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Crystal structure of bis(5-methoxy-2-(((2-oxidoethyl)imino)methyl)phenolate- $\kappa^3 O, N, O'$)manganes(IV), $C_{20}H_{22}N_2O_6Mn$

The crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	Black block
Size:	0.16 × 0.12 × 0.10 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.71 mm ⁻¹
Diffractometer, scan mode:	Bruker APEX, ω -scans
$\theta_{\max}$, completeness:	25.0°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	41463, 3458, 0.036
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 3060
$N(\text{param})_{\text{refined}}$:	265
Programs:	Bruker [1], SHELX [2, 3]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Mn1	0.2500	0.7500	0.22830(4)	0.0297(2)
Mn2	0.2500	0.2500	0.28592(4)	0.0286(2)
N1	0.25570(17)	0.61275(18)	0.23685(15)	0.0336(6)
N2	0.38819(18)	0.24913(17)	0.27819(14)	0.0322(6)
O1	−0.09137(19)	0.6151(2)	0.02074(14)	0.0582(8)
O2	0.15803(16)	0.73900(14)	0.15605(13)	0.0378(5)
O3	0.34519(18)	0.74677(16)	0.29354(13)	0.0445(6)
O4	0.25679(15)	0.15931(18)	0.35801(14)	0.0457(6)
O5	0.25675(14)	0.34313(15)	0.21969(13)	0.0378(6)
O6	0.3657(2)	−0.1022(2)	0.48561(17)	0.0666(9)
C1	−0.0197(2)	0.6077(3)	0.06722(18)	0.0437(8)
C2	−0.0060(3)	0.5176(3)	0.0934(2)	0.0509(10)
H2	−0.0445	0.4687	0.0791	0.061*
C3	0.0644(3)	0.5026(2)	0.1399(2)	0.0480(9)
H3	0.0741	0.4426	0.1566	0.058*
C4	0.1234(2)	0.5758(2)	0.16372(17)	0.0347(7)
C5	0.1084(2)	0.6667(2)	0.13710(17)	0.0323(7)
C6	0.0367(2)	0.6810(2)	0.08762(17)	0.0381(7)
H6	0.0274	0.7400	0.0688	0.046*
C7	0.1963(2)	0.5540(2)	0.21161(17)	0.0361(8)
H7	0.2015	0.4923	0.2258	0.043*
C8	0.3274(2)	0.5834(2)	0.28768(19)	0.0440(8)
H8A	0.3866	0.5686	0.2649	0.053*
H8B	0.3062	0.5291	0.3132	0.053*
C9	0.3390(3)	0.6657(3)	0.3350(2)	0.0535(10)

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Abstract

$C_{20}H_{22}N_2O_6Mn$, orthorhombic, *Pccn* (no. 56), $a = 14.1678(16)$ Å, $b = 14.3469(18)$ Å, $c = 19.335(2)$ Å, $V = 3930.1(8)$ Å³, $Z = 8$, $R_{\text{gt}}(F) = 0.0504$, $wR_{\text{ref}}(F^2) = 0.1441$, $T = 293(2)$ K.

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Table 2 (continued)

Atom	x	y	z	U_{iso}^*/U_{eq}
H18A	0.2854	0.6702	0.3660	0.064*
H18B	0.3958	0.6587	0.3625	0.064*
C10	0.4182(2)	0.1112(2)	0.34563(17)	0.0344(7)
C11	0.4871(3)	0.0469(3)	0.3673(2)	0.0526(10)
H20	0.5483	0.0532	0.3503	0.063*
C12	0.4682(3)	−0.0235(3)	0.4117(2)	0.0614(12)
H21	0.5149	−0.0663	0.4234	0.074*
C13	0.3766(3)	−0.0313(3)	0.44012(19)	0.0470(9)
C14	0.3075(2)	0.0313(2)	0.42150(18)	0.0393(8)
H23	0.2478	0.0265	0.4412	0.047*
C15	0.3254(2)	0.1024(2)	0.37326(16)	0.0328(7)
C16	0.4442(2)	0.1862(2)	0.30112(17)	0.0320(7)
H31	0.5071	0.1897	0.2876	0.038*
C17	0.4216(2)	0.3260(2)	0.2343(2)	0.0426(8)
H32A	0.4795	0.3090	0.2107	0.051*
H32B	0.4330	0.3816	0.2617	0.051*
C18	0.3426(2)	0.3420(2)	0.1832(2)	0.0440(8)
H36A	0.3518	0.4009	0.1594	0.053*
H36B	0.3420	0.2925	0.1489	0.053*
C19	−0.1147(4)	0.7048(4)	−0.0053(3)	0.0774(15)
H37A	−0.1308	0.7452	0.0324	0.116*
H37B	−0.1675	0.6997	−0.0362	0.116*
H37C	−0.0616	0.7300	−0.0298	0.116*
C20	0.2802(3)	−0.1060(4)	0.5241(2)	0.0723(14)
H39A	0.2692	−0.0469	0.5459	0.108*
H39B	0.2850	−0.1536	0.5589	0.108*
H39C	0.2287	−0.1202	0.4936	0.108*

Source of material

Ligand was synthesized according to the reference method [4]. All other reagents were commercially available and used as purchased. A mixture of 2-((2-hydroxyethyl)imino)methyl)-5-methoxyphenol (156.17 mg, 0.4 mmol), 1,2,4-triazole (69.21 mg, 0.4 mmol) and methanol (10 mL) was heated at 60 °C for 10 h, and then cooled to room temperature. The resulting black block crystals of the title compound were obtained and washed with distilled water. The yield is ca. 30%. IR(KBr): 3257(s), 1588(s), 1559(s), 1456(s), 1455(s), 1349(s), 1286(s), 1156(s), 1115(s), 1052(s), 1001(s), 925(s), 859(s), 814(m), 761(m), 721(m), 600(m), 444(m) cm^{−1}.

Comment

The design and synthesis of manganese complexes have progressed extensively in recent years [5–7]. Recently, many manganese complexes have been synthesized and proposed for various applications [8–10].

The title compound crystallizes in the orthorhombic space group *Pccn* with eight formula units in the unit cell. There are two C₂ symmetrically complexes in the asymmetric unit. As shown in the figure, one formula unit consists of two schiff ligands and one Mn atom. Each Mn ion is in an octahedral coordination environment, with two nitrogen atoms and four oxygen atoms from the two schiff ligands. Geometric parameters are similar to the literature [11].

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