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trans-Diaquabis[5-carboxy-2-(3-pyridyl)-1*H*-imidazole-4-carboxylato-κ^2N^3,O^4]-manganese(II)

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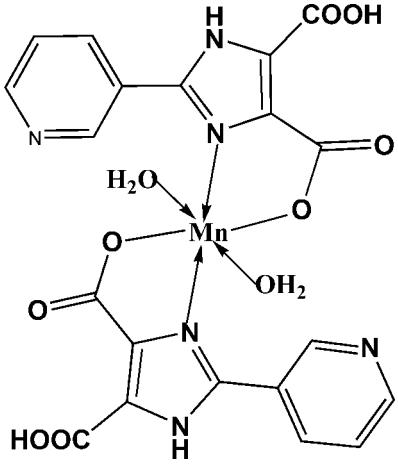
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.048; wR factor = 0.165; data-to-parameter ratio = 13.6.

In the title compound, $[Mn(C_{10}H_6N_3O_4)_2(H_2O)_2]$, synthesized by hydrothermal reaction, the Mn^{II} ion lies on an inversion centre and displays a distorted octahedral coordination geometry defined by the two imidazole N atoms and two carboxylate O atoms of the two *trans*-standing chelate ligands, and two O atoms of the water molecules. A two-dimensional supramolecular architecture is formed *via* N—H···O, O—H···N and O—H···O hydrogen-bonding interactions.

Related literature

For the chemistry of imidazoles, see: Xiao *et al.* (2004); Zhang *et al.* (2004); Lu *et al.* (2006).



Experimental

Crystal data

$[Mn(C_{10}H_6N_3O_4)_2(H_2O)_2]$
M_r = 555.33
Triclinic, $P\overline{1}$
a = 6.9574 (7) Å
b = 8.5636 (7) Å
c = 9.4409 (16) Å
α = 81.90 (3)°
β = 83.42 (4)°
γ = 72.10 (2)°
V = 528.41 (11) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.70 mm^{-1}
T = 298 (2) K
0.25 × 0.20 × 0.20 mm

Data collection

Rigaku Mercury2 diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.845, T_{max} = 0.869
5416 measured reflections
2378 independent reflections
1871 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.165
S = 1.11
2378 reflections
175 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.54 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O4^{i}	0.86	2.00	2.840 (3)	164
O5—H5···N3^{ii}	0.82	1.97	2.779 (3)	171
O5—H5B···O3^{iii}	0.839 (17)	2.074 (18)	2.908 (3)	173 (3)
O3—H3···O2	0.82	1.69	2.456 (3)	155

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

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

This work was supported by a start-up grant from Southeast University to Professor Ren-Gen Xiong.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2177).

References

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Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
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supplementary materials

Acta Cryst. (2008). E**64**, m1286 [**doi:10.1107/S1600536808029073**]

trans-Diaquabis[5-carboxy-2-(3-pyridyl)-1*H*-imidazole-4-carboxylato-κ^2N^3,O^4]manganese(II)

L.-Z. Chen

Comment

N-Heterocyclic carboxylic acids, such as imidazole-4,5-dicarboxylic acid, are recognized as efficient N,*O*-donors, exhibiting diverse modes of coordination (Zhang *et al.*, 2004; Xiao *et al.*, 2004; Lu *et al.*, 2006). In this work, we have chosen 2-Pyridin-3-yl-1*H*-imidazole-4,5-dicarboxylic acid as the building block to obtain the title compound, and we present its crystal structure here. Mn^{II} ion lies on an inversion centre and displaying distorted octahedral coordination geometry defined by the two imidazole N atoms, two O toms of the carboxylate groups and two O atoms of the water molecules. The pyridine ring and imidazole rings are twisted from each other by a dihedral angle of 20.78 (2)° (Fig. 1). The crystal structure is stabilized by intermolecular O—H···N, O—H···O and N—H···O, hydrogen bonds. A two-dimensional supramolecular architecture is formed *via* hydrogen-bond interactions (Table 1 and Fig. 2).

Experimental

A mixture of 2-Pyridin-3-yl-1*H*-imidazole-4,5-dicarboxylic acid (0.1 mmol, 23 mg) and $MnCl_2$ (20 mg, 0.1 mmol) and water (1 ml) sealed in a glass tube was maintained at 100°C for 3 d then cooled to room temperature to obtain suitable single crystals for X-ray analysis.

Refinement

All H atoms attached to C atoms, O atoms and N atoms except H5B were fixed geometrically and treated as riding with C—H = 0.93 Å (aromatic), O—H = 0.82 Å and N—H = 0.86 Å with U_{iso}(H) = 1.2U_{eq}(C and N) or U_{iso}(H) = 1.5U_{eq}(O). H5B atom of H_2O were located in difference Fourier maps.

Figures

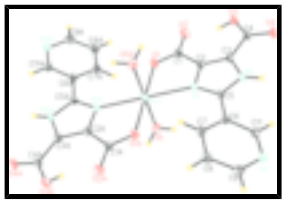

Fig. 1. A view of the title compound with the atomic numbering scheme. Displacement ellipsoids were drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii. Unlabelled atoms are related to labelled atoms by the symmetry code (-x+1, -y+1, -z).

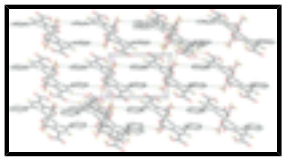

Fig. 2. The crystal packing of the title compound viewed along the *b* axis and all hydrogen atoms not involved in hydrogen bonding (dashed lines) were omitted for clarity.

trans-Diaquabis[5-carboxy-2-(3-pyridyl)-1*H*-imidazole-4- carboxylato-κ^2N^3,O^4]manganese(II)

Crystal data

$[Mn(C_{10}H_6N_3O_4)_2(H_2O)_2]$	$Z = 1$
$M_r = 555.33$	$F_{000} = 283$
Triclinic, $P\overline{1}$	$D_x = 1.745$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 6.9574$ (7) Å	Cell parameters from 1463 reflections
$b = 8.5636$ (7) Å	$\theta = 3.1$–27.5º
$c = 9.4409$ (16) Å	$\mu = 0.70$ mm^{-1}
$\alpha = 81.90$ (3)º	$T = 298$ (2) K
$\beta = 83.42$ (4)º	Block, colourless
$\gamma = 72.10$ (2)º	0.25 × 0.20 × 0.20 mm
$V = 528.41$ (11) Å^3	

Data collection

Rigaku Mercury2 diffractometer	2378 independent reflections
Radiation source: fine-focus sealed tube	1871 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.029$
Detector resolution: 13.6612 pixels mm^{-1}	$\theta_{max} = 27.5$º
$T = 298$(2) K	$\theta_{min} = 2.5$º
ω scans	$h = -8 \rightarrow 8$
Absorption correction: multi-scan (CrystalClear; Rigaku, 2005)	$k = -11 \rightarrow 11$
$T_{min} = 0.845$, $T_{max} = 0.869$	$l = -12 \rightarrow 12$
5416 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.047$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.165$	$w = 1/[\sigma^2(F_o^2) + (0.1003P)^2 + 0.0122P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.11$	$(\Delta/\sigma)_{max} < 0.001$
2378 reflections	$\Delta\rho_{max} = 0.54$ e Å^{-3}
175 parameters	$\Delta\rho_{min} = -0.44$ e Å^{-3}
2 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Mn1	0.5000	0.5000	0.0000	0.0299 (2)
C1	0.3266 (4)	0.8677 (4)	−0.0160 (3)	0.0290 (6)
C2	0.2634 (4)	0.8148 (3)	0.1332 (3)	0.0253 (6)
C3	0.1577 (4)	0.9082 (3)	0.2405 (3)	0.0260 (6)
C4	0.0487 (5)	1.0861 (4)	0.2425 (3)	0.0308 (6)
C5	0.2472 (4)	0.6428 (3)	0.3206 (3)	0.0229 (5)
C6	0.2698 (4)	0.4926 (3)	0.4203 (3)	0.0253 (6)
C7	0.3049 (5)	0.3401 (4)	0.3713 (3)	0.0336 (7)
H7A	0.3120	0.3314	0.2737	0.040*
C8	0.3291 (5)	0.2013 (4)	0.4703 (3)	0.0369 (7)
H8A	0.3592	0.0972	0.4399	0.044*
C9	0.3080 (5)	0.2195 (4)	0.6156 (3)	0.0345 (7)
H9A	0.3215	0.1261	0.6817	0.041*
N3	0.2692 (4)	0.3661 (3)	0.6640 (3)	0.0332 (6)
C11	0.2491 (5)	0.4986 (4)	0.5688 (3)	0.0300 (6)
H11A	0.2196	0.6010	0.6025	0.036*
N1	0.3172 (3)	0.6504 (3)	0.1834 (2)	0.0255 (5)
N2	0.1531 (4)	0.7971 (3)	0.3573 (2)	0.0269 (5)
H2A	0.0992	0.8207	0.4412	0.032*
O1	0.4330 (4)	0.7595 (3)	−0.0912 (2)	0.0380 (5)
O2	0.2722 (4)	1.0220 (3)	−0.0599 (2)	0.0408 (6)
O3	0.0641 (4)	1.1816 (3)	0.1292 (2)	0.0397 (6)
H3	0.1602	1.1348	0.0764	0.060*
O4	−0.0526 (4)	1.1310 (3)	0.3540 (2)	0.0457 (6)
O5	0.7793 (4)	0.5087 (3)	0.0738 (2)	0.0414 (6)
H5	0.7544	0.5539	0.1476	0.062*
H5B	0.867 (5)	0.416 (3)	0.083 (3)	0.042 (10)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0369 (4)	0.0247 (4)	0.0204 (3)	0.0026 (3)	0.0007 (3)	−0.0056 (2)

C1	0.0337 (15)	0.0254 (14)	0.0204 (13)	0.0004 (11)	0.0015 (11)	−0.0017 (10)
C2	0.0307 (14)	0.0207 (13)	0.0197 (13)	−0.0006 (10)	−0.0005 (11)	−0.0035 (10)
C3	0.0315 (14)	0.0231 (14)	0.0205 (12)	−0.0040 (11)	0.0015 (11)	−0.0049 (10)
C4	0.0366 (16)	0.0242 (14)	0.0257 (14)	0.0005 (12)	−0.0005 (12)	−0.0061 (11)
C5	0.0233 (13)	0.0235 (13)	0.0184 (12)	−0.0021 (10)	0.0020 (10)	−0.0047 (9)
C6	0.0270 (13)	0.0265 (14)	0.0208 (13)	−0.0063 (11)	0.0028 (11)	−0.0041 (10)
C7	0.0455 (17)	0.0288 (15)	0.0212 (14)	−0.0052 (13)	0.0077 (13)	−0.0064 (11)
C8	0.0493 (19)	0.0225 (14)	0.0336 (16)	−0.0033 (12)	−0.0003 (14)	−0.0048 (11)
C9	0.0404 (17)	0.0279 (15)	0.0303 (16)	−0.0074 (13)	0.0003 (13)	0.0039 (12)
N3	0.0419 (15)	0.0327 (13)	0.0209 (12)	−0.0075 (11)	0.0023 (10)	−0.0012 (9)
C11	0.0388 (16)	0.0271 (14)	0.0226 (14)	−0.0065 (12)	−0.0030 (12)	−0.0041 (11)
N1	0.0310 (12)	0.0214 (11)	0.0200 (11)	−0.0021 (9)	−0.0007 (10)	−0.0028 (9)
N2	0.0334 (12)	0.0246 (12)	0.0185 (11)	−0.0032 (10)	0.0038 (9)	−0.0058 (8)
O1	0.0503 (14)	0.0304 (11)	0.0210 (10)	0.0023 (10)	0.0077 (9)	−0.0028 (8)
O2	0.0578 (14)	0.0251 (11)	0.0257 (11)	0.0011 (10)	0.0082 (10)	0.0035 (8)
O3	0.0508 (14)	0.0229 (11)	0.0330 (12)	0.0038 (9)	0.0059 (10)	−0.0031 (8)
O4	0.0650 (16)	0.0303 (12)	0.0291 (12)	0.0059 (11)	0.0040 (11)	−0.0123 (9)
O5	0.0423 (13)	0.0434 (14)	0.0309 (12)	0.0012 (11)	−0.0015 (10)	−0.0119 (10)

Geometric parameters (Å, °)

Mn1—O5^{i}	2.163 (2)	C5—N2	1.356 (3)
Mn1—O5	2.163 (2)	C5—C6	1.460 (4)
Mn1—O1^{i}	2.194 (2)	C6—C7	1.389 (4)
Mn1—O1	2.194 (2)	C6—C11	1.399 (4)
Mn1—N1^{i}	2.322 (2)	C7—C8	1.383 (4)
Mn1—N1	2.322 (2)	C7—H7A	0.9300
C1—O1	1.246 (3)	C8—C9	1.388 (4)
C1—O2	1.279 (3)	C8—H8A	0.9300
C1—C2	1.477 (4)	C9—N3	1.335 (4)
C2—N1	1.370 (3)	C9—H9A	0.9300
C2—C3	1.380 (4)	N3—C11	1.326 (4)
C3—N2	1.355 (3)	C11—H11A	0.9300
C3—C4	1.480 (4)	N2—H2A	0.8600
C4—O4	1.238 (3)	O3—H3	0.8200
C4—O3	1.267 (4)	O5—H5	0.8200
C5—N1	1.331 (3)	O5—H5B	0.839 (17)
O5^{i}—Mn1—O5	180.00 (11)	N2—C5—C6	123.9 (2)
O5^{i}—Mn1—O1^{i}	90.51 (10)	C7—C6—C11	117.7 (3)
O5—Mn1—O1^{i}	89.49 (10)	C7—C6—C5	121.3 (2)
O5^{i}—Mn1—O1	89.49 (10)	C11—C6—C5	121.0 (2)
O5—Mn1—O1	90.51 (10)	C8—C7—C6	118.9 (3)
O1^{i}—Mn1—O1	180.0	C8—C7—H7A	120.6
O5^{i}—Mn1—N1^{i}	90.00 (8)	C6—C7—H7A	120.6
O5—Mn1—N1^{i}	90.00 (8)	C7—C8—C9	119.2 (3)
O1^{i}—Mn1—N1^{i}	74.86 (8)	C7—C8—H8A	120.4

O1—Mn1—N1^{i}	105.14 (8)	C9—C8—H8A	120.4
O5^{i}—Mn1—N1	90.00 (8)	N3—C9—C8	122.5 (3)
O5—Mn1—N1	90.00 (8)	N3—C9—H9A	118.8
O1^{i}—Mn1—N1	105.14 (8)	C8—C9—H9A	118.8
O1—Mn1—N1	74.86 (8)	C11—N3—C9	118.2 (3)
N1^{i}—Mn1—N1	180.0	N3—C11—C6	123.5 (3)
O1—C1—O2	123.7 (3)	N3—C11—H11A	118.2
O1—C1—C2	118.1 (3)	C6—C11—H11A	118.2
O2—C1—C2	118.2 (3)	C5—N1—C2	105.7 (2)
N1—C2—C3	110.3 (2)	C5—N1—Mn1	145.47 (18)
N1—C2—C1	119.8 (2)	C2—N1—Mn1	108.75 (16)
C3—C2—C1	129.9 (3)	C3—N2—C5	109.1 (2)
N2—C3—C2	104.8 (2)	C3—N2—H2A	125.5
N2—C3—C4	121.9 (2)	C5—N2—H2A	125.5
C2—C3—C4	133.1 (3)	C1—O1—Mn1	118.36 (18)
O4—C4—O3	124.5 (3)	C4—O3—H3	109.5
O4—C4—C3	117.8 (3)	Mn1—O5—H5	109.5
O3—C4—C3	117.7 (2)	Mn1—O5—H5B	113 (2)
N1—C5—N2	110.0 (2)	H5—O5—H5B	112.4
N1—C5—C6	126.0 (2)		
O1—C1—C2—N1	−1.9 (4)	C6—C5—N1—C2	−179.2 (3)
O2—C1—C2—N1	179.4 (3)	N2—C5—N1—Mn1	176.6 (2)
O1—C1—C2—C3	175.6 (3)	C6—C5—N1—Mn1	−2.2 (5)
O2—C1—C2—C3	−3.1 (5)	C3—C2—N1—C5	−0.6 (3)
N1—C2—C3—N2	1.4 (3)	C1—C2—N1—C5	177.3 (3)
C1—C2—C3—N2	−176.2 (3)	C3—C2—N1—Mn1	−178.84 (19)
N1—C2—C3—C4	−173.1 (3)	C1—C2—N1—Mn1	−0.9 (3)
C1—C2—C3—C4	9.3 (6)	O5^{i}—Mn1—N1—C5	95.6 (3)
N2—C3—C4—O4	−1.9 (5)	O5—Mn1—N1—C5	−84.4 (3)
C2—C3—C4—O4	171.9 (3)	O1^{i}—Mn1—N1—C5	5.0 (4)
N2—C3—C4—O3	178.8 (3)	O1—Mn1—N1—C5	−175.0 (4)
C2—C3—C4—O3	−7.4 (5)	O5^{i}—Mn1—N1—C2	−87.49 (19)
N1—C5—C6—C7	−22.7 (4)	O5—Mn1—N1—C2	92.51 (19)
N2—C5—C6—C7	158.6 (3)	O1^{i}—Mn1—N1—C2	−178.01 (18)
N1—C5—C6—C11	159.7 (3)	O1—Mn1—N1—C2	1.99 (18)
N2—C5—C6—C11	−18.9 (4)	C2—C3—N2—C5	−1.7 (3)
C11—C6—C7—C8	−3.7 (4)	C4—C3—N2—C5	173.6 (3)
C5—C6—C7—C8	178.7 (3)	N1—C5—N2—C3	1.4 (3)
C6—C7—C8—C9	3.1 (5)	C6—C5—N2—C3	−179.8 (2)
C7—C8—C9—N3	−1.4 (5)	O2—C1—O1—Mn1	−177.4 (2)
C8—C9—N3—C11	0.4 (5)	C2—C1—O1—Mn1	3.9 (4)
C9—N3—C11—C6	−1.1 (5)	O5^{i}—Mn1—O1—C1	86.8 (2)
C7—C6—C11—N3	2.8 (4)	O5—Mn1—O1—C1	−93.2 (2)
C5—C6—C11—N3	−179.6 (3)	N1^{i}—Mn1—O1—C1	176.7 (2)
N2—C5—N1—C2	−0.4 (3)	N1—Mn1—O1—C1	−3.3 (2)

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2A···O4^{ii}	0.86	2.00	2.840 (3)	164
O5—H5···N3^{iii}	0.82	1.97	2.779 (3)	171
O5—H5B···O3^{iv}	0.839 (17)	2.074 (18)	2.908 (3)	173 (3)
O3—H3···O2	0.82	1.69	2.456 (3)	155

Symmetry codes: (ii) −*x*, −*y*+2, −*z*+1; (iii) −*x*+1, −*y*+1, −*z*+1; (iv) *x*+1, *y*−1, *z*.

Fig. 1

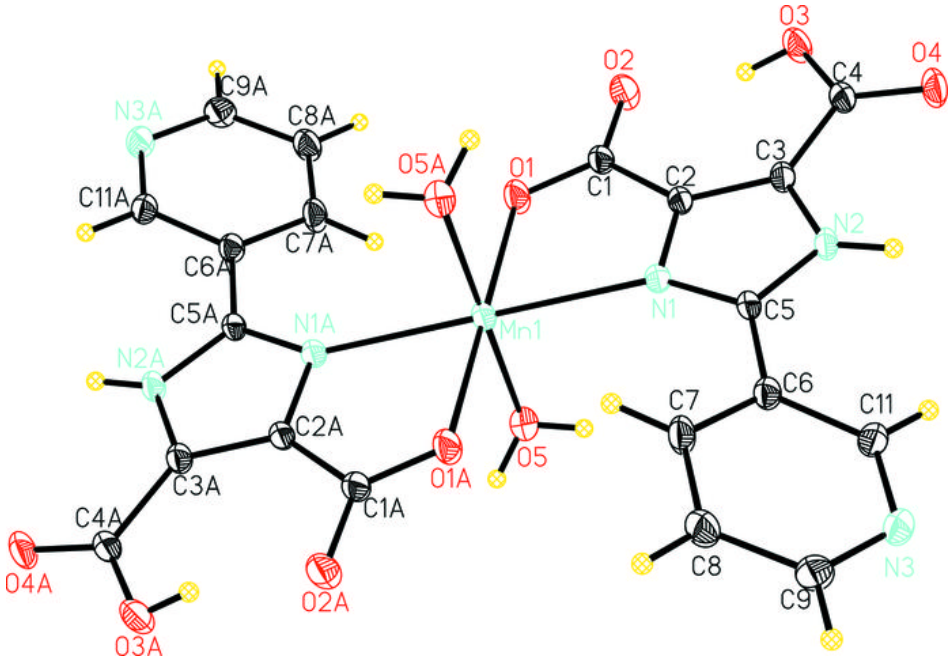
O3
O4
C4
O2
C9A
N3A
C8A
O5A
O1
C1
C2
C3
C11A
C7A
N2
C6A
C5A
N1A
Mn1
N1
C5
N2A
C6
C7
C11
C2A
O1A
O5
C3A
C1A
C4A
C8
N3
O4A
O2A
C9
O3A

Fig. 2