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Diaquabis(1*H*-imidazole-κN^3)bis(nitrobenzoato-κO)manganese(II)

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In the title complex, $[Mn(C_7H_4NO_4)_2(C_3H_4N_2)_2(H_2O)_2]$, the Mn^{II} atom, located on an inversion center, assumes an octahedral coordination geometry formed by four O and two N atoms. The nitrobenzoate mean plane is inclined to the coordination plane formed by the four O atoms, with a dihedral angle of 23.98 (6)°. The interplanar distance of 3.624 (16) Å implies there is no π–π stacking between parallel imidazole rings.

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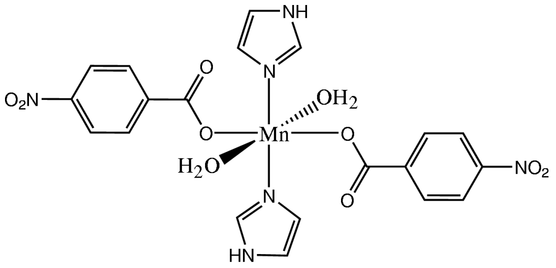
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 Å
R factor = 0.031
wR factor = 0.082
Data-to-parameter ratio = 11.4

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

Comment

Several metal complexes incorporating imidazole have been prepared in our laboratory in order to investigate π–π stacking interactions between imidazole rings. The X-ray structure of the title Mn^{II} complex of imidazole, (I), shows no π–π stacking occurring between imidazole rings.



(I)

The molecular structure of (I) is shown in Fig. 1. The Mn^{II} atom is located on an inversion center and has an octahedral coordination geometry (Table 1) formed by nitrobenzoate anions, imidazole molecules and water molecules. The nitrobenzoate anions are planar [the maximum atomic deviation being 0.0751 (16) Å for atom O2] and are tilted with respect to

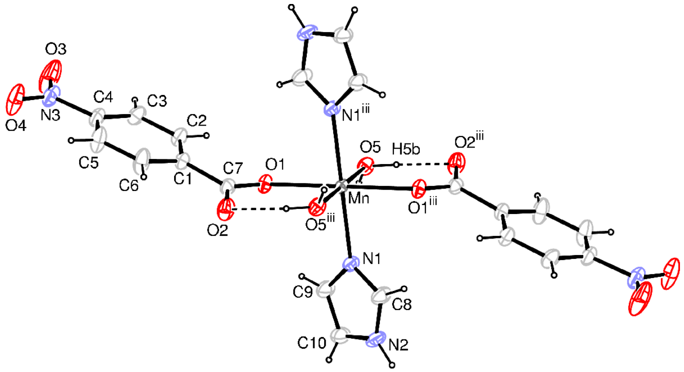


Figure 1
The molecular structure of (I) drawn with 30% probability displacement ellipsoids. Dashed lines indicate the intramolecular hydrogen bonding. [Symmetry code: (iii) $1 - x, 1 - y, 1 - z$.]

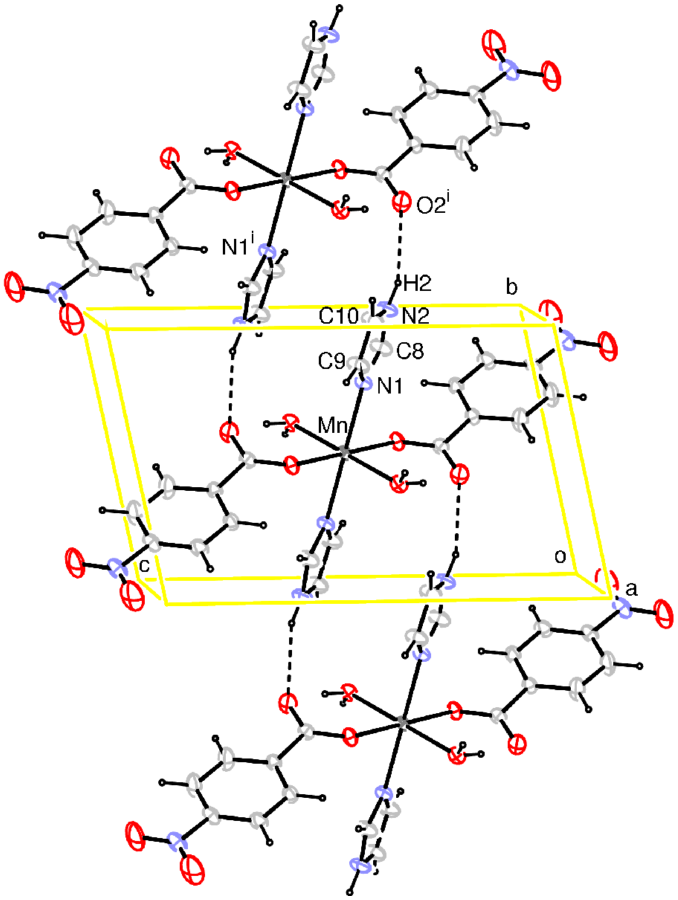


Figure 2
A packing diagram of (I), showing the parallel displacement of imidazole rings. Dashed lines indicate intermolecular N—H···O hydrogen bonds [Symmetry code: (i) $1 - x, 2 - y, 1 - z$.]

the coordination plane formed by the four O atoms at an angle of 23.98 (6)°. This is similar to the situation found in the Ni^{II} (Xu & Xu, 2004*a*) and Co^{II} analogs (Xu & Xu, 2004*b*).

The Mn^{II} complex molecules are linked to each other *via* intermolecular hydrogen bonding, either between imidazole ligands and carboxyl groups (as shown in Fig. 2) or between coordinated water molecules and carboxyl groups (Table 2). The parallel displacement of imidazole rings of neighboring complex molecules can be seen in Fig. 2. The interplanar distance of 3.624 (16) Å between the N1- and N1^{i}-containing rings [symmetry code: (i) $1 - x, 2 - y, 1 - z$] is longer than the value of 3.555 (14) Å found in the Co^{II} analog and the value of 3.535 (14) Å in the Ni^{II} analog mentioned above. This suggests normal van der Waals contacts but not π–π stacking interactions between parallel imidazole rings in the crystal structure.

Experimental

$MnCl_2 \cdot 2H_2O$ (0.32 g, 2 mmol) was dissolved in an aqueous solution (10 ml) containing *p*-nitrobenzoic acid (0.33 g, 2 mmol) and NaOH (0.08 g, 2 mmol). The solution was refluxed for 30 min; an ethanol solution (10 ml) of imidazole (0.14 g, 2 mmol) was then added with continuous stirring. The resulting mixture was refluxed for a further 4 h. After cooling to room temperature, the solution was filtered and yellow single crystals were obtained from the filtrate after two weeks.

Crystal data

$[Mn(C_7H_4NO_4)_2(C_3H_4N_2)_2(H_2O)_2]$
$M_r = 559.36$
Triclinic, $P\overline{1}$
$a = 5.6745$ (3) Å
$b = 8.1082$ (3) Å
$c = 12.8399$ (6) Å
$\alpha = 76.7284$ (15)°
$\beta = 88.139$ (2)°
$\gamma = 86.3319$ (13)°
$V = 573.71$ (5) Å^3
$Z = 1$
$D_x = 1.619$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2279 reflections
$\theta = 3.0$–24.0°
$\mu = 0.65$ mm^{-1}
$T = 295$ (2) K
Prism, yellow
0.30 × 0.24 × 0.21 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.821$, $T_{max} = 0.870$
4189 measured reflections
1997 independent reflections
1903 reflections with $I > 2\sigma(I)$
$R_{int} = 0.014$
$\theta_{max} = 25.0$°
$h = -6 \rightarrow 6$
$k = -9 \rightarrow 9$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.082$
$S = 1.10$
1997 reflections
175 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0441P)^2 + 0.2558P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.23$ e Å^{-3}
$\Delta\rho_{min} = -0.29$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Mn—N1	2.2127 (14)	Mn—O5	2.2180 (13)
Mn—O1	2.2376 (12)		
N1—Mn—O1	93.52 (5)	O1—Mn—O5	88.44 (5)
N1—Mn—O5	89.43 (5)		

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O2^{i}	0.86	2.34	3.091 (2)	146
O5—H5*A*···O1^{ii}	0.83 (3)	2.01 (3)	2.8070 (17)	163 (2)
O5—H5*B*···O2^{iii}	0.85 (2)	1.85 (2)	2.668 (2)	161 (2)

Symmetry codes: (i) $1 - x, 2 - y, 1 - z$; (ii) $2 - x, 1 - y, 1 - z$; (iii) $1 - x, 1 - y, 1 - z$.

Water H atoms were located in a difference Fourier map and independently refined with fixed isotropic displacement parameters of 0.05 Å^2. H atoms on aromatic rings were placed in calculated positions, with C—H = 0.93 Å and N—H = 0.86 Å, and were included in the final cycles of refinement in a riding model, with $U_{iso}(H) = 1.2U_{eq}$ of the carrier atoms.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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References

Altomare, A., Cascarano, G., Giacovazzo, C. & Guagliardi, A. (1993). *J. Appl. Cryst.* **26**, 343–350.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Rigaku (1998). *PROCESS-AUTO*. Rigaku Corporation, Tokyo, Japan.
Rigaku/MSC (2002). *CrystalStructure*. Version 3.00. Rigaku/MSC, 9009 New Trails Drive, The Woodlands, TX 77381–5209, USA.
Sheldrick, G. M. (1997). *SHELXL*97. University of Göttingen, Germany.
Xu, T.-G. & Xu, D.-J. (2004*a*). *Acta Cryst.* E**60**, m27–m29.
Xu, T.-G. & Xu, D.-J. (2004*b*). *Acta Cryst.* E**60**, m1131–m1133.