# Crystal structure of aqua(biphenyl-2,4′-dicarboxylato)-manganese(II), $Mn(H_2O)(C_{14}H_8O_4)$

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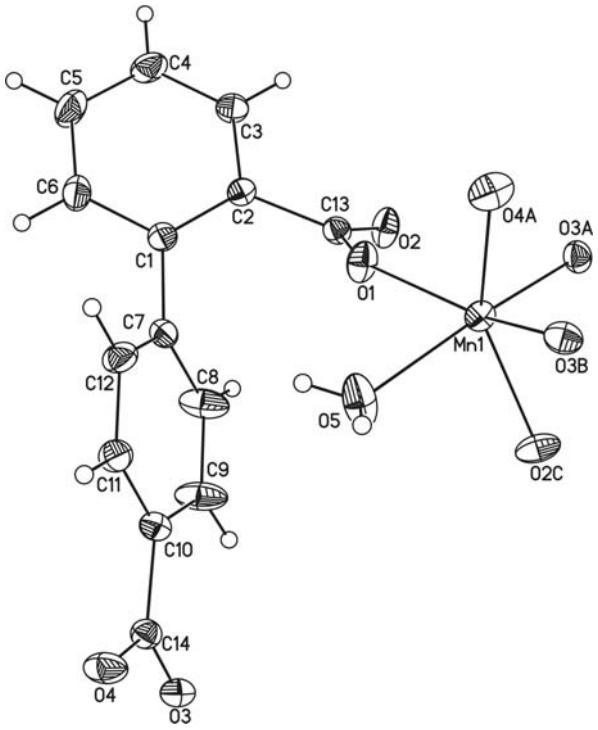


**Abstract**

$C_{14}H_{10}MnO_5$, orthorhombic, *Pbca* (no. 61), $a$ = 7.3872(5) Å, $b$ = 15.3323(9) Å, $c$ = 23.120(1) Å, $V$ = 2618.6 Å$^3$, $Z$ = 8, $R_{gt}(F)$ = 0.029, $wR_{ref}(F^2)$ = 0.085, $T$ = 298 K.

**Source of material**

A mixture of $MnSO_4 \cdot H_2O$ (0.5 mmol, 0.085 g), biphenyl-2,4′-dicarboxylic acid ($H_2$bpdc, 0.5 mmol, 0.17 g), NaOH (1.0 mmol, 0.04 g) and $H_2O$ (15 ml) was placed in a Parr Teflon-lined stainless steel vessel (23 ml), which was sealed and heated at 403 K for four days. After the mixture had been cooled slowly to room temperature, colorless crystals of the title compound were obtained.

**Experimental details**

Water H atoms were located in difference Fourier maps and refined with restraints $d$(O—H) = 0.85(3) Å and $d$(H···H) = 1.34(3) Å. All the remaining H atoms were positioned geometrically and treated as riding with $d$(C—H) = 0.93 Å and $U_{iso}$(H) = 1.2 $U_{eq}$(C).

**Discussion**

Biphenyl-2,4′-dicarboxylic acid ($H_2$bpdc) is a flexible ligand coordinating transition metals, with two carboxyl groups that can supply four potential O donor atoms. Moreover, the two rings can be rotated around the bridging C—C single bond and the two carboxyl groups are located asymmetrically, which makes it a good candidate for constructing various supramolecular compounds. So far, only few supramolecular compounds involving $H_2$bpdc have been reported [1-3].

The asymmetric unit of the title crystal structure comprises one $Mn^{2+}$ ion, one bpdc anion and one coordinating water molecule. Each $Mn^{2+}$ ion is coordinated by one water molecule and five oxygen atoms from four bpdc anions, two of which are from one chelated carboxylate group, two from the bis(monodentate) carboxylate group and one oxygen atom is from the tris(dentate) chelated carboxylate group. Two neighbour asymmetric units are linked together by bpdc forming a dimeric unit. Then adjacent dimeric units are interconnected into an infinite chain along [100] through oxygen atoms from bpdc ligands. Adjacent one-dimensional chains are further arranged into a two-dimensional network parallel to the (001) plane.

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

| | |
|---|---|
| Crystal: | colorless block, size 0.10 × 0.12 × 0.15 mm |
| Wavelength: | Mo $K_\alpha$ radiation (0.71073 Å) |
| $\mu$: | 10.23 cm$^{-1}$ |
| Diffractometer, scan mode: | Bruker SMART Apex CCD, $\omega$ |
| $2\theta_{max}$: | 52° |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$: | 25426, 2561 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\ \sigma(I_{obs})$, 2268 |
| $N(param)_{refined}$: | 187 |
| Programs: | SHELXS-97, SHELXL-97 [4] |

**Table 2.** Atomic coordinates and displacement parameters (in Å$^2$).

| Atom | Site | $x$ | $y$ | $z$ | $U_{iso}$ |
|---|---|---|---|---|---|
| H(6) | 8$c$ | 0.7791 | 0.0534 | 0.0010 | 0.056 |
| H(5) | 8$c$ | 1.0106 | 0.1196 | –0.0492 | 0.062 |
| H(4) | 8$c$ | 1.1761 | 0.2297 | –0.0056 | 0.054 |
| H(3) | 8$c$ | 1.1038 | 0.2751 | 0.0863 | 0.043 |
| H(12) | 8$c$ | 0.4522 | 0.0939 | 0.0451 | 0.049 |
| H(11) | 8$c$ | 0.2334 | 0.0106 | 0.0904 | 0.045 |
| H(9) | 8$c$ | 0.5753 | –0.0361 | 0.2202 | 0.066 |
| H(8) | 8$c$ | 0.7947 | 0.0457 | 0.1751 | 0.061 |
| H(5A) | 8$c$ | 0.209(3) | 0.206(2) | 0.185(1) | 0.086 |
| H(5B) | 8$c$ | 0.359(3) | 0.175(2) | 0.159(1) | 0.086 |

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**Table 3.** Atomic coordinates and displacement parameters (in $Å^2$).

| Atom | Site | $x$ | $y$ | $z$ | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| Mn(1) | 8*c* | 0.49606(3) | 0.30265(2) | 0.22401(1) | 0.0194(2) | 0.0315(2) | 0.0290(2) | 0.00336(8) | 0.00046(8) | 0.00031(9) |
| C(2) | 8*c* | 0.8953(2) | 0.19231(9) | 0.09972(7) | 0.0232(7) | 0.0300(8) | 0.0282(8) | 0.0018(6) | 0.0014(6) | 0.0009(6) |
| C(1) | 8*c* | 0.7964(2) | 0.1248(1) | 0.07396(7) | 0.0300(8) | 0.0313(8) | 0.0312(8) | –0.0015(6) | 0.0037(6) | –0.0006(6) |
| C(6) | 8*c* | 0.8434(3) | 0.0985(1) | 0.01838(8) | 0.053(1) | 0.050(1) | 0.037(1) | –0.0138(9) | 0.0094(8) | –0.0141(8) |
| C(5) | 8*c* | 0.9829(3) | 0.1376(2) | –0.01177(8) | 0.055(1) | 0.065(1) | 0.035(1) | –0.0053(9) | 0.0168(8) | –0.0105(9) |
| C(4) | 8*c* | 1.0808(3) | 0.2035(1) | 0.01409(8) | 0.039(1) | 0.056(1) | 0.040(1) | –0.0066(8) | 0.0141(8) | 0.0050(8) |
| C(3) | 8*c* | 1.0372(2) | 0.2305(1) | 0.06918(8) | 0.0289(8) | 0.0399(9) | 0.0398(9) | –0.0073(7) | 0.0050(7) | 0.0003(7) |
| C(7) | 8*c* | 0.6503(2) | 0.0764(1) | 0.10433(7) | 0.0322(8) | 0.0269(7) | 0.0330(8) | –0.0044(6) | 0.0035(6) | –0.0029(6) |
| C(12) | 8*c* | 0.4788(2) | 0.0665(1) | 0.07997(8) | 0.043(1) | 0.053(1) | 0.0257(8) | –0.0148(8) | –0.0038(7) | 0.0054(8) |
| C(11) | 8*c* | 0.3474(2) | 0.0163(1) | 0.10709(7) | 0.0340(9) | 0.049(1) | 0.0307(8) | –0.0140(7) | –0.0047(7) | 0.0007(7) |
| C(10) | 8*c* | 0.3853(2) | –0.0254(1) | 0.15875(7) | 0.0289(8) | 0.0288(8) | 0.0352(8) | –0.0030(6) | 0.0014(6) | 0.0016(6) |
| C(9) | 8*c* | 0.5513(3) | –0.0116(1) | 0.18426(9) | 0.039(1) | 0.064(1) | 0.062(1) | –0.015(1) | –0.0164(9) | 0.039(1) |
| C(8) | 8*c* | 0.6829(2) | 0.0381(1) | 0.15728(9) | 0.0292(9) | 0.057(1) | 0.067(1) | –0.0120(8) | –0.0147(8) | 0.030(1) |
| C(14) | 8*c* | 0.2501(2) | –0.0841(1) | 0.18655(7) | 0.0294(8) | 0.0282(8) | 0.0335(8) | 0.0001(6) | 0.0037(6) | –0.0001(7) |
| C(13) | 8*c* | 0.8462(2) | 0.2290(1) | 0.15797(7) | 0.0234(7) | 0.0276(7) | 0.0322(8) | –0.0024(6) | 0.0026(6) | –0.0014(6) |
| O(1) | 8*c* | 0.6847(1) | 0.24483(8) | 0.16781(5) | 0.0230(6) | 0.0554(8) | 0.0420(7) | 0.0049(5) | 0.0033(5) | –0.0154(6) |
| O(2) | 8*c* | 0.9743(1) | 0.24265(9) | 0.19268(6) | 0.0245(6) | 0.0600(9) | 0.0389(7) | –0.0007(5) | –0.0019(5) | –0.0199(6) |
| O(3) | 8*c* | 0.2916(2) | –0.12543(7) | 0.23249(5) | 0.0297(6) | 0.0315(6) | 0.0375(6) | 0.0010(5) | 0.0039(5) | 0.0067(5) |
| O(4) | 8*c* | 0.0954(2) | –0.09298(8) | 0.16526(5) | 0.0313(7) | 0.0542(8) | 0.0452(7) | –0.0135(6) | –0.0043(5) | 0.0126(6) |
| O(5) | 8*c* | 0.3264(2) | 0.2003(1) | 0.18803(8) | 0.0275(7) | 0.0600(9) | 0.085(1) | 0.0023(6) | –0.0004(7) | –0.0377(8) |

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