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Bis[(1*H*-benzimidazol-2-yl)methanol-κ^2N,O]-(nitrato-κ^2O,O')zinc(II) nitrate monohydrate

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Key indicators

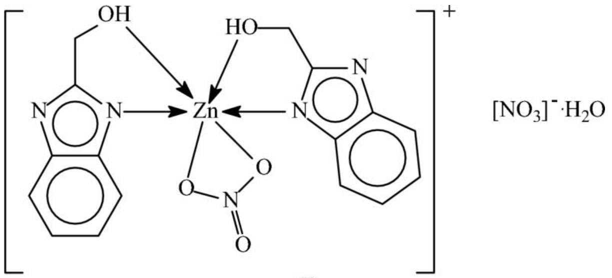
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.042
wR factor = 0.114
Data-to-parameter ratio = 11.0

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

The title compound, $[Zn(NO_3)(C_8H_8N_2O)_2]NO_3\cdot H_2O$, consists of a tris-chelated zinc cation and a nitrate anion, along with an uncoordinated water molecule. These interact through O—H···O and N—H···O hydrogen bonds, giving rise to a three-dimensional network structure. The Zn^{II} ion has an octahedral coordination.

Comment

The benzimidazol-2-ylmethanol ligand has been shown to bind to cobalt(II) as a neutral chelate (Zeng *et al.*, 2006). This feature is also preserved in the present zinc nitrate complex; of the two nitrate anions, only one is involved in coordination. The compound crystallizes as a monohydrate, (I) (Fig. 1), and the metal shows an octahedral coordination. The heterocycle as well as the nitrate group engage in chelation. The structure is consolidated by hydrogen bonds (Table 1) between the cation, anion and the uncoordinated water molecule, leading to a three-dimensional network.



(I)

Experimental

(1*H*-Benzimidazol-2-yl)methanol (0.15 g, 1 mmol), zinc(II) nitrate hexahydrate (0.15 g, 0.5 mmol) and zinc(II) acetate (0.12 g, 0.5 mmol) were dissolved in water (10 ml). Pale-yellow platelets separated from the solution after two weeks.

Crystal data

$[Zn(NO_3)(C_8H_8N_2O)_2]NO_3\cdot H_2O$
M_r = 503.73
Triclinic, $P\overline{1}$
a = 8.2287 (8) Å
b = 9.6745 (9) Å
c = 13.542 (1) Å
α = 81.506 (2)°
β = 80.678 (2)°
γ = 69.867 (2)°
V = 993.89 (15) Å^3
Z = 2
D_x = 1.683 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 1.30 mm^{-1}
T = 293 (2) K
Thick plate, pale yellow
0.20 × 0.15 × 0.08 mm

Data collection

Bruker APEX2 area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.781$, $T_{\max} = 0.903$
5025 measured reflections
3444 independent reflections
2947 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.020$
$\theta_{\max} = 25.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.114$
$S = 1.06$
3444 reflections
313 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0636P)^2 + 0.1377P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.42$ e Å^{-3}
$\Delta\rho_{\min} = -0.38$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	2.246 (3)	Zn1—O4	2.213 (3)
Zn1—O2	2.173 (3)	Zn1—N1	1.997 (2)
Zn1—O3	2.195 (2)	Zn1—N3	1.993 (3)
O1—Zn1—O2	117.3 (1)	O2—Zn1—N3	77.1 (1)
O1—Zn1—O3	96.2 (1)	O3—Zn1—O4	58.1 (1)
O1—Zn1—O4	154.1 (1)	O3—Zn1—N1	99.5 (1)
O1—Zn1—N1	76.2 (1)	O3—Zn1—N3	98.8 (1)
O1—Zn1—N3	85.3 (1)	O4—Zn1—N1	103.1 (1)
O2—Zn1—O3	145.4 (1)	O4—Zn1—N3	100.8 (1)
O2—Zn1—O4	88.6 (1)	N1—Zn1—N3	155.2 (1)
O2—Zn1—N1	96.7 (1)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1*o*···O1*w*	0.85 (1)	1.80 (1)	2.635 (4)	172 (5)
O2—H2*o*···O6$^{\rm i}$	0.84 (1)	2.08 (2)	2.877 (4)	159 (4)
O1*w*—H1*w*1···O5$^{\rm ii}$	0.85 (1)	2.07 (2)	2.908 (5)	168 (5)
O1*w*—H1*w*2···O6$^{\rm iii}$	0.85 (1)	2.29 (3)	3.038 (5)	148 (5)
N2—H2*n*···O6	0.85 (1)	2.14 (2)	2.922 (4)	154 (4)
N4—H4*n*···O7$^{\rm iv}$	0.85 (1)	2.14 (2)	2.959 (4)	163 (3)

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

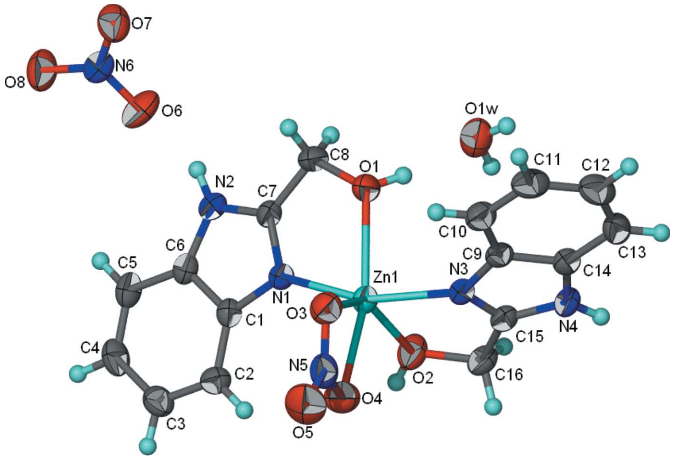


Figure 1
The asymmetric unit of (I). Displacement ellipsoids are drawn at the 50% probability level, and H atoms as spheres of arbitrary radii.

The C-bound H atoms were placed in calculated positions (C—H = 0.93–0.97 Å) and included in the refinement in the riding-model approximation, with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$. The amino, hydroxy and water H atoms were located in a difference Fourier map and refined isotropically with distance restraints of O(N)—H = 0.85 (1) Å and H···H = 1.39 (1) Å.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *SHELXL97*.

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