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Tetrakis[3-(pyrazin-2-yloxy)pyridine-κN]-dithiocyanatomanganese(II)

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.053
wR factor = 0.120
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.

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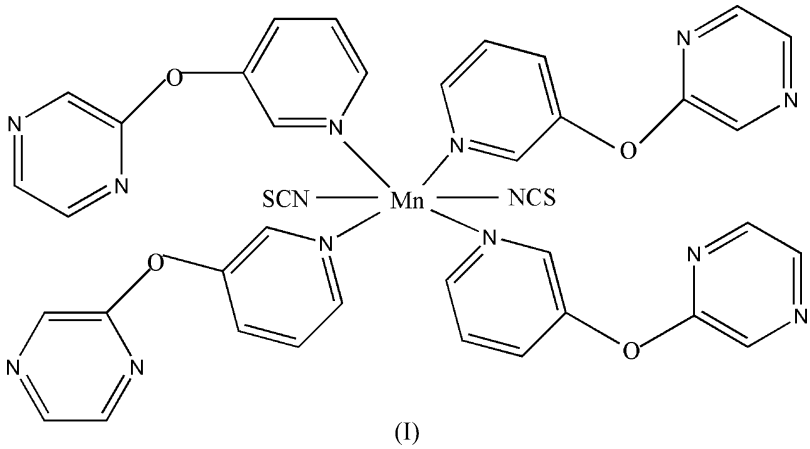
In the title compound, $[Mn(NCS)_2(C_9H_7N_3O)_4]$, the Mn^{II} ion lies on an inversion centre and assumes a distorted octahedral MnN_6 coordination geometry. Weak C—H···N and π–π stacking interactions consolidate the crystal packing.

Comment

Metal complexes with *N*-heterocyclic rings as ligands play a pivotal role in modern coordination chemistry: however, ligand molecules that consist of pyrazinyl and pyridyl are less well studied (Mcmorran & Steel, 2002). Our interest in these ligands resulted in the synthesis of the title complex, (I) (Fig. 1)



(I)

The Mn^{II} ion lies on an inversion centre and assumes a distorted octahedral coordination geometry (Table 1) from four N-bonded 3-(pyrazin-2-yloxy)pyridine ligands and two N-bonded thiocyanate anions. In the crystal structure of (I) there are weak C—H···N intra- and intermolecular interactions (Table 2). In addition, weak π–π stacking interactions occur between the pyridyl and pyrazine rings; the relevant distances are $Cg1\cdots Cg2^{i}$ = 3.766 (2) and $Cg1\cdots Cg2^{i}_{perp}$ = 3.595Å [symmetry code: (i) $1-x, 1-y, 1-z$; $Cg1$ and $Cg2$ are the centroids of the N5/C1–C5 and N3/N4/C9/C11–C13 rings, respectively; $Cg1\cdots Cg2^{i}_{perp}$ is the perpendicular distance from the $Cg1$ ring plane to the $Cg2^{i}$ ring plane].

Experimental

A methanol solution (5 ml) of 3-(pyrazin-2-yloxy)pyridine (0.0627 g, 0.362 mmol) was added to an aqueous solution (10 ml) of $Mn(ClO_4)_2\cdot 6H_2O$ (0.2621 g, 0.724 mmol) and NaNCS (0.1174 g, 1.45 mmol). The mixture was stirred for a few minutes and colorless single crystals of (I) were obtained after allowing the solution to stand at room temperature for two weeks.

Crystal data

$[Mn(NCS)_2(C_9H_7N_3O)_4]$
M_r = 863.80
Triclinic, $P\overline{1}$
a = 9.421 (2) Å
b = 9.729 (2) Å
c = 11.650 (3) Å
α = 76.749 (4)°
β = 68.154 (3)°
γ = 88.666 (4)°
V = 962.4 (4) Å^3
Z = 1
D_x = 1.490 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.51 mm^{-1}
T = 298 (2) K
Prism, colorless
0.41 × 0.38 × 0.07 mm

Data collection

Bruker SMART APEX CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.817, T_{max} = 0.965
5227 measured reflections
3708 independent reflections
2946 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 26.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.120
S = 1.03
3708 reflections
268 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0569P)^2 + 0.0965P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Table 1
Selected bond lengths (Å).

Mn1—N1	2.146 (2)	Mn1—N2	2.342 (2)
Mn1—N5	2.305 (2)		

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···N7^{i}	0.93	2.57	3.441 (5)	156
C14—H14···N1^{ii}	0.93	2.60	3.201 (4)	123
C15—H15···N1	0.93	2.61	3.220 (4)	124

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

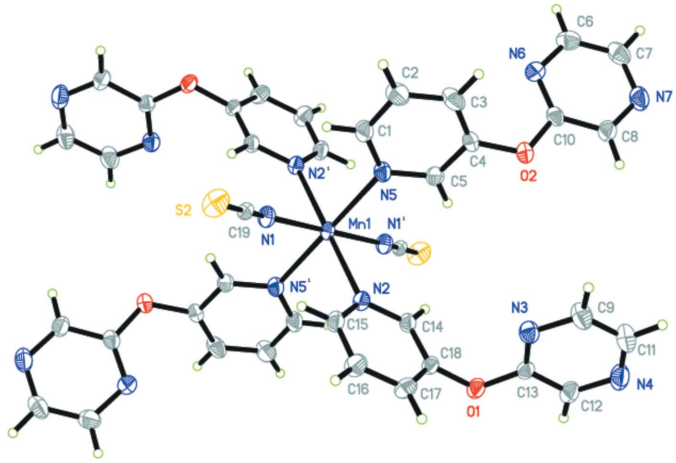


Figure 1
The molecular structure of (I), showing 30% displacement ellipsoids (arbitrary spheres for the H atoms). [Symmetry code: (i) $1-x, 1-y, -z$.]

All H atoms were placed in calculated positions (C—H = 0.93 Å) and refined as riding, with $U_{iso}(H) = 1.2U_{eq}(C)$.

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

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References

Bruker (1997). *SMART* (Version 5.6) and *SAINT* (Version 5. A06). Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2001). *SHELXTL*. Version 6.12. Bruker AXS Inc., Madison, Wisconsin, USA.
Mcmorran, D. A. & Steel, P. J. (2002). *Dalton Trans.* pp. 3321–3326.
Sheldrick, G. M. (1996). *SADABS*. Version 2.10. University of Göttingen, Germany.