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Tetrakis(1*H*-imidazole-κN^3)zinc(II) bis(2-hydroxy-3,5-dinitrobenzoate)

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The title complex, $[Zn(C_3H_4N_2)_4](C_7H_3N_2O_7)_2$, consists of a tetrakis(1*H*-imidazole-κN^3)zinc(II) cation and two 2-hydroxy-3,5-dinitrobenzoate anions. In the cation, the Zn^{II} atom, located on a twofold axis, is tetrahedrally coordinated by four N atoms from four imidazole ligands. Intermolecular hydrogen bonds between cations and anions form a supramolecular network.

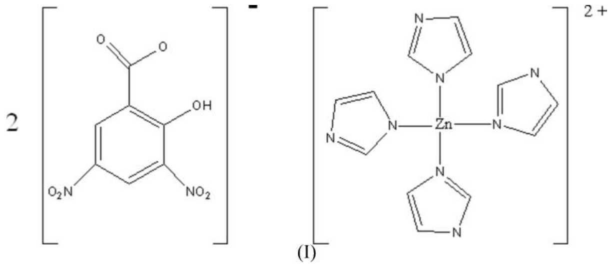
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.042
wR factor = 0.102
Data-to-parameter ratio = 15.1

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

Comment

In recent years, much attention has been paid to the design and construction of metal-organic frameworks because of their interesting structural motifs (Dakanali *et al.*, 2003), fluorescent properties (Shi *et al.*, 2004) and potential applications (Seo *et al.*, 2000; Kitaura *et al.*, 2002; Rowsell *et al.*,2004) in molecular-based materials. 3,5-Dinitrosalicylate, which contains carboxylate and hydroxy groups, is a member of a family of flexible ligands with versatile binding modes. We report here a tetra(imidazole)zinc(II) complex, (I), with 2-hydroxy-3,5-dinitrobenzoate as counter-ion.



(I)

The asymmetric unit of (I) consists of one half of a mononuclear tetrakis(1*H*-imidazole-κN^3)zinc(II) cation and one 2-hydroxy-3,5-dinitrobenzoate anion (Fig. 1). The Zn^{II} atom, located on a twofold axis, is tetrahedrally coordinated by four N donor atoms from four imidazole ligands, with nearly identical Zn—N distances of 1.988 (2) and 1.990 (2)Å. Cations and anions are connected through N—H$\cdots$O hydrogen bonds involving the NH of imidazole ligands as donors and the O atoms of NO_2 groups as acceptors, forming a supramolecular network (Table 1).

Experimental

The title complex was prepared by the addition of stoichiometric amounts of zinc acetate (20 mmol) and imidazole (20 mmol) to a hot aqueous solution of 3,5-dinitrosalicylic acid (20 mmol). The pH was then adjusted to 7–8 with NaOH (30 mmol). The resulting solution was filtered and yellow single crystals were obtained after several days at room temperature (yield 64%).

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Crystal data

$[Zn(C_3H_4N_2)_4](C_7H_3N_2O_7)_2$
$M_r = 791.93$
Monoclinic, $C2/c$
$a = 25.0809\ (15)$ Å
$b = 6.7251\ (4)$ Å
$c = 18.9145\ (10)$ Å
$\beta = 97.658\ (6)^\circ$
$V = 3161.9\ (3)$ Å^3
$Z = 4$
$D_x = 1.664$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.87$ mm^{-1}
$T = 293\ (2)$ K
Block, yellow
$0.20 \times 0.18 \times 0.10$ mm

Data collection

Bruker APEX-II area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.846$, $T_{max} = 0.918$
20634 measured reflections
3635 independent reflections
2431 reflections with $I > 2\sigma(I)$
$R_{int} = 0.058$
$\theta_{max} = 27.6^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.102$
$S = 1.05$
3635 reflections
241 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0425P)^2 + 0.9736P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.37$ e Å^{-3}
$\Delta\rho_{min} = -0.43$ e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4A···O1^{i}	0.86	1.97	2.787 (3)	159
N2—H2A···O3	0.86	2.00	2.843 (3)	168
O1—H1A···O2	0.82	1.75	2.502 (2)	152

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

All H atoms were positioned geometrically and refined as riding, with C—H = 0.93, N—H = 0.86 and O—H = 0.82 Å, and with U_{iso}(H) = $1.2U_{eq}$(C,N,O).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXTL* (Bruker, 1998).

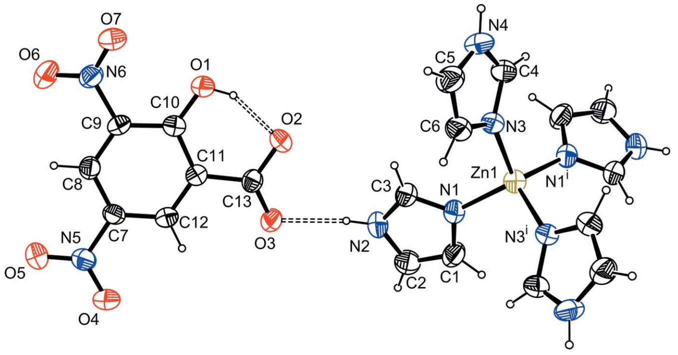

Figure 1
The structures of the cation and anion of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radius. [Symmetry code: (i) $1 - x, y, \frac{3}{2} - z$.]

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