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Key indicators

Single-crystal X-ray study
 $T = 293$ K
 Mean $\sigma(\text{C}-\text{C}) = 0.007$ Å
 R factor = 0.065
 wR factor = 0.172
 Data-to-parameter ratio = 16.4

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

Bis(2-formylphenolato- $\kappa^2\text{O},\text{O}'$)manganese(II)

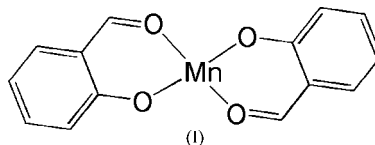
The title compound, $[\text{Mn}(\text{C}_7\text{H}_5\text{O}_2)_2]$, is a mononuclear manganese(II) complex. The Mn^{II} atom, lying on an inversion centre, is four-coordinated by four O atoms from two salicylaldehyde ligands, forming a square-planar geometry.

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Comment

Manganese(II) complexes are very important in biological chemistry and supramolecular chemistry (Miyasaka *et al.*, 1996; Ciringh *et al.*, 1997; Mabad *et al.*, 1986). We report here the crystal structure of the new title manganese(II) complex, (I).



The Mn^{II} ion in complex (I), lying on an inversion centre, is four-coordinated by four O atoms from two salicylaldehyde ligands, forming a square-planar geometry (Fig. 1). The bond lengths and angles (Table 1) involving the Mn^{II} ion are comparable with the values observed in other manganese complexes (Nakasuka *et al.*, 1985; Zhang, 2006; Gao & Liu, 2005; Okabe & Koizumi, 1998).

Experimental

Salicylaldehyde (1.0 mmol, 122.1 mg) and $\text{Mn}(\text{CH}_3\text{COO})_2 \cdot 2\text{H}_2\text{O}$ (0.5 mmol, 104.5 mg) were dissolved in ethanol (80 ml). The mixture was refluxed at 345 K under an argon atmosphere for about 1 h to give a red solution. After allowing this solution to stand in air for 7 d, deep-brown plate-shaped crystals were formed at the bottom of the vessel.

Crystal data

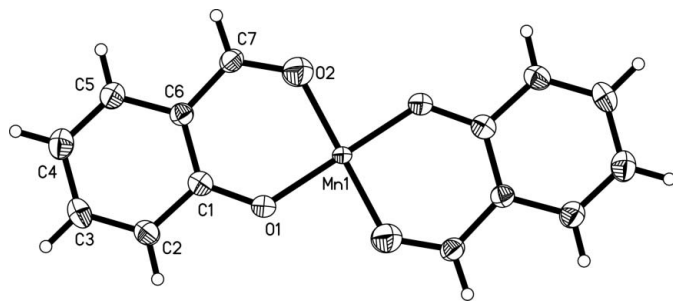
$[\text{Mn}(\text{C}_7\text{H}_5\text{O}_2)_2]$
 $M_r = 297.16$
 Monoclinic, $P2_1/c$
 $a = 12.918$ (2) Å
 $b = 5.831$ (1) Å
 $c = 8.101$ (3) Å
 $\beta = 95.54$ (3)°
 $V = 607.4$ (3) Å³

$Z = 2$
 $D_x = 1.625$ Mg m⁻³
 Mo $K\alpha$ radiation
 $\mu = 1.09$ mm⁻¹
 $T = 293$ (2) K
 Plate, brown
 $0.10 \times 0.10 \times 0.03$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\text{min}} = 0.899$, $T_{\text{max}} = 0.968$

5037 measured reflections
 1446 independent reflections
 1133 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.049$
 $\theta_{\text{max}} = 28.3^\circ$


Figure 1

The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. Unlabelled atoms are related to the labelled atoms by the symmetry operation $(-x, 2 - y, 1 - z)$.

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.065$
 $wR(F^2) = 0.172$
 $S = 1.07$
 1446 reflections
 88 parameters
 H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0704P)^2 + 1.5184P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.48 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.75 \text{ e } \text{\AA}^{-3}$

Table 1

Selected geometric parameters (\AA , $^\circ$).

Mn1—O1	1.833 (3)	Mn1—O2	1.844 (4)
O1 ⁱ —Mn1—O1	180	O1—Mn1—O2	94.90 (17)
O1—Mn1—O2 ⁱ	85.10 (17)	O2 ⁱ —Mn1—O2	180

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

All H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.93 Å and with $U_{\text{iso}}(\text{H})$ set to $1.2U_{\text{eq}}(\text{C})$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINTE* (Bruker, 1998); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997a); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997a); molecular graphics: *SHELXTL* (Sheldrick, 1997b); software used to prepare material for publication: *SHELXTL*.

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