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Bis(methanol)bis[(*E*)-4-methoxy-*N*-(4-pyridylmethylene)aniline]dithiocyanatomanganese(II)

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.042
wR factor = 0.097
Data-to-parameter ratio = 16.8

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

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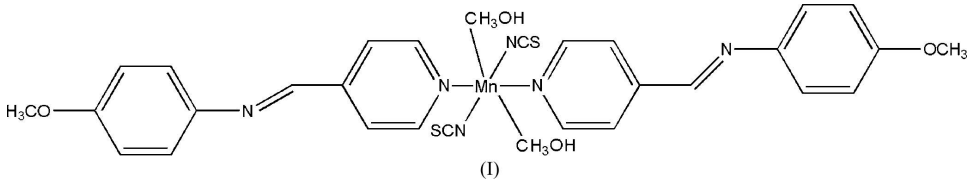
The title compound, $[Mn(NCS)_2(C_{13}H_{12}N_2O)_2(CH_3OH)_2]$, has been synthesized and structurally characterized. The Mn atom is located on a crystallographic inversion centre. O—H···N hydrogen bonds connect the Mn^{II} monomers into a one-dimensional tape structure.

Comment

Transition-metal complexes with (*E*)-4-methoxy-*N*-(4-pyridylmethylene)aniline (*L*) represent an active area of research in view of their interesting optical, photophysical and liquid-crystalline properties. However, only a few solid-state structures of these complexes have been reported (Wong *et al.*, 1999). In this paper, we report the synthesis and characterization of a new Mn^{II} monomer, (I), containing ligand *L*.



(I)

The structure analysis shows that the Mn^{II} atom is located on a crystallographic inversion centre and is six-coordinated in an MnO_2N_4 octahedral geometry, formed by two N atoms from ligands *L*, two SCN^- N atoms and two CH_3OH O atoms (Fig. 1). The Mn—N bond length to the coordinated SCN^- ion (Table 1) is slightly longer than that to *L*; the Mn—O/N bond lengths are in the range 2.150 (2)–2.336 (2) Å, which are comparable with those obsevered in other Mn^{II}-containing compounds (Hou *et al.*, 2004). The dihedral angle between the two aromatic rings within one ligand is 34.27 (15)°. Mn^{II} monomers are linked *via* hydrogen bonds into a one-dimensional tape running along the *a* axis (Table 2 and Fig. 2). The stacking mode suggests no significant π–π interactions.

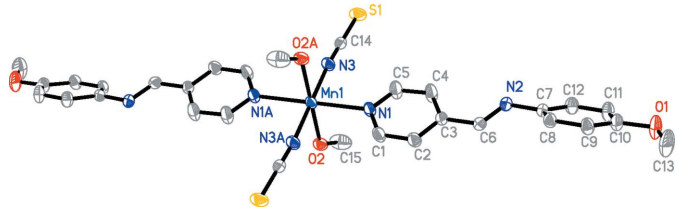


Figure 1
The molecular structure of the title compound with displacement ellipsoids drawn at the 30% probability level. H atoms have been omitted. [Symmetry code: (A) $-x+2, -y, -z+1$.]

Experimental

Ligand *L* was synthesized acoording to the method of Wong & Wong (1999). A mixture of *L* (0.2 ml) and $Mn(ClO_4)\cdot 6H_2O$ (0.1 mmol) in methanol (10 ml) was stirred for 20 min. Potassium thiocyanate (0.4 mmol) was added and the resulting yellow solution was filtered. After several days, yellow crystals were obtained in 67% yield (based on Mn). Elemental analysis (%) calculated for $C_{15}H_{16}Mn_{0.5}N_3O_2S$: C 49.78 H 4.46 N 11.61%; found: C 49.56 H 4.65 N 11.78%.

Crystal data

$[Mn(NCS)_2(C_{13}H_{12}N_2O)_2(CH_4O)_2]$
M_r = 659.70
Monoclinic, $P2_1/n$
a = 8.4046 (15) Å
b = 16.724 (3) Å
c = 12.306 (2) Å
β = 106.737 (3)°
V = 1656.4 (5) Å^3
Z = 2
D_x = 1.323 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.57 mm^{-1}
T = 294 (2) K
Block, yellow
0.24 × 0.22 × 0.18 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.876, T_{max} = 0.905
9254 measured reflections
3379 independent reflections
1963 reflections with $I > 2\sigma(I)$
R_{int} = 0.049
θ_{max} = 26.4°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.097
S = 1.00
3379 reflections
201 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0302P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

Table 1
Selected bond lengths (Å).

Mn1—N3^{i}	2.150 (2)	Mn1—O2	2.219 (2)
Mn1—N3	2.150 (2)	Mn1—N1	2.336 (2)
Mn1—O2^{i}	2.219 (2)	Mn1—N1^{i}	2.336 (2)

Symmetry code: (i) $-x+2, -y, -z+1$.

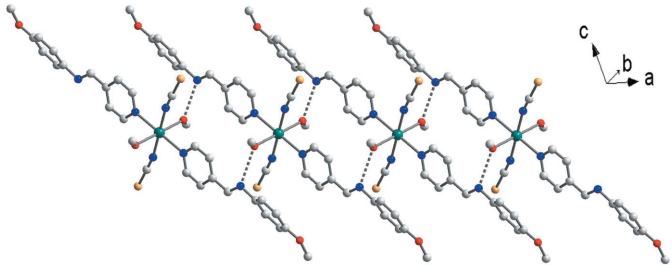


Figure 2
A view along *b* of the one-dimensional tape structure of the title compound.

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2A···N2^{ii}	0.818 (10)	2.016 (11)	2.831 (3)	174 (3)

Symmetry code: (ii) $x+1, y, z$.

H atoms were positioned geometrically and refined as riding, with C—H = 0.93–0.96 Å and O—H = 0.90 Å and U_{iso}(H) = 1.5U_{eq}(methyl C) or 1.2U_{eq}(C,O).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP*-III (Burnett & Johnson, 1996); software used to prepare material for publication: *SHELXTL* (Bruker, 1998).

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References

Bruker (1998). *SMART-NT*, *SAINT-NT* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Burnett, M. N. & Johnson, C. K. (1996). *ORTEPIII*. Report ORNL-6895. Oak Ridge National Laboratory, Tennessee, USA.
Hou, H., Li, L., Zhu, Y., Fan, Y.-T. & Qiao, Y.-Q. (2004). *Inorg. Chem.* **43**, 4767–4774.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Wong, W.-Y. & Wong, W.-T. (1999). *J. Organomet. Chem.* **584**, 48–57.