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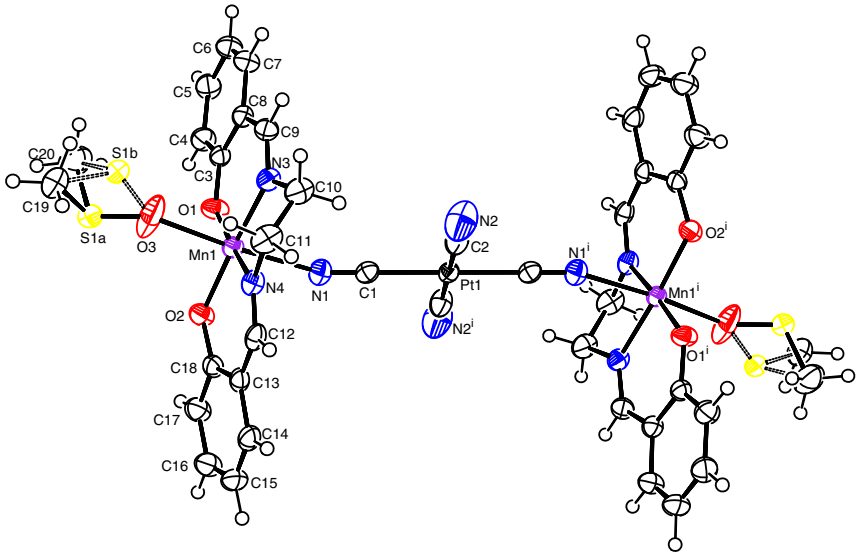
Crystal structure of [di(μ$_2$-cyanido)-dicyanido-bis(dimethyl sulfoxide-κ*O*)-bis(2,2′-(ethane-1,2-diylbis(azanylylidenemethanylylidene)) diphenolato-κ^4,*N*,*N*′,*O*,*O*′)-dimanganese(III)-platinum(II)], $C_{40}H_{40}Mn_2N_8O_6PtS_2$



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Abstract

$C_{40}H_{40}Mn_2N_8O_6PtS_2$, monoclinic, $P2_1/n$ (no. 14), a = 10.5707(3) Å, b = 18.5331(5) Å, c = 12.0293(3) Å, β = 114.6276(10)°, V = 2142.26(10) Å^3, Z = 2, $R_{gt}(F)$ = 0.0148, $wR_{ref}(F^2)$ = 0.0380, T = 223 K.

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The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	Brown block
Size:	0.20 × 0.14 × 0.08 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	3.99 mm^{-1}
Diffractometer, scan mode:	PHOTON 100 CMOS, φ and ω
θ_{max}, completeness:	26.0°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	54955, 4209, 0.032
Criterion for I_{obs}, $N(hkl)_{gt}$:	I_{obs} > 2 σ(I_{obs}), 3888
$N(param)_{refined}$:	280
Programs:	Bruker [1], SHELX [2], ORTEP-3 [3], PLATON [4]

Source of material

To a solution of [Mn(salen)(CH_3CO_2)] (salen = *N*,*N*′-bis(salicylidene)ethylenediiminato; 1.2211 g; 3.211 mmol) in MeOH (30 mL) was added $K_2Pt(CN)_4$ (0.5785 g, 1.533 mmol) in H_2O (20 mL) and stirred for 3 h at room temperature. The formed precipitate was separated by filtration, washed with H_2O and MeOH, and dried at 60 °C, to give a dark

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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	0.02610 (4)
Mn1	0.30412 (3)	0.19126 (2)	0.72037 (2)	0.02576 (7)
S1A[a]	0.14083 (9)	0.30270 (4)	0.85769 (7)	0.0408 (3)
S1B[b]	0.0957 (2)	0.24076 (10)	0.85744 (19)	0.0414 (6)
O1	0.41388 (15)	0.16562 (8)	0.88294 (12)	0.0348 (3)
O2	0.40579 (16)	0.27587 (7)	0.72683 (12)	0.0342 (3)
O3	0.1489 (2)	0.24779 (13)	0.77796 (18)	0.0747 (7)
N1	0.43320 (18)	0.12506 (10)	0.64233 (16)	0.0353 (4)
N2	0.1795 (2)	−0.02919 (16)	0.3597 (2)	0.0674 (7)
N3	0.18340 (17)	0.10542 (9)	0.69420 (14)	0.0298 (3)
N4	0.17338 (16)	0.21285 (9)	0.54983 (14)	0.0293 (3)
C1	0.4591 (2)	0.07944 (11)	0.59122 (17)	0.0294 (4)
C2	0.2962 (2)	−0.01900 (13)	0.4105 (2)	0.0406 (5)
C3	0.3954 (2)	0.11259 (10)	0.94875 (17)	0.0279 (4)
C4	0.4927 (2)	0.10530 (12)	1.07025 (18)	0.0359 (5)
H4	0.5670	0.1381	1.1027	0.043*
C5	0.4807 (2)	0.05055 (12)	1.14273 (19)	0.0388 (5)
H5	0.5480	0.0461	1.2237	0.047*
C6	0.3714 (3)	0.00191 (11)	1.0985 (2)	0.0414 (5)
H6	0.3632	−0.0347	1.1492	0.050*
C7	0.2756 (3)	0.00795 (11)	0.9799 (2)	0.0380 (5)
H7	0.2017	−0.0252	0.9493	0.046*
C8	0.2849 (2)	0.06251 (10)	0.90263 (18)	0.0292 (4)
C9	0.1853 (2)	0.06142 (11)	0.77702 (18)	0.0321 (4)
H9	0.1160	0.0256	0.7538	0.039*
C10	0.0831 (2)	0.09614 (13)	0.56540 (18)	0.0395 (5)
H10A	0.0002	0.0705	0.5612	0.047*
H10B	0.1254	0.0682	0.5206	0.047*
C11	0.0444 (2)	0.17031 (14)	0.51073 (19)	0.0406 (5)
H11A	−0.0008	0.1672	0.4213	0.049*
H11B	−0.0203	0.1932	0.5392	0.049*
C12	0.1945 (2)	0.25720 (11)	0.47741 (17)	0.0301 (4)
H12	0.1273	0.2595	0.3962	0.036*
C13	0.3136 (2)	0.30361 (10)	0.51157 (17)	0.0292 (4)
C14	0.3289 (2)	0.34511 (11)	0.41966 (19)	0.0367 (5)
H14	0.2623	0.3407	0.3384	0.044*
C15	0.4379 (3)	0.39158 (12)	0.4455 (2)	0.0432 (5)
H15	0.4476	0.4178	0.3826	0.052*
C16	0.5341 (3)	0.39952 (12)	0.5661 (2)	0.0441 (5)
H16	0.6085	0.4319	0.5847	0.053*
C17	0.5218 (2)	0.36047 (11)	0.6588 (2)	0.0387 (5)
H17	0.5878	0.3669	0.7398	0.046*
C18	0.4128 (2)	0.31139 (10)	0.63418 (17)	0.0296 (4)
C19	−0.0358 (3)	0.31338 (15)	0.8307 (3)	0.0540 (6)
H19A	−0.0890	0.3287	0.7468	0.081*
H19B	−0.0434	0.3495	0.8859	0.081*
H19C	−0.0721	0.2678	0.8444	0.081*
C20	0.1993 (3)	0.26498 (17)	1.0094 (2)	0.0639 (8)
H20A	0.2862	0.2394	1.0297	0.096*
H20B	0.1297	0.2318	1.0120	0.096*
H20C	0.2135	0.3035	1.0680	0.096*

[a]Occupancy: 0.7045(19), [b]Occupancy: 0.2955(19).

brown powder (1.4698 g). Crystals suitable for X-ray diffraction analysis were obtained by slow evaporation from a dimethyl sulfoxide (DMSO) solution at 90 °C.

Experimental details

Hydrogen atoms were positioned geometrically and allowed to ride on their parent atoms with *d*(C—H) = 0.94, 0.98 or 0.97 Å and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C) with the help of the SHELXL program (AFIX 43, 23 or 137 options) [2].

Comment

The crystal structure of the related heterometallic cyanido-bridged polymeric complex $[\{Mn(salen)\}_2Pt(CN)_4]_n$ (salen = *N*,*N*′-bis(salicylidene)ethylenediiminato) has been determined previously [5, 6].

The title complex has a heterometallic trinuclear structure, in which two cationic $[Mn(salen)(DMSO)]^+$ units are formally connected by the anionic $[Pt(CN)_4]^{2-}$ bridge (see the figure). In the complex, Pt(II) is four-coordinated in a slightly distorted square-planar environment by four C atoms of four CN^- ligands and is located on an inversion center; the asymmetric unit contains one half of the compound. The Mn(III) atom is six-coordinated in a distorted octahedral environment by an anionic tetradentate salen ligand, and two axial N and O atoms from the cyanido ligand of the bridging $[Pt(CN)_4]^{2-}$ unit and the DMSO solvent molecule, respectively. The Pt–C and C≡N bond lengths are almost equal with *d*(Pt–C) = 1.989(2) and 1.998(2) Å and *d*(C≡N) = 1.144(3) and 1.142(3) Å, respectively. The Mn–N/O axial bonds [Mn1–N1 = 2.3055(17) Å; Mn1–O3 = 2.2843(18) Å] are slightly longer than the Mn–N/O(salen) equatorial bonds [Mn1–N3/4 = 1.9808(16) and 1.9788(16) Å; Mn1–O1/2 = 1.8723(13) and 1.8843(14) Å]. In the refinement, the S atom of DMSO was found to be disordered over two sites with the site-occupancy factor of 0.705(2) for the major component (see the figure; O3 is also affected). The complex molecules are stacked in columns along [100]. In the columns, several intermolecular π-π-stacking interactions between adjacent aryl rings are present. For Cg1 (the centroid of ring C3—C8) and Cg1^i (symmetry code *i*: 1–*x*, –*y*, 2–*z*), the centroid-centroid distance is 3.4652(14) Å [4].

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

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