metal complexes incorporating imidazole ligands have been prepared, among which some structures showed π–π stacking between imidazole rings (Xu & Xu, 2004). However, in the present imidazole–cobalt(II) complex, (I) (Fig. 1), no such π–π stacking occurs.



(I)

The Co^{II} atom in (I) is located on an inversion centre and assumes an octahedral coordination geometry formed by six imidazole molecules. The imidazole ring planes are nearly perpendicular to each other, with dihedral angles of

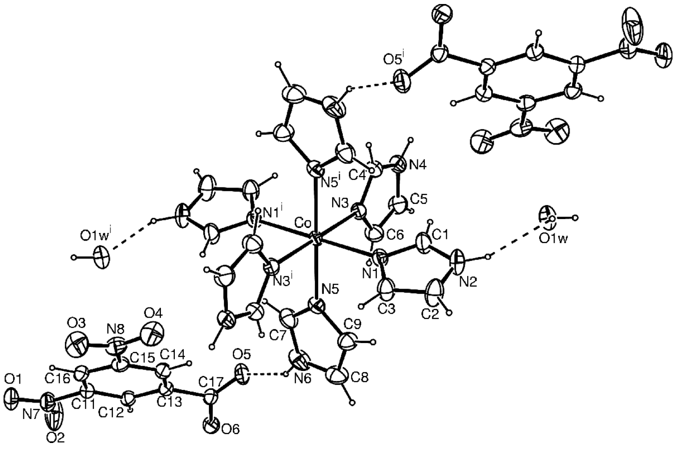


Figure 1
The molecular structure of (I), shown with 30% probability displacement ellipsoids. Dashed lines indicate hydrogen bonds. [Symmetry codes: (i) $1-x, 1-y, 1-z$].

89.38 (6) (between the N1- and N3-containing rings), 88.50 (7) (between the N3- and N5-containing rings) and 77.37 (8)° (between the N1- and N5-containing rings). While two imidazole ligands are hydrogen bonded to extra cluster water molecules (Fig. 1), the other four are hydrogen bonded to carboxyl groups of dinitrobenzoate anions (Fig. 2). Weak C—H···π interactions occur between imidazole rings, as evidenced by the following geometrical data (*Cg* is the centroid of the relevant ring): H1···*Cg*(N3-ring) = 2.98 Å and C1—H1···*Cg*(N3-ring) = 134°; H4···*Cg*(N5-ring) = 3.02 Å and C4—H4···*Cg*(N5-ring) = 137°; H9···*Cg*(N1-ring) = 3.03 Å and C9—H9···*Cg*(N1-ring) = 133°. No π–π stacking is observed in the crystal structure of (I).

The dinitrobenzoate does not coordinates to the Co^{II} atom but bridges neighboring complex cations *via* the N—H···O hydrogen bonds (Table 2 and Fig. 2).

Experimental

A mixed acetonitrile–water solution (20 ml *v*/*v*) containing 3,5-dinitrobenzoic acid (0.21 g, 2 mmol), NaOH (0.08 g, 2 mmol) and $CoCl_2·6H_2O$ (0.24 g, 1 mmol) was refluxed for 30 min. Imidazole (0.24 g, 1 mmol) was then added to the solution which was refluxed for a further 9 h. After cooling to room temperature, the solution was filtered and red single crystals of (I) were obtained after 3 d from the filtrate.

Crystal data

$[Co(C_3H_4N_2)_6](C_7H_3N_2O_6)_2·2H_2O$
M_r = 925.68
Monoclinic, $P2_1/n$
a = 15.1912 (13) Å
b = 8.2285 (10) Å
c = 16.7012 (12) Å
β = 104.058 (12)°
V = 2025.1 (4) Å^3
Z = 2

D_x = 1.518 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 10 399 reflections
θ = 2.8–25.0°
μ = 0.51 mm^{-1}
T = 295 (2) K
Prism, red
0.35 × 0.32 × 0.17 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.831, T_{max} = 0.912
17 920 measured reflections

4613 independent reflections
3847 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 27.4°
$h = -19 \rightarrow 19$
$k = -10 \rightarrow 10$
$l = -21 \rightarrow 21$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.084
S = 1.05
4613 reflections
286 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0384P)^2 + 0.6491P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

Table 1
Selected bond lengths (Å).

Co—N3	2.1497 (13)	Co—N5	2.1582 (13)
Co—N1	2.1536 (13)		

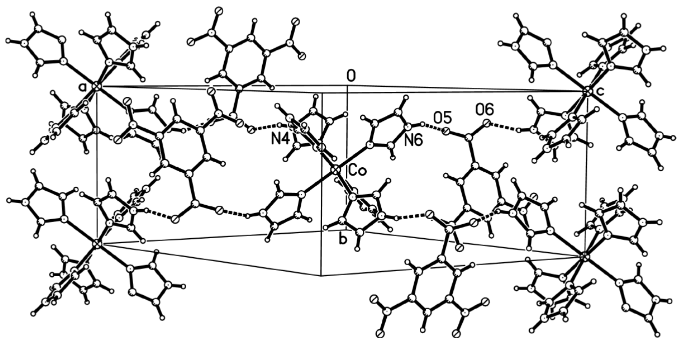


Figure 2
The molecular packing diagram for (I). Dashed lines indicate hydrogen bonds between cations and anions.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···O1*W*	0.86	2.01	2.794 (2)	151
N4—H4*A*···O6^{iii}	0.86	1.96	2.804 (2)	166
N6—H6*A*···O5	0.86	2.02	2.798 (2)	150
O1*W*—H1*A*···O6^{ii}	0.87	1.96	2.7976 (19)	160
O1*W*—H1*B*···O5^{i}	0.83	1.92	2.7408 (19)	169

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

The water H atoms (H1*A* and H1*B*) were located in a difference Fourier map and modelled with fixed positions and fixed isotropic displacement parameters of 0.08 Å^2. The other H atoms were placed in calculated positions with C—H = 0.93 Å and N—H = 0.86 Å, and were refined using a riding model, with $U_{iso}(H) = 1.2U_{eq}$ of their carrier atoms.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 for Windows (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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