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Diaquabis[5-(pyrazin-2-yl)tetrazolato]manganese(II)

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Key indicators

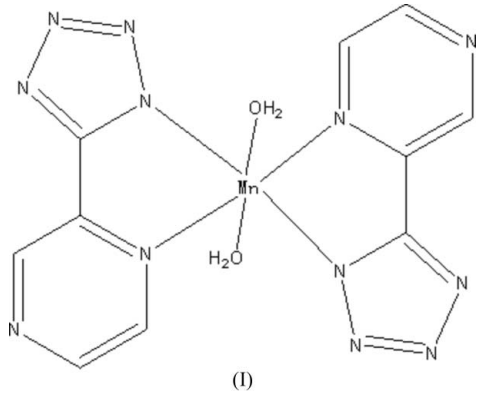
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.025
wR factor = 0.069
Data-to-parameter ratio = 13.8

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

In the title complex, $[Mn(C_5H_3N_3)_2(H_2O)_2]$, the Mn^{II} atom, located on an inversion center, is coordinated by four N atoms from two 5-(2-pyrazinyl)tetrazolate ligands and two water molecules in a distorted octahedral geometry. The packing is governed by intermolecular O—H···N hydrogen bonds.

Comment

The design, synthesis, characterization, and properties of supramolecular networks formed by using functionalized organic molecules as bridges between metal centers are of great interest (Rizk *et al.*, 2005; Eddaoudi *et al.*, 2001). Reports on tetrazoles are increasing rapidly, since tetrazoles play an important role as a ligand in coordination chemistry (Song & Xi, 2006). Recently, 5-substituted 1*H*-tetrazoles have been synthesized by a facile approach (Demko & Sharpless, 2001*a*,*b*). In the general reaction, the tetrazoles are prepared by the addition of an azide to a nitrile in water with the aid of a Lewis acid such as Zn^{2+}. In this paper, we selected 2-cyanopyrazine, NaN_3 and a Lewis acid $MnCl_2$ as reagents to yield, in one-step, the title mononuclear complex, (I), under hydrothermal conditions.



(I)

In (I), the Mn^{II} atom, located on an inversion center, is coordinated by four N atoms from two 5-(2-pyrazinyl)tetrazolate ligands and two water molecules in a distorted octahedral geometry. In each ligand, the pyrazinyl and tetrazolyl rings are almost coplanar, making a dihedral angle of 2.51 (5)°. Intermolecular O—H···N hydrogen bonds (Table 2) stabilize the crystal packing.

Experimental

Hydrothermal treatment of $MnCl_2{\cdot}4H_2O$ (1.0 mmol, 0.197 g), 2-cyanopyrazine (1 mmol, 0.105 g), NaN_3 (1 mmol, 0.065 g), and water

(3 ml) over 50 h at 422 K yielded red block-shaped crystals (yield: 60%).

Crystal data

$[Mn(C_5H_3N_3)_2(H_2O)_2]$
M_r = 385.24
Monoclinic, $P2_1/n$
a = 5.9840 (3) Å
b = 11.7421 (5) Å
c = 10.8646 (5) Å
β = 104.731 (2)°
V = 738.31 (6) Å^3
Z = 2
D_x = 1.733 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.93 mm^{-1}
T = 293 (2) K
Block, yellow
0.25 × 0.20 × 0.17 mm

Data collection

Bruker APEX-II area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.800, T_{max} = 0.858
9055 measured reflections
1700 independent reflections
1576 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.069
S = 1.05
1700 reflections
123 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0389P)^2 + 0.1934P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1W···N6^{i}	0.83 (2)	1.92 (2)	2.7425 (16)	169 (2)
O1W—H2W···N4^{ii}	0.77 (3)	2.04 (3)	2.7939 (18)	167 (2)

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

H atoms of the water molecule were located in a difference Fourier map and were refined isotropically. Other H atoms were placed in calculated positions and treated as riding on their parent atoms, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C).

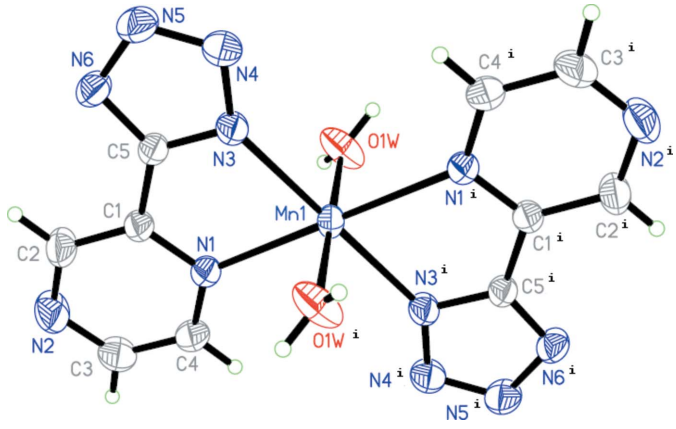


Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Non-H atoms are shown as 50% probability displacement ellipsoids. H atoms are represented as small spheres of arbitrary radii. [Symmetry code: (i) $2-x, 2-y, 1-z$.]

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: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

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