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Tetraaquabis(isothiocyanato)manganese(II) bis(2-methylpyrazine-1,4-dioxide)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.035
wR factor = 0.097
Data-to-parameter ratio = 11.9

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

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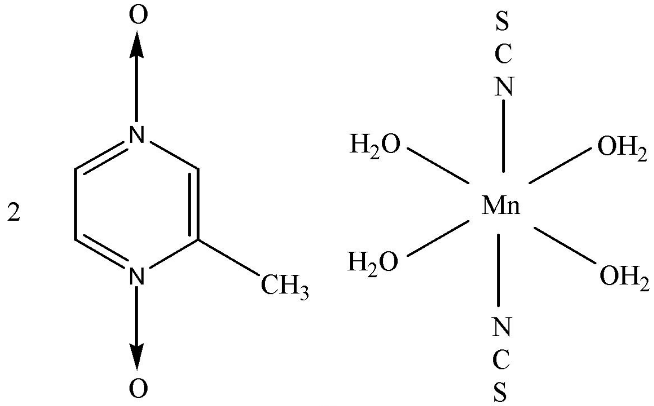
In the title molecular complex, $[Mn(NCS)_2(H_2O)_4]\cdot 2C_5H_6N_2O_2$, the manganese(II) atom has a slightly distorted octahedral coordination, formed by four O atoms from the water molecules and two N atoms from the thiocyanate anions. The Mn complrx lies on a special position of site symmetry 2 and $\overline{1}$, and the 2-methylpyrazine-1,4-dioxide molecule is located on a mirror plane. The crystal packing is stabilized by intermolecular OH(water)$\cdots$O$\leftarrow$N hydrogen bonds.

Comment

In the title molecular complex, (I), the manganese(II) atom is coordinated by four O atoms from the water molecules and two N atoms from the thiocyanate anions. Atom Mn1 lies on a twofold axis and an inversion centre. The Mn1–O3 and Mn1–N3 bond lengths are 2.1918 (14) Å and 2.188 (3) Å, respectively; the manganese(II) atom has a slightly distorted octahedral coordination. The non-H atoms of the 2-methylpyrazine-1,4-dioxide molecules lie on mirror planes. In the crystal structure, the 2-methylpyrazine-1,4-dioxide molecules are packed as columns along the b axis, with the manganese(II) complexes positioned between the columns. The crystal packing (Fig. 2) is stabilized by intermolecular OH(water)$\cdots$O$\leftarrow$N hydrogen bonds (Table 1).



(I)

Experimental

To 15 ml of an aqueous solution of $Mn(ClO_4)_2\cdot 6H_2O$ (0.1425 g, 0.394 mmol) and sodium thiocyanate (0.0652 g, 0.804 mmol), 2-methylpyrazine-1,4-dioxide (0.0511 g, 0.405 mmol) was added. The resulting solution was stirred for a few minutes. Colorless single crystals were obtained after the solution was allowed to stand at room temperature for three weeks.

Crystal data

$[Mn(NCS)_2(H_2O)_4]\cdot 2C_5H_6N_2O_2$
$M_r = 495.40$
Monoclinic, $C2/m$
$a = 17.027\ (6)$ Å
$b = 6.828\ (3)$ Å
$c = 10.126\ (4)$ Å
$\beta = 111.844\ (4)^\circ$
$V = 1092.7\ (8)$ Å^3
$Z = 2$
$D_x = 1.506$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2372 reflections
$\theta = 2.6$–26.9°
$\mu = 0.84$ mm^{-1}
$T = 293\ (2)$ K
Prism, colorless
$0.20 \times 0.15 \times 0.11$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.848$, $T_{max} = 0.911$
2787 measured reflections
1103 independent reflections
1026 reflections with $I > 2\sigma(I)$
$R_{int} = 0.028$
$\theta_{max} = 25.5^\circ$
$h = -20 \rightarrow 14$
$k = -8 \rightarrow 8$
$l = -10 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.097$
$S = 1.09$
1103 reflections
93 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0634P)^2 + 0.3225P]$, where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.47$ e Å^{-3}
$\Delta\rho_{min} = -0.47$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H7A···O2^{i}	0.89	1.84	2.716 (2)	170
O3—H6B···O1^{ii}	0.82	1.96	2.748 (2)	162

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

The methyl H atoms (H4A and H5B) and atom H7A from the coordinated water molecule were found in a difference Fourier map. The rest of the H atoms were positioned geometrically. All H atoms were included in the final cycles of the refinement using a riding model (C—H = 0.93–0.97 Å, O—H = 0.82–0.89 Å, U_{iso}(H) = 1.2–1.5 U_{eq} of the carrier atom).

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

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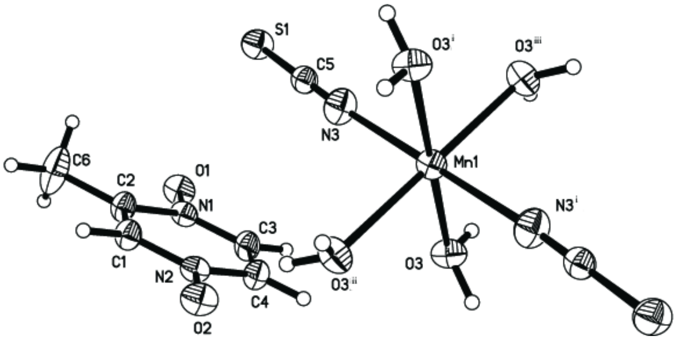

Figure 1
View of (I), showing 30% probability displacement ellipsoids. [Symmetry codes: (i) $-x, -y, -z$; (ii) $x, -y, z$; (iii) $-x, y, -z$].

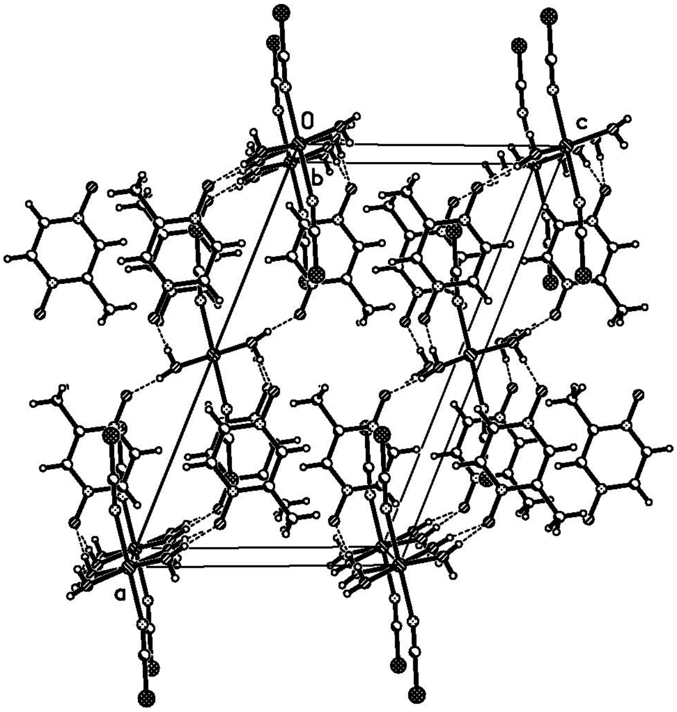

Figure 2
The packing of (I). The intermolecular O—H···O hydrogen bonds are indicated by dashed lines.

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