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Poly[[[μ_3-1,3,5-tris(imidazol-1-ylmethyl)-2,4,6-trimethylbenzene]manganese(II)] methylbenzenesulfonate dihydrate]

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Key indicators

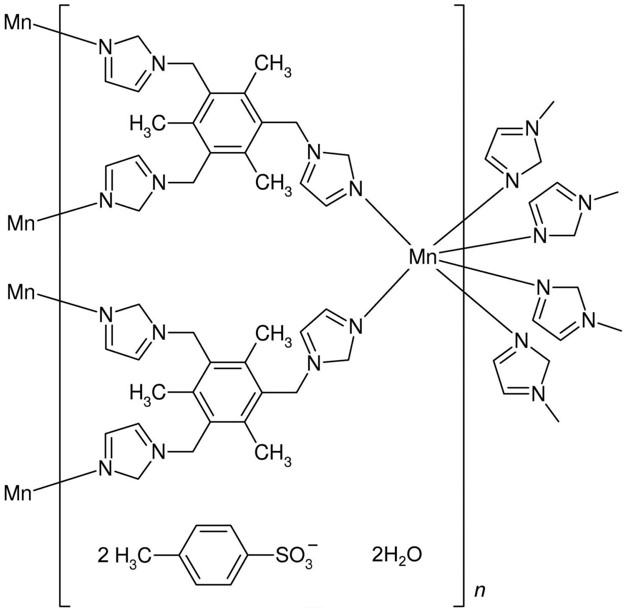
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.007 Å
Disorder in solvent or counterion
R factor = 0.060
wR factor = 0.167
Data-to-parameter ratio = 12.2

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

The title compound, $[Mn(C_{21}H_{24}N_6)_2](C_7H_7SO_3)_2\cdot 2H_2O$, comprises a two-dimensional network structure in which each Mn^{II} atom lies on a centre of inversion and is coordinated by six 1,3,5-tris(imidazol-1-ylmethyl)-2,4,6-trimethylbenzene ligands, each of which coordinates to three Mn atoms.

Comment

The use of multidentate organic ligands and suitable metal salts to construct supramolecular architectures has been demonstrated extensively in recent years. One-, two- and three-dimensional frameworks including adamantoid, cubic, ladder, honeycomb and helical structures have been synthesized (Zhao *et al.*, 2005; Fan *et al.*, 2002, 2003). We have used the multidentate ligand 1,3,5-tris(imidazol-1-ylmethyl)-2,4,6-trimethylbenzene (denoted L) to synthesize the title compound, (I), which adopts a two-dimensional network structure based on a honeycomb motif.



(I)

In (I) (Fig. 1), each Mn^{II} atom lies on a centre of inversion and is coordinated by six imidazole N atoms from different L ligands, each of which coordinates to three Mn atoms. The local coordination environment of Mn^{II} is a slightly distorted octahedron with Mn—N bond distances in the range 2.270 (3)–2.319 (3) Å and N—Mn—N bond angles in the range 85.55 (12)–180°. The network structure is two-dimensional, lying in the (001) plane (Fig. 2).

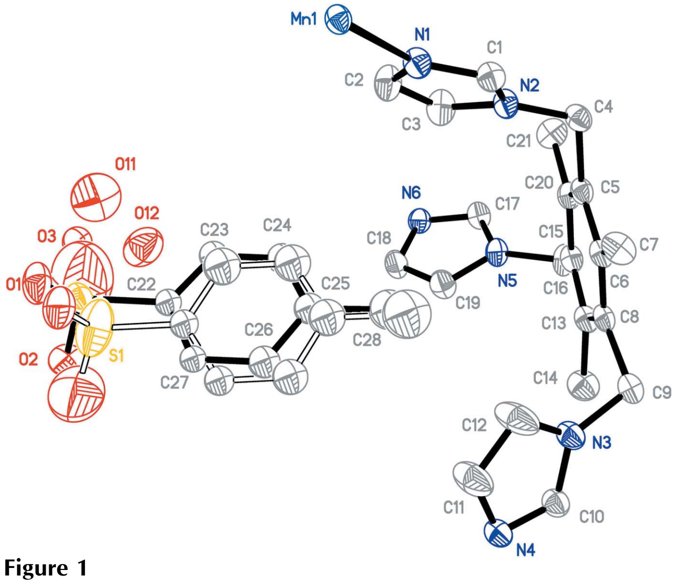


Figure 1
The asymmetric unit of (I), showing displacement ellipsoids at the 30% probability level. H atoms have been omitted. The two disorder components of the methylbenzenesulfonate anion are shown with open and solid bonds, respectively.

Experimental

1,3,5-Tris(imidazol-1-ylmethyl)-2,4,6-trimethylbenzene) (*L*) was prepared according to a literature method (Liu *et al.*, 1999). A solution of $[Mn(OH_2)_4](C_7H_7SO_3)_2$ (0.0943 g,0.2 mmol) in 10 ml of water was added to a solution of *L* (0.0360 g,0.1 mmol) in 10 ml of methanol. The mixture was stirred for 3 h at room temperature and then filtered. The filtrate was allowed to stand in air at room temperature for several days, and colourless crystals suitable for X-ray diffraction were obtained. Elemental analysis found: C 58.22, H 5.72%; calculated: C 58.20, H 5.73%.

Crystal data

$[Mn(C_{21}H_{24}N_6)_2](C_7H_7O_3S)_2 \cdot 2H_2O$
$M_r = 1154.27$
Triclinic, $P\bar{1}$
$a = 11.481$ (3) Å
$b = 11.635$ (3) Å
$c = 13.170$ (3) Å
$\alpha = 64.764$ (4)°
$\beta = 88.190$ (5)°
$\gamma = 63.025$ (4)°
$V = 1389.4$ (6) Å^3
$Z = 1$
$D_x = 1.380$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.38$ mm^{-1}
$T = 293$ (2) K
Block, colourless
0.30 × 0.20 × 0.18 mm

Data collection

Bruker SMART 1000 CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.890$, $T_{max} = 0.932$
7123 measured reflections
4878 independent reflections
2988 reflections with $I > 2\sigma(I)$
$R_{int} = 0.028$
$\theta_{max} = 25.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.060$
$wR(F^2) = 0.167$
$S = 1.03$
4878 reflections
399 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0717P)^2 + 0.9438P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.004$
$\Delta\rho_{max} = 0.70$ e Å^{-3}
$\Delta\rho_{min} = -0.47$ e Å^{-3}

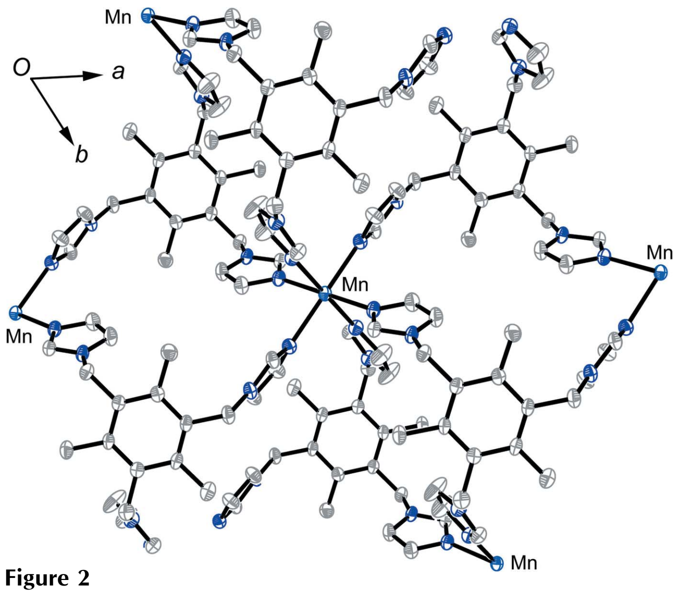


Figure 2
The network structure of (I), viewed approximately along the *c* axis. Displacement ellipsoids are shown at the 30% probability level. H atoms, water molecules and methylbenzenesulfonate anions have been omitted.

C-bound H atoms were included in calculated positions and refined as riding with C—H distances in the range 0.93–0.97 Å and $U_{iso}(H) = 1.2U_{eq}(C)$, or $1.5U_{eq}$(C methyl). The methyl groups of the ligand *L* (C7, C14 and C21) were allowed to rotate about their local threefold axes. The methylbenzenesulfonate anion was refined as disordered over two positions with site occupancy factors constrained to 0.5. The two components were restrained to have similar geometries, and the C atoms were refined with isotropic displacement parameters. The S and O atoms were refined with anisotropic displacement parameters, but with the O atoms restrained to approximate isotropic behaviour. The water molecules O11 and O12 are also disordered and included with site occupancy factor 0.5. The H atoms of these molecules were placed in suitable positions to form O—H···O hydrogen bonds, with O—H = 0.85 Å, and were refined as riding with $U_{iso}(H) = 1.5U_{eq}(O)$.

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

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References

Bruker (1998). *SMART-NT*, *SAINT-NT* and *SHELXTL-NT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Fan, J., Sui, B., Okamura, T., Sun, W.-Y., Tang, W.-X. & Ueyama, N. (2002). *Dalton Trans.* pp. 3868–3873.
Fan, J., Zhu, H.-F., Okamura, T., Sun, W.-Y., Tang, W.-X. & Ueyama, N. (2003). *Inorg. Chem.* **42**, 158–162.
Liu, H.-K., Sun, W.-Y., Zhu, H.-L., Yu, K.-B. & Tang, W.-X. (1999). *Inorg. Chim. Acta*, **295**, 129–135.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Zhao, W., Song, Y., Okamura, T., Fan, J., Sun, W.-Y., Tang, W.-X. & Ueyama, N. (2005). *Inorg. Chem.* **44**, 3330–3336.

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