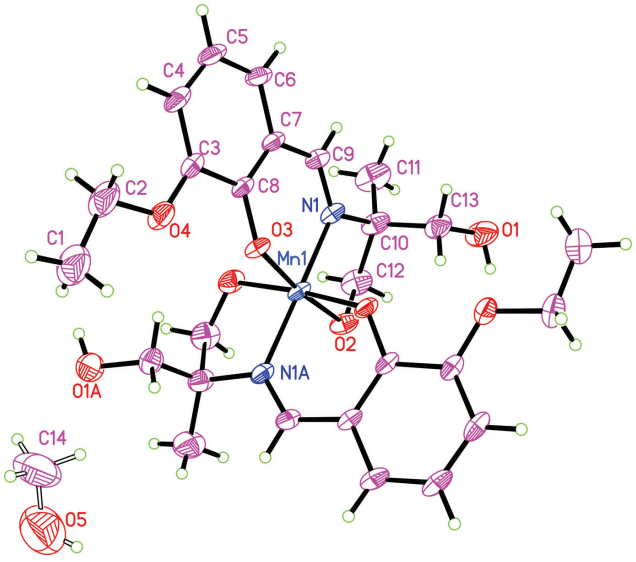
Ge Yuan, Wang Dengwu, Huo Xiaoping, Yang Liguo and Zhang Cuihong*

# Crystal structure of bis(5-ethoxy-2-(((1-hydroxy-2-methyl-3-oxidopropan-2-yl)imino)methyl)phenolato-κ$^3$*N*,*O*,*O*')manganese(IV) – methanol (1/1), $C_{27}H_{38}MnN_2O_9$

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## Abstract

$C_{27}H_{38}MnN_2O_9$, monoclinic, *C*2/*c* (no. 15), $a = 14.9473(14)$ Å, $b = 17.8744(16)$ Å, $c = 12.5536(11)$ Å, $\beta = 122.596(5)°$, $V = 2825.7(5)$ Å$^3$, $Z = 4$, $R_{gt}(F) = 0.0423$, $wR_{ref}(F^2) = 0.1295$, $T = 298$ K [1–3].

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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.

***Corresponding author: Zhang Cuihong,** Key Laboratory of Organic Polymer Photoelectric Materials, School of Science, Xijing University, Xi'an 710123, Shaanxi, P.R. China, e-mail: cuicui1008@126.com
**Ge Yuan, Wang Dengwu and Huo Xiaoping:** Key Laboratory of Organic Polymer Photoelectric Materials, School of Science, Xijing University, Xi'an 710123, Shaanxi, P.R. China
**Yang Liguo:** College of Chemistry and Environmental Engineering, Anyang Institute of Technology, Anyang 455000, Henan, P.R. China. https://orcid.org/0000-0003-4899-8298

**Table 1:** Data collection and handling.

| | |
|---|---|
| Crystal: | Black block |
| Size: | 0.10 × 0.08 × 0.06 mm |
| Wavelength: | Mo *Kα* radiation (0.71073 Å) |
| $\mu$: | 0.52 mm$^{-1}$ |
| Diffractometer, scan mode: | Bruker APEX-II, $\varphi$ and $\omega$ |
| $\theta_{max}$, completeness: | 27.7°, >99% |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$, $R_{int}$: | 17608, 3293, 0.031 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\ \sigma(I_{obs})$, 2815 |
| $N(param)_{refined}$: | 190 |
| Programs: | Bruker [1], SHELX [2, 3] |

## Source of material

The organic ligand was synthesized from the reaction of *o*-vanillin (100 mg, 0.65 mmol) and 2-amino-2-methylpropane-1,3-diol (70 mg, 0.65 mmol) according to the procedure reported earlier [4]. The ligand (0.010 mol) and manganese acetate (0.01 mol) was added to methanolic solution (30 mL), the mixture refluxed for 24 h with the formation of a yellow powder. The solid was filtered off washed with water, methanol and ether and dried under vacuum. Yield (2.5 g, 32%).

## Experimental details

The C-bound H atoms were geometrically placed (C—H = 0.95–0.98 Å) and refined as riding with $U_{iso}(H) = 1.2$–$1.5\ U_{eq}(C)$ [1–3]. The methanol molecule has a large ellipsoid due to the disorder around a center of twofold axis.

## Comment

Schiff base compounds show photochromism and thermochromism in the solid state by proton transfer from the hydroxy O atom to the imine N atom. Lots of the complexes with the schiff base ligand have been synthesized. One new schiff base ligand was synthesized by our group. Then one manganese complex with the new ligand has been synthesized. The similar complexes have been reported [4–8].

As shown in the Figure, the asymmetric unit of the title structure contains one half of the manganes complex (located on a twofold axis) and one half of methanol molecule (near a twofold axis). The bond lengths of Mn1—O2,

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

| Atom | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Mn1 | 0.5000 | 0.32403(2) | 0.2500 | 0.03507(15) |
| N1 | 0.41569(14) | 0.31641(9) | 0.32834(15) | 0.0399(4) |
| O1 | 0.13220(17) | 0.27866(15) | 0.09058(19) | 0.0830(7) |
| H1 | 0.1230 | 0.2678 | 0.0219 | 0.124* |
| C1 | 0.9096(3) | 0.5192(3) | 0.5444(4) | 0.1122(15) |
| H1A | 0.9251 | 0.4694 | 0.5300 | 0.168* |
| H1B | 0.9748 | 0.5456 | 0.5986 | 0.168* |
| H1C | 0.8689 | 0.5450 | 0.4651 | 0.168* |
| O2 | 0.40465(13) | 0.25313(9) | 0.13883(14) | 0.0519(4) |
| C2 | 0.8481(2) | 0.5154(2) | 0.6048(3) | 0.0847(10) |
| H2A | 0.8887 | 0.4899 | 0.6856 | 0.102* |
| H2B | 0.8313 | 0.5653 | 0.6190 | 0.102* |
| C3 | 0.68750(16) | 0.45971(11) | 0.56169(17) | 0.0412(4) |
| O3 | 0.58391(11) | 0.40026(8) | 0.36528(12) | 0.0401(3) |
| O4 | 0.75377(13) | 0.47538(10) | 0.52193(15) | 0.0559(4) |
| C4 | 0.70129(19) | 0.48240(12) | 0.67480(19) | 0.0503(5) |
| H4 | 0.7604 | 0.5109 | 0.7308 | 0.060* |
| C5 | 0.6281(2) | 0.46338(13) | 0.70632(19) | 0.0544(6) |
| H5 | 0.6378 | 0.4799 | 0.7821 | 0.065* |
| O5[a] | 0.9823(18) | 0.2709(5) | 0.2212(15) | 0.184(5) |
| H5A[a] | 0.9315 | 0.2824 | 0.1512 | 0.276* |
| C14[a] | 0.9832(11) | 0.3169(8) | 0.3160(12) | 0.149(4) |
| H14A[a] | 1.0314 | 0.3580 | 0.3368 | 0.223* |
| H14B[a] | 1.0058 | 0.2876 | 0.3904 | 0.223* |
| H14C[a] | 0.9131 | 0.3360 | 0.2839 | 0.223* |
| C6 | 0.54248(19) | 0.42071(13) | 0.62626(19) | 0.0485(5) |
| H6 | 0.4938 | 0.4080 | 0.6477 | 0.058* |
| C7 | 0.52667(16) | 0.39528(11) | 0.51017(16) | 0.0380(4) |
| C9 | 0.43811(17) | 0.34812(12) | 0.43249(18) | 0.0420(4) |
| H9 | 0.3919 | 0.3392 | 0.4592 | 0.050* |
| C8 | 0.59748(15) | 0.41624(10) | 0.47493(16) | 0.0350(4) |
| C10 | 0.3213(2) | 0.26645(13) | 0.2568(2) | 0.0527(6) |
| C11 | 0.2938(3) | 0.22313(18) | 0.3405(3) | 0.0822(10) |
| H11A | 0.3565 | 0.1991 | 0.4077 | 0.123* |
| H11B | 0.2411 | 0.1860 | 0.2908 | 0.123* |
| H11C | 0.2666 | 0.2571 | 0.3757 | 0.123* |
| C12 | 0.3539(2) | 0.21321(14) | 0.1884(3) | 0.0642(7) |
| H12A | 0.4017 | 0.1754 | 0.2469 | 0.077* |
| H12B | 0.2916 | 0.1882 | 0.1204 | 0.077* |
| C13 | 0.2291(2) | 0.31772(15) | 0.1639(2) | 0.0581(6) |
| H13A | 0.2205 | 0.3569 | 0.2111 | 0.070* |
| H13B | 0.2467 | 0.3413 | 0.1079 | 0.070* |

[a]Occupancy. 0.5.

Mn1—O3 and Mn1—N1 are 1.854, 1.889 and 1.976 Å, respectively, which are similar with the Ni complex [9]. In the Ni complex, the coordination environment is the same with the compound one.

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