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Diaquabis[4-(3-pyridyl)-1*H*-1,2,4-triazole]-dithiocyanatomanganese(II)

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.005 Å
R factor = 0.045
wR factor = 0.120
Data-to-parameter ratio = 12.4

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

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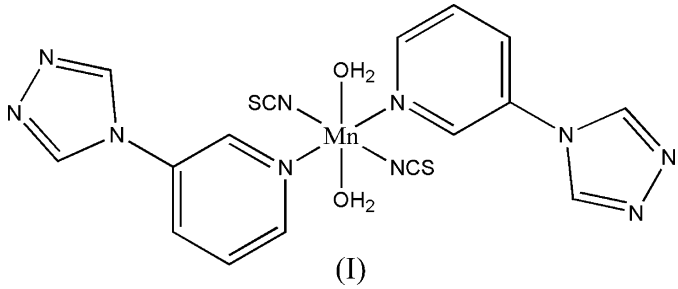
The crystal structure of the title compound, $[Mn(NCS)_2(C_7H_6N_4)_2(H_2O)_2]$, is stabilized by O—H···N hydrogen bonding.

Comment

Transition metal complexes with 1,2,4-triazole derivatives as ligands are of great interest from both theoretical and practical viewpoints as they are the subject of magnetic studies (Shakirova *et al.*, 2002). In the present paper, the title compound, (I), has been synthesized.



(I)

The structure of compound (I) is shown in Fig. 1. The bond lengths and angles of the molecule are shown in Table 1. The crystal structure is stabilized by O—H···N hydrogen bonds (Fig. 2 and Table 2). The Mn atoms are octahedrally coordinated by two water O atoms in one axis, two thiocyanate N atoms in another axis and two N atoms of the 4-(3-pyridyl)-1*H*-1,2,4-triazole ligands in the third axis.

Experimental

The title compound was prepared by adding a hot ethanol solution (2 ml) of 3-(4*H*-1,2,4-triazol-4-yl)pyridine (2 mmol, 0.292 g) to a solution of the metal salt $MnCl_2$ (1 mmol, 0.126 g) and NaSCN (2 mmol, 0.162 g) in hot water (3 ml). The mixture was stirred for several hours. A precipitate was obtained after partial evaporation of the resulting solution followed by cooling. Suitable crystals were obtained by slow evaporation of a solution of the compound in water.

Crystal data

$[Mn(NCS)_2(C_7H_6N_4)_2(H_2O)_2]$
M_r = 499.45
Triclinic, $P\overline{1}$
a = 9.829 (3) Å
b = 10.150 (3) Å
c = 10.826 (3) Å
α = 88.111 (4)°
β = 74.483 (4)°
γ = 85.562 (5)°
V = 1037.5 (5) Å^3
Z = 2
D_x = 1.599 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.88 mm^{-1}
T = 294 (2) K
Block, colourless
0.22 × 0.20 × 0.16 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.820, T_{max} = 0.873
5268 measured reflections
3623 independent reflections
2387 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.121
S = 1.05
3623 reflections
292 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0568P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.51 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Mn1—N1	2.161 (3)	Mn1—N3	2.334 (3)
Mn1—N2	2.162 (3)	Mn1—N7	2.349 (3)
Mn1—O1	2.189 (3)	S1—C1	1.622 (4)
Mn1—O2	2.214 (3)	S2—C2	1.621 (4)
N1—Mn1—N2	178.56 (12)	O1—Mn1—N3	92.17 (10)
N1—Mn1—O1	88.72 (11)	O2—Mn1—N3	83.74 (10)
N2—Mn1—O1	92.56 (11)	N1—Mn1—N7	90.68 (11)
N1—Mn1—O2	90.56 (11)	N2—Mn1—N7	88.65 (11)
N2—Mn1—O2	88.21 (11)	O1—Mn1—N7	89.94 (10)
O1—Mn1—O2	175.83 (9)	O2—Mn1—N7	94.18 (10)
N1—Mn1—N3	91.60 (11)	N3—Mn1—N7	176.93 (10)
N2—Mn1—N3	89.02 (11)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···N6^{i}	0.84 (2)	2.02 (2)	2.843 (4)	171 (4)
O1—H1B···N5^{ii}	0.87 (2)	1.95 (2)	2.816 (4)	174 (4)
O2—H2A···N10^{iii}	0.86 (2)	1.97 (2)	2.821 (4)	171 (3)
O2—H2B···N9^{iv}	0.84 (2)	2.00 (2)	2.836 (4)	176 (4)

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

C-bound H atoms were positioned geometrically and refined in the riding-model approximation, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C). Water H atoms were located in a difference map and then restrained to O—H = 0.85 (3) Å and U_{iso}(H) = 1.5U_{eq}(O).

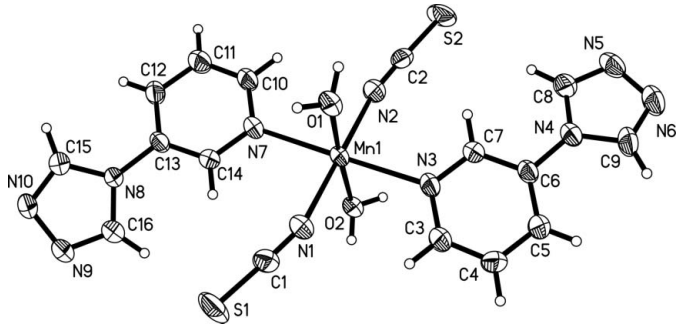


Figure 1
The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

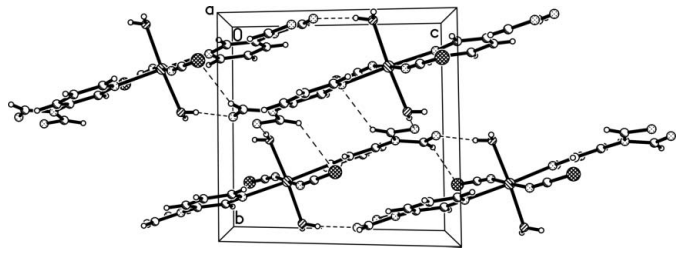


Figure 2
A packing diagram for (I), viewed down the *a* axis. Hydrogen-bonding interactions are illustrated by dashed lines.

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* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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