

Dicyanatobis(1,10-phenanthroline)manganese(II)

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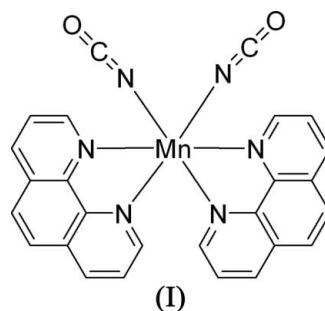
In the title compound, [Mn(NCO)₂(C₁₂H₈N₂)₂], the Mn atom, on a twofold rotation axis, is chelated by the two phenanthroline ligands, with two cyanate groups in *cis* positions.

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Comment

The ligand behavior of the cyanate ion (NCO⁻) is of interest because of its potential ambidentate character. In contrast to the situation with the pseudohalide NCS⁻, which has been studied in more detail, rather fewer NCO⁻ complexes have been reported (Anderson & Marshall, 1978; Schonherr, 1986; Luo *et al.*, 2003). Some Mn monomeric complexes have been reported (Cheng *et al.*, 2004; Wang *et al.*, 2004; Wu & Xu, 2004). Extending this research, we report here another new monomeric complex, namely dicyanatobis(1,10-phenanthroline)manganese(II), (I).



Two 1,10-phenanthroline molecules, one manganese(II) cation and two cyanate anions constitute the monomeric

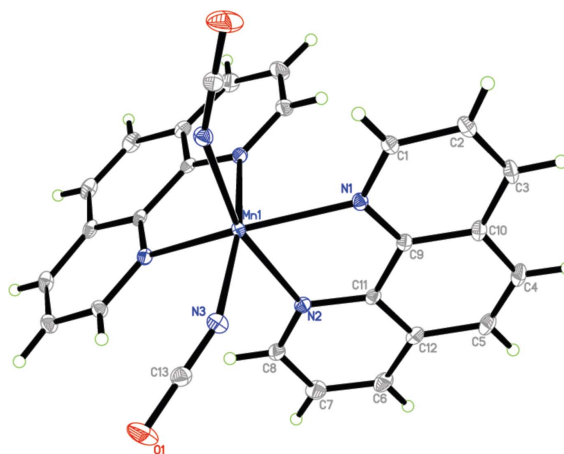


Figure 1

The molecular structure of the title complex. Displacement ellipsoids are drawn at the 30% probability level. Unlabeled atoms are related to labeled atoms by the symmetry operator $(-x + 1, y, -z + \frac{1}{2})$.

complex, with Mn lying on a twofold rotation axis. The metal atom adopts a distorted MnN_6 octahedral geometry defined by four N atoms from two 1,10-phenanthroline ligands and two cyanate anions that occupy *cis* positions (Fig. 1). The geometry of the manganese center is not significantly different from that found in the diaqua(1,10-phenanthroline) analog (Fan *et al.*, 2005).

Experimental

A mixture of manganese(II) perchlorate (1 mmol, 0.36 g), 1,10-phenanthroline (2 mmol, 0.40 g) and sodium cyanate (2 mmol, 0.11 g) in a water (30 ml) and ethanol mixture (1:1 *v/v*) was stirred for several hours at room temperature. The mixture was filtered and the resulting solution was evaporated at room temperature until yellow crystals formed. Analysis found C 62.06, H 3.33, N 16.73%; calculated for $\text{C}_{26}\text{H}_{16}\text{MnN}_6\text{O}_2$ C 62.53, H 3.23, N 16.83%.

Crystal data

$[\text{Mn}(\text{NCO})_2(\text{C}_{12}\text{H}_8\text{N}_2)_2]$
 $M_r = 499.39$
 Orthorhombic, *Pbcn*
 $a = 13.603$ (3) Å
 $b = 9.4010$ (19) Å
 $c = 16.749$ (3) Å
 $V = 2141.9$ (7) Å³
 $Z = 4$
 $D_x = 1.549$ Mg m⁻³

Mo $K\alpha$ radiation
 Cell parameters from 2133 reflections
 $\theta = 2.5\text{--}22.1^\circ$
 $\mu = 0.66$ mm⁻¹
 $T = 292$ (3) K
 Block, yellow
 $0.40 \times 0.28 \times 0.24$ mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
 Oscillation φ scans
 Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
 $T_{\min} = 0.805$, $T_{\max} = 0.858$
 15679 measured reflections

2423 independent reflections
 2133 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.045$
 $\theta_{\text{max}} = 27.5^\circ$
 $h = -17 \rightarrow 16$
 $k = -11 \rightarrow 11$
 $l = -21 \rightarrow 21$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.032$
 $wR(F^2) = 0.067$
 $S = 1.05$
 2423 reflections
 159 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.001P)^2 + 2P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.29$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.31$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Mn1—N3	2.1340 (14)	O1—C13	1.206 (2)
Mn1—N1	2.2874 (13)	N3—C13	1.162 (2)
Mn1—N2	2.3440 (13)		
N3—Mn1—N1	105.83 (5)	N3—C13—O1	179.2 (2)
N1—Mn1—N2 ⁱ	86.39 (5)		

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

H atoms were constrained to an ideal geometry, with C—H distances of 0.93 Å and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Data collection: *CrystalStructure* (Rigaku/MS, 2004); cell refinement: *CrystalStructure*; data reduction: *SHELXTL* (Bruker, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* (Sheldrick, 1998); software used to prepare material for publication: *SHELXTL*.

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References

- Anderson, O. P. & Marshall, J. C. (1978). *Inorg. Chem.* **17**, 1258–1263.
 Bruker (1997). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
 Cheng, Y., Hu, M., Fan, S. & Zhang, W. (2004). *Acta Cryst.* **E60**, m212–m213.
 Fan, S.-R., Zhu, L.-G., Xiao, H.-P. & Ng, S. W. (2005). *Acta Cryst.* **E61**, m563–m565.
 Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
 Luo, J., Zhou, X., Weng, L. & Hou, X. (2003). *Acta Cryst.* **C59**, m519–m522.
 Rigaku/MS (2004). *CrystalStructure*. Version 3.6.0. Rigaku/MS, 9009 New Trails Drive, The Woodlands, TX 77381-5209, USA.
 Schonherr, T. (1986). *Inorg. Chem.* **25**, 171–175.
 Sheldrick, G. M. (1990). *Acta Cryst.* **A46**, 467–473.
 Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.
 Wang, J., Ping, L., Chen, Y. & Liu, Z. (2004). *Acta Cryst.* **E60**, m628–m630.
 Wu, Z. & Xu, D. (2004). *Acta Cryst.* **E60**, m839–m841.