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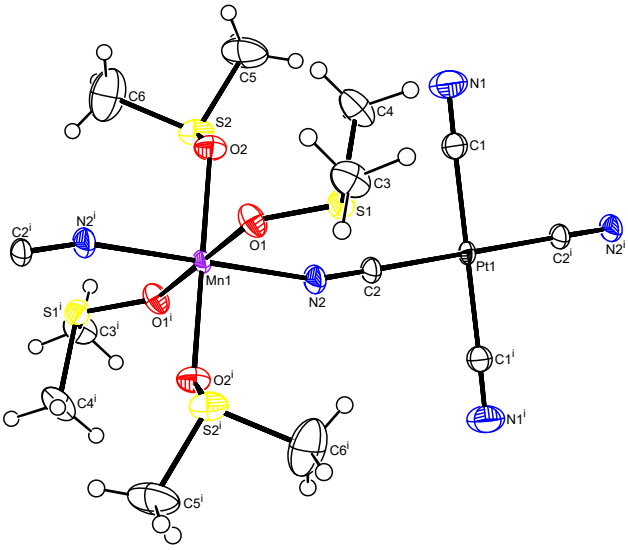
Crystal structure of *catena*-poly[di(μ_2-cyanido-κ^2C:N)-dicyanido-tetrakis(dimethyl sulfoxide-κO)-manganese(II)-platinum(II)], $C_{12}H_{24}MnN_4O_4PtS_4$



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Abstract

$C_{12}H_{24}MnN_4O_4PtS_4$, triclinic, $P\bar{1}$ (no. 2), a = 7.5234(2) Å, b = 9.2143(2) Å, c = 9.4188(2) Å, α = 68.9266(7)°, β = 76.5614(8)°, γ = 85.8639(8)°, V = 592.54(2) Å^3, Z = 1, $R_{gt}(F)$ = 0.0175, $wR_{ref}(F^2)$ = 0.0409, T = 223 K.

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A part of the polymeric title crystal structure is shown in Figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

The suspension of [$MnCl_2$(terpy)] (terpy = 2,2′:6′,2″-terpyridine; 0.3582 g; 1.001 mmol) and $K_2Pt(CN)_4$ (0.3744 g, 1.000 mmol) in H_2O (50 mL) was refluxed for 3 h. After cooling, the formed precipitate was separated by filtration, washed with H_2O and acetone, and dried at 50 °C, to give an ivory colored powder (0.5614 g). Crystals suitable for X-ray diffraction analysis were obtained by slow evaporation from a dimethyl sulfoxide (DMSO) solution at 90 °C.

Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.27 × 0.22 × 0.10 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	6.80 mm^{-1}
Diffractometer, scan mode:	PHOTON 100 CMOS, φ and ω
θ_{max}, completeness:	28.3°, 94%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	16,474, 2794, 0.064
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 2793
$N(param)_{refined}$:	125
Programs:	BRUKER [1], SHELX [2], ORTEP-3 [3], PLATON [4]

Experimental details

Hydrogen atoms were positioned geometrically and allowed to ride on their parent atoms with d(C—H) = 0.97 Å and U_{iso}(H) = 1.5U_{eq}(C) with the help of the SHELXL program (AFIX 137 options) [2].

Comment

The crystal structures of the related heterometallic cyanido-bridged Mn–Pt-complexes [{Mn(salen)}$_2$Pt(CN)$_4$]$_n$ (salen = *N*,*N*′-bis(salicylidene)ethylenediiminato) [5, 6], [Mn(L)Pt(CN)$_4$]$_n$ (L = 2,13-dimethyl-3,12-diaza-6,9-dioxa-1(2,6)-pyridinacyclotridecaphane-2,12-diene) [7] and [Mn(phen)Pt(CN)$_4$]$_n$ (phen = 1,10-phenanthroline) [8] have been determined previously.

The title complex exhibits one-dimensional cyanido-bridged chain structure along the [01$\bar{1}$] direction [4], in which two trans-cyanido ligands of the unit [Pt(CN)$_4$]$^{2-}$ are connected to two Mn(II) units [Mn(DMSO)$_4$]$^{2+}$ (DMSO = dimethyl

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	x	y	z	U_{iso}*/U_{eq}
Pt1	0.5000	0.0000	0.5000	0.01992 (5)
Mn1	0.5000	0.5000	0.0000	0.01939 (9)
S1	0.16671 (7)	0.24650 (6)	0.08218 (7)	0.02969 (11)
S2	0.40896 (8)	0.63399 (8)	0.28672 (7)	0.03753 (13)
O1	0.2583 (2)	0.4018 (2)	−0.02187 (19)	0.0332 (3)
O2	0.3319 (2)	0.5695 (2)	0.1872 (2)	0.0338 (3)
N1	0.1455 (4)	0.1482 (3)	0.6396 (3)	0.0547 (6)
N2	0.5449 (3)	0.2803 (2)	0.1848 (2)	0.0327 (4)
C1	0.2745 (3)	0.0953 (3)	0.5877 (3)	0.0325 (5)
C2	0.5301 (3)	0.1783 (2)	0.2991 (2)	0.0256 (4)
C3	−0.0059 (4)	0.2262 (4)	−0.0098 (3)	0.0425 (6)
H3A	0.0502	0.2072	−0.1051	0.064*
H3B	−0.0764	0.3208	−0.0345	0.064*
H3C	−0.0859	0.1394	0.0599	0.064*
C4	0.0243 (4)	0.2815 (4)	0.2456 (3)	0.0469 (7)
H4A	−0.0520	0.3706	0.2095	0.070*
H4B	0.0996	0.3022	0.3070	0.070*
H4C	−0.0525	0.1907	0.3093	0.070*
C5	0.2392 (5)	0.5929 (6)	0.4631 (4)	0.0677 (10)
H5A	0.1254	0.6411	0.4399	0.102*
H5B	0.2789	0.6339	0.5323	0.102*
H5C	0.2209	0.4813	0.5131	0.102*
C6	0.3754 (8)	0.8379 (4)	0.2065 (6)	0.0814 (13)
H6A	0.4131	0.8884	0.2692	0.122*
H6B	0.2472	0.8579	0.2060	0.122*
H6C	0.4477	0.8786	0.1005	0.122*

sulfoxide). In the complex, the Pt(II) ion is four-coordinated in a slightly distorted square-planar environment by four C atoms of four CN^- ligands, whereas the Mn(II) ion is six-coordinated in a slightly distorted octahedral environment by two N atoms from two bridging $[Pt(CN)_4]^{2-}$ units and four O atoms from the four DMSO solvent molecules, and the two metal ions are located on an inversion center, respectively; the asymmetric unit of the polymer contains one half of the repeat unit $[Mn(DMSO)_4Pt(CN)_4]$. The Pt–C and C≡N bond lengths are almost equal with d(Pt–C) = 1.987(2) and 1.997(2) Å and d(C≡N) = 1.140(4) and 1.135(3) Å, respectively. The Mn–O bonds [Mn1–O1/O2 = 2.1713(15) and 2.1862(16) Å] are slightly shorter than the Mn–N bonds [Mn1–N2 = 2.2097(19) Å]. In the crystal structure, the complexes display very weak intermolecular C–H···N and C–H···O hydrogen bonds with distances of 3.5432(1) and 3.3658(1) Å between the donor and acceptor atoms, respectively, to stabilize the three-dimensional packing [4].

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Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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