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Diaquatetraimidazolecobalt(II) dibromide

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Key indicators

Single-crystal X-ray study
T = 223 K
Mean σ(C–C) = 0.003 Å
R factor = 0.021
wR factor = 0.050
Data-to-parameter ratio = 19.6

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

In the title compound, $[Co(C_3H_4N_2)_4(H_2O)_2]Br_2$, the Co atom is situated on an inversion center. It is coordinated by four N atoms of four imidazole ligands and two O atoms of water molecules and has an octahedral geometry. In the crystal structure, water molecules, imidazole NH groups and Br atoms contribute to the formation of a three-dimensional hydrogen-bonded network.

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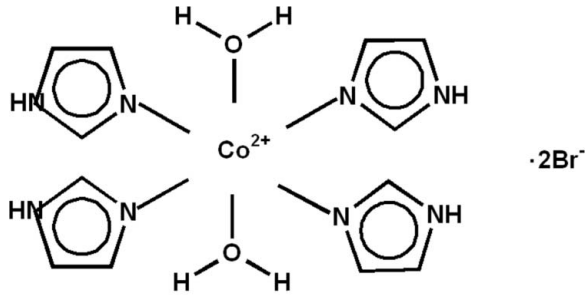
Comment

In the title complex, (I), the centrosymmetric coordination environment of cobalt is similar to that in $[Co(C_3H_4N_2)_4(H_2O)_2]Cl_2$, (II) (Furenlid *et al.*, 1986). For example, the bond distances in (II) [Co—N = 2.103 (2) and 2.169 (2) Å, and Co—O = 2.171 (2) Å] are similar to those in (I) (Table 1).



(I)

Experimental

Crystals of (I) were obtained from $CoBr_2{\cdot}6H_2O$ (5 mmol) and imidazole (10 mmol) in an aqueous solution (30 ml) at room temperature. After a few days, pink prism-shaped crystals appeared.

Crystal data

$[Co(C_3H_4N_2)_4(H_2O)_2]Br_2$
M_r = 527.11
Monoclinic, $C2/c$
a = 12.6213 (18) Å
b = 11.2582 (16) Å
c = 14.291 (2) Å
β = 109.869 (3)°
V = 1909.7 (5) Å^3
Z = 4
D_x = 1.833 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 12889 reflections
θ = 2.5–28.3°
μ = 5.11 mm^{-1}
T = 223 (2) K
Prism, pink
0.30 × 0.25 × 0.19 mm

Data collection

Bruker AXS APEX CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS* in *SAINT*; Bruker 1998)
T_{min} = 0.24, T_{max} = 0.38
12889 measured reflections
2377 independent reflections
2121 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 28.3°
$h = -16 \rightarrow 16$
$k = -14 \rightarrow 14$
$l = -18 \rightarrow 18$

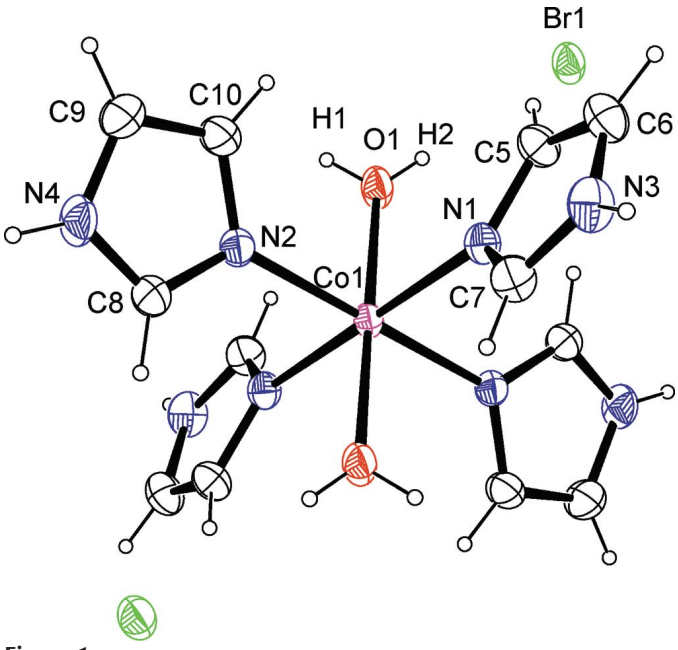


Figure 1
The crystal structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme. Unlabeled atoms are related to labeled atoms by $\frac{1}{2}-x, \frac{1}{2}-y, 1-z$.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.021$
$wR(F^2) = 0.050$
$S = 1.09$
2377 reflections
121 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0204P)^2 + 1.4558P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.32$ e Å^{-3}
$\Delta\rho_{min} = -0.46$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—N2	2.1120 (15)	O1—H1	0.82 (2)
Co1—N1	2.1657 (14)	O1—H2	0.76 (2)
Co1—O1	2.1672 (13)		
N2—Co1—N1	89.28 (5)	N1—Co1—O1	89.92 (5)
N2—Co1—O1	89.32 (6)	H1—O1—H2	107 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H2···Br1^{i}	0.76 (2)	2.54 (3)	3.2965 (14)	180 (2)
O1—H1···Br1^{ii}	0.82 (2)	2.46 (2)	3.2659 (14)	170 (2)
N4—H4···Br1	0.86	2.61	3.3875 (16)	151
N3—H3···Br1^{iii}	0.86	2.67	3.4607 (16)	154

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

The imidazole H atoms were constrained to an ideal geometry, with C—H = 0.93 Å and N—H = 0.86 Å. Water H atoms were located in a difference Fourier map and their positions were refined freely.

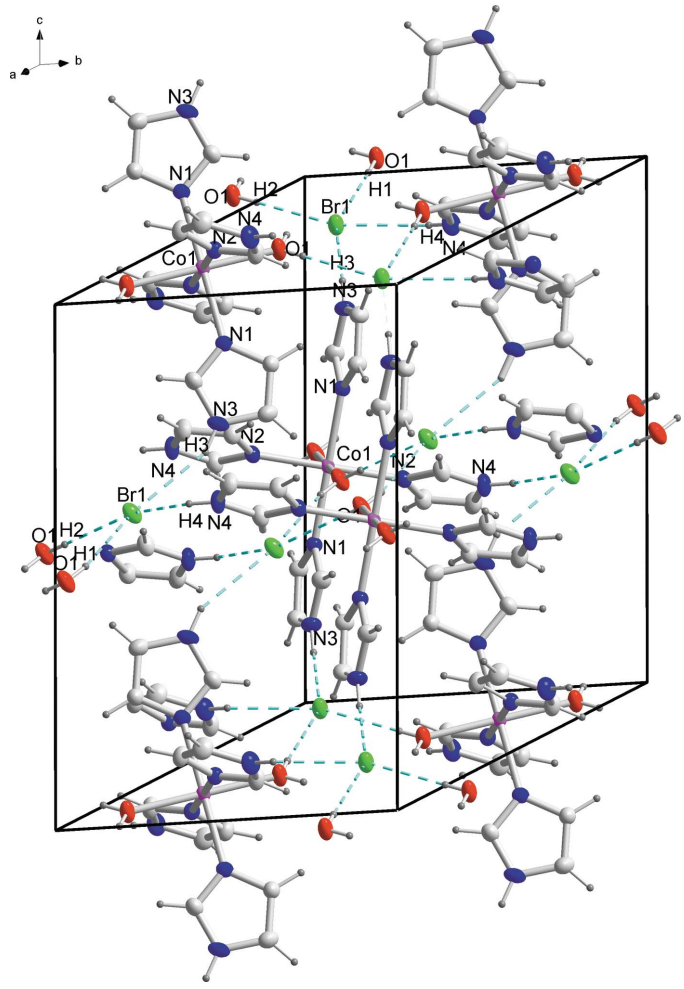


Figure 2
The crystal packing of (I), showing the hydrogen-bonding interactions as dashed lines.

All H atoms were assigned isotropic displacement parameters $U_{iso}(H) = 1.2U_{eq}(C,N,O)$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *ORTEP3* (Farrugia, 1997) and *DIAMOND* (Brandenburg & Berndt, 1999); software used to prepare material for publication: *SHELXTL*.

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