

## Bis(acetato- $\kappa^2O,O'$ )[2,6-bis(1*H*-pyrazol-3-yl)- $\kappa N^2$ ]pyridine- $\kappa N$ ]manganese(II)

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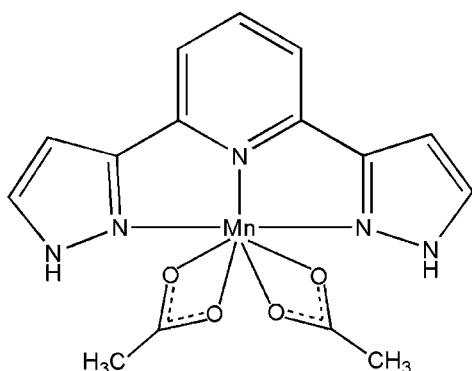
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Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(C-C) = 0.004$  Å;  $R$  factor = 0.034;  $wR$  factor = 0.117; data-to-parameter ratio = 13.3.

In the title complex,  $[Mn(CH_3CO_2)_2(C_{11}H_9N_5)]$ , the Mn<sup>II</sup> atom is coordinated by the pyridine N atom and two pyrazole N atoms from a 2,6-bis(pyrazol-3-yl)pyridine ligand and four O atoms from two bidentate acetate ligands. The complex molecules are linked by intermolecular N—H...O hydrogen bonds into a chain along [010].  $\pi$ - $\pi$  interactions between the pyridine rings and between the pyrazole rings [centroid-centroid distances = 3.772 (2) and 3.546 (2) Å] connect the chains.

### Related literature

 For a related structure, see: Rich *et al.* (2010).


### Experimental

#### Crystal data

 $[Mn(C_2H_3O_2)_2(C_{11}H_9N_5)]$ 
 $M_r = 384.26$ 

 Triclinic,  $P\bar{1}$ 
 $a = 8.2386$  (16) Å

 $b = 9.4324$  (19) Å

 $c = 11.081$  (2) Å

 $\alpha = 98.32$  (3)°

 $\beta = 95.01$  (3)°

 $\gamma = 106.11$  (3)°  
 $V = 811.2$  (3) Å<sup>3</sup>  
 $Z = 2$   
 Mo  $K\alpha$  radiation

 $\mu = 0.85$  mm<sup>-1</sup>  
 $T = 293$  K  
 $0.30 \times 0.20 \times 0.20$  mm

#### Data collection

 Rigaku R-Axis RAPID  
 diffractometer  
 Absorption correction: multi-scan  
 (ABSCOR; Higashi, 1995)  
 $T_{min} = 0.816$ ,  $T_{max} = 0.849$ 

 5563 measured reflections  
 3001 independent reflections  
 2386 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.030$ 

#### Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.034$   
 $wR(F^2) = 0.117$   
 $S = 1.10$   
 3001 reflections

 226 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{max} = 0.51$  e Å<sup>-3</sup>  
 $\Delta\rho_{min} = -0.43$  e Å<sup>-3</sup>
**Table 1**

Selected bond lengths (Å).

Mn1—O1	2.480 (2)	Mn1—N2	2.262 (2)
Mn1—O2	2.192 (2)	Mn1—N3	2.235 (2)
Mn1—O3	2.596 (2)	Mn1—N4	2.270 (2)
Mn1—O4	2.160 (2)		

**Table 2**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1B...O4 <sup>i</sup>	0.86	1.91	2.751 (3)	165
N5—H5B...O2 <sup>ii</sup>	0.86	1.85	2.712 (3)	180

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MS, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2414).

### References

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**supplementary materials**

*Acta Cryst.* (2011). E67, m502 [ doi:10.1107/S1600536811010506 ]

**Bis(acetato- $\kappa^2O,O'$ )[2,6-bis(1*H*-pyrazol-3-yl- $\kappa N^2$ )pyridine- $\kappa N$ ]manganese(II)**

**F. Yu and B. Li**

**Experimental**

2,6-Bis(pyrazol-3-yl)pyridine (0.1 mmol) was dissolved in methanol (2.5 ml) with 0.2 mmol of trimethylamine. Mn(OAc)<sub>2</sub> (0.2 mmol) in methanol (2.5 ml) was added into the resulting solution. After stirring at room temperature for 1 h, the resulting yellow solution was put into a tube layered with ether. Yellow crystals were obtained in three days.

**Refinement**

H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 (aromatic), 0.96 (CH<sub>3</sub>) and N—H = 0.86 Å and with  $U_{\text{iso}}(\text{H}) = 1.2(1.5 \text{ for methyl})U_{\text{eq}}(\text{C}, \text{N})$ .

**Figures**

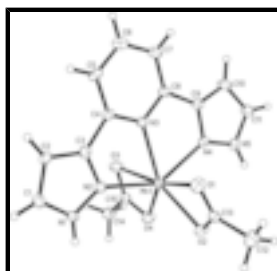


Fig. 1. Molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

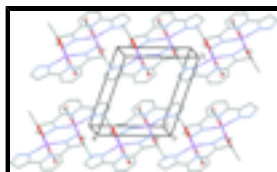


Fig. 2. Crystal packing of the title compound, showing the chain structures along the *b* axis. Dashed lines denote hydrogen bonds. H atoms have been omitted for clarity.

**Bis(acetato- $\kappa^2O,O'$ )[2,6-bis(1*H*-pyrazol-3-yl- $\kappa N^2$ )pyridine- $\kappa N$ ]manganese(II)**

*Crystal data*

[Mn(C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>)<sub>2</sub>(C<sub>11</sub>H<sub>9</sub>N<sub>5</sub>)]

$M_r = 384.26$

Triclinic,  $P\bar{1}$

Hall symbol: -P 1

$a = 8.2386(16) \text{ \AA}$

$b = 9.4324(19) \text{ \AA}$

$c = 11.081(2) \text{ \AA}$

$\alpha = 98.32(3)^\circ$

$Z = 2$

$F(000) = 394$

$D_x = 1.573 \text{ Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 2386 reflections

$\theta = 6.1\text{--}54.9^\circ$

$\mu = 0.85 \text{ mm}^{-1}$

$T = 293 \text{ K}$

# supplementary materials

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$\beta = 95.01 (3)^\circ$   
 $\gamma = 106.11 (3)^\circ$   
 $V = 811.2 (3) \text{ \AA}^3$

Block, yellow  
 $0.30 \times 0.20 \times 0.20 \text{ mm}$

## Data collection

Rigaku R-Axis RAPID  
diffractometer  
Radiation source: rotation anode  
graphite  
 $\omega$  scans  
Absorption correction: multi-scan  
(*ABSCOR*; Higashi, 1995)  
 $T_{\min} = 0.816$ ,  $T_{\max} = 0.849$   
5563 measured reflections

3001 independent reflections  
2386 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.030$   
 $\theta_{\max} = 26.0^\circ$ ,  $\theta_{\min} = 3.4^\circ$   
 $h = -10 \rightarrow 10$   
 $k = -11 \rightarrow 9$   
 $l = -13 \rightarrow 13$

## Refinement

Refinement on  $F^2$   
Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.034$   
 $wR(F^2) = 0.117$   
 $S = 1.10$   
3001 reflections  
226 parameters  
0 restraints

Primary atom site location: structure-invariant direct methods  
Secondary atom site location: difference Fourier map  
Hydrogen site location: inferred from neighbouring sites  
H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0565P)^2]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.51 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = -0.43 \text{ e \AA}^{-3}$

## Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{Å}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Mn1	0.67466 (5)	0.89985 (4)	0.81715 (4)	0.01323 (17)
N1	0.3285 (3)	1.0204 (2)	0.7643 (2)	0.0155 (5)
H1B	0.3327	1.0677	0.8375	0.019*
N2	0.4400 (3)	0.9459 (2)	0.7303 (2)	0.0155 (5)
N3	0.6132 (3)	0.7810 (2)	0.6217 (2)	0.0131 (5)
N4	0.8712 (3)	0.7781 (2)	0.7766 (2)	0.0148 (5)
N5	1.0113 (3)	0.7595 (3)	0.8392 (2)	0.0179 (5)
H5B	1.0537	0.8029	0.9135	0.021*
C1	0.2104 (4)	1.0115 (3)	0.6700 (3)	0.0187 (6)
H1A	0.1217	1.0545	0.6732	0.022*
C2	0.2431 (4)	0.9274 (3)	0.5670 (3)	0.0169 (6)
H2A	0.1842	0.9025	0.4877	0.020*
C3	0.3877 (3)	0.8887 (3)	0.6116 (3)	0.0156 (6)
C4	0.4818 (3)	0.7946 (3)	0.5476 (2)	0.0135 (6)
C5	0.4382 (4)	0.7223 (3)	0.4265 (2)	0.0181 (6)

H5A	0.3462	0.7324	0.3771	0.022*
C6	0.5374 (4)	0.6335 (3)	0.3808 (3)	0.0225 (7)
H6A	0.5109	0.5824	0.2999	0.027*
C7	0.6738 (4)	0.6213 (3)	0.4548 (3)	0.0204 (7)
H7A	0.7413	0.5638	0.4244	0.025*
C8	0.7087 (4)	0.6962 (3)	0.5750 (2)	0.0145 (6)
C9	0.8480 (4)	0.6925 (3)	0.6657 (3)	0.0158 (6)
C10	0.9715 (4)	0.6183 (4)	0.6587 (3)	0.0252 (7)
H10A	0.9825	0.5508	0.5922	0.030*
C11	1.0740 (4)	0.6645 (3)	0.7698 (3)	0.0213 (7)
H11A	1.1696	0.6353	0.7926	0.026*
C12	1.0613 (4)	1.3063 (3)	0.8677 (3)	0.0306 (8)
H12A	1.0919	1.3407	0.7931	0.046*
H12B	1.1568	1.2860	0.9100	0.046*
H12C	1.0294	1.3823	0.9194	0.046*
C13	0.9129 (4)	1.1649 (3)	0.8373 (3)	0.0166 (6)
O1	0.8498 (3)	1.1097 (2)	0.7299 (2)	0.0253 (5)
O2	0.8561 (3)	1.1034 (2)	0.92644 (17)	0.0196 (5)
C14	0.3975 (4)	0.6485 (3)	1.0567 (3)	0.0228 (7)
H14A	0.3170	0.5539	1.0197	0.034*
H14B	0.3380	0.7142	1.0935	0.034*
H14C	0.4766	0.6332	1.1188	0.034*
C15	0.4932 (4)	0.7179 (3)	0.9591 (3)	0.0153 (6)
O3	0.4611 (3)	0.6531 (2)	0.85024 (18)	0.0227 (5)
O4	0.6077 (3)	0.8442 (2)	0.99224 (18)	0.0195 (5)

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Mn1	0.0131 (3)	0.0136 (3)	0.0113 (2)	0.00332 (17)	0.00028 (18)	-0.00105 (16)
N1	0.0176 (13)	0.0184 (12)	0.0118 (12)	0.0079 (10)	0.0042 (10)	0.0006 (9)
N2	0.0136 (13)	0.0139 (12)	0.0192 (13)	0.0045 (10)	0.0024 (10)	0.0029 (10)
N3	0.0139 (12)	0.0139 (12)	0.0114 (12)	0.0035 (10)	0.0023 (10)	0.0024 (9)
N4	0.0146 (12)	0.0180 (12)	0.0110 (12)	0.0050 (10)	-0.0001 (10)	0.0011 (9)
N5	0.0161 (13)	0.0185 (13)	0.0185 (13)	0.0047 (10)	-0.0002 (10)	0.0037 (10)
C1	0.0177 (16)	0.0223 (15)	0.0179 (15)	0.0082 (13)	0.0028 (13)	0.0052 (12)
C2	0.0176 (15)	0.0212 (15)	0.0110 (14)	0.0052 (12)	-0.0009 (12)	0.0031 (11)
C3	0.0128 (14)	0.0119 (14)	0.0216 (16)	0.0020 (11)	0.0035 (12)	0.0039 (11)
C4	0.0158 (15)	0.0142 (14)	0.0099 (14)	0.0021 (11)	0.0026 (12)	0.0038 (11)
C5	0.0221 (16)	0.0204 (15)	0.0103 (14)	0.0053 (13)	-0.0028 (12)	0.0031 (11)
C6	0.0296 (18)	0.0196 (16)	0.0186 (16)	0.0085 (14)	0.0045 (14)	0.0012 (12)
C7	0.0250 (17)	0.0215 (16)	0.0172 (16)	0.0113 (13)	0.0050 (13)	0.0010 (12)
C8	0.0176 (15)	0.0153 (14)	0.0106 (14)	0.0047 (12)	0.0021 (12)	0.0026 (11)
C9	0.0164 (15)	0.0170 (14)	0.0143 (15)	0.0049 (12)	0.0041 (12)	0.0022 (11)
C10	0.0300 (19)	0.0326 (18)	0.0166 (16)	0.0195 (15)	0.0017 (14)	-0.0033 (13)
C11	0.0212 (17)	0.0286 (17)	0.0176 (16)	0.0141 (14)	0.0006 (13)	0.0032 (13)
C12	0.0286 (19)	0.0187 (16)	0.039 (2)	-0.0018 (14)	0.0063 (16)	0.0045 (14)
C13	0.0159 (15)	0.0148 (14)	0.0201 (16)	0.0086 (12)	0.0002 (13)	0.0000 (12)

## supplementary materials

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O1	0.0234 (12)	0.0237 (12)	0.0262 (12)	0.0056 (10)	0.0001 (10)	0.0003 (9)
O2	0.0236 (11)	0.0167 (10)	0.0145 (11)	0.0011 (9)	0.0007 (9)	0.0004 (8)
C14	0.0275 (17)	0.0185 (15)	0.0200 (16)	0.0025 (13)	0.0024 (14)	0.0044 (12)
C15	0.0186 (15)	0.0174 (14)	0.0144 (15)	0.0127 (12)	0.0007 (12)	0.0041 (11)
O3	0.0272 (12)	0.0271 (12)	0.0158 (11)	0.0123 (10)	0.0026 (9)	0.0017 (9)
O4	0.0219 (11)	0.0206 (11)	0.0147 (11)	0.0035 (9)	0.0039 (9)	0.0034 (8)

### *Geometric parameters (Å, °)*

Mn1—O1	2.480 (2)	C5—C6	1.399 (4)
Mn1—O2	2.192 (2)	C5—H5A	0.9300
Mn1—O3	2.596 (2)	C6—C7	1.373 (4)
Mn1—O4	2.160 (2)	C6—H6A	0.9300
Mn1—N2	2.262 (2)	C7—C8	1.380 (4)
Mn1—N3	2.235 (2)	C7—H7A	0.9300
Mn1—N4	2.270 (2)	C8—C9	1.469 (4)
N1—C1	1.341 (4)	C9—C10	1.387 (4)
N1—N2	1.349 (3)	C10—C11	1.370 (4)
N1—H1B	0.8600	C10—H10A	0.9300
N2—C3	1.332 (4)	C11—H11A	0.9300
N3—C4	1.347 (3)	C12—C13	1.510 (4)
N3—C8	1.353 (3)	C12—H12A	0.9600
N4—C9	1.336 (3)	C12—H12B	0.9600
N4—N5	1.361 (3)	C12—H12C	0.9600
N5—C11	1.338 (4)	C13—O1	1.233 (3)
N5—H5B	0.8600	C13—O2	1.275 (3)
C1—C2	1.383 (4)	C14—C15	1.512 (4)
C1—H1A	0.9300	C14—H14A	0.9600
C2—C3	1.410 (4)	C14—H14B	0.9600
C2—H2A	0.9300	C14—H14C	0.9600
C3—C4	1.478 (4)	C15—O3	1.241 (3)
C4—C5	1.382 (4)	C15—O4	1.278 (3)
O4—Mn1—O2	85.32 (8)	N3—C4—C5	122.6 (2)
O4—Mn1—N3	135.59 (8)	N3—C4—C3	112.7 (2)
O2—Mn1—N3	138.38 (8)	C5—C4—C3	124.6 (3)
O4—Mn1—N2	103.71 (8)	C4—C5—C6	117.6 (3)
O2—Mn1—N2	111.90 (8)	C4—C5—H5A	121.2
N3—Mn1—N2	71.44 (8)	C6—C5—H5A	121.2
O4—Mn1—N4	103.09 (8)	C7—C6—C5	120.3 (3)
O2—Mn1—N4	95.79 (8)	C7—C6—H6A	119.8
N3—Mn1—N4	71.19 (8)	C5—C6—H6A	119.8
N2—Mn1—N4	142.63 (8)	C6—C7—C8	118.8 (3)
O4—Mn1—O1	140.27 (8)	C6—C7—H7A	120.6
O2—Mn1—O1	55.33 (7)	C8—C7—H7A	120.6
N3—Mn1—O1	84.13 (8)	N3—C8—C7	122.0 (3)
N2—Mn1—O1	88.11 (8)	N3—C8—C9	112.8 (2)
N4—Mn1—O1	87.66 (8)	C7—C8—C9	125.2 (3)
O4—Mn1—O3	54.13 (7)	N4—C9—C10	109.9 (3)
O2—Mn1—O3	139.25 (7)	N4—C9—C8	117.9 (2)

N3—Mn1—O3	81.62 (7)	C10—C9—C8	132.1 (3)
N2—Mn1—O3	84.46 (7)	C11—C10—C9	106.1 (3)
N4—Mn1—O3	90.63 (7)	C11—C10—H10A	127.0
O1—Mn1—O3	165.39 (6)	C9—C10—H10A	127.0
C1—N1—N2	111.6 (2)	N5—C11—C10	107.3 (3)
C1—N1—H1B	124.2	N5—C11—H11A	126.4
N2—N1—H1B	124.2	C10—C11—H11A	126.4
C3—N2—N1	104.9 (2)	C13—C12—H12A	109.5
C3—N2—Mn1	117.16 (17)	C13—C12—H12B	109.5
N1—N2—Mn1	137.93 (18)	H12A—C12—H12B	109.5
C4—N3—C8	118.8 (2)	C13—C12—H12C	109.5
C4—N3—Mn1	120.55 (17)	H12A—C12—H12C	109.5
C8—N3—Mn1	120.66 (18)	H12B—C12—H12C	109.5
C9—N4—N5	105.9 (2)	O1—C13—O2	121.1 (3)
C9—N4—Mn1	117.09 (18)	O1—C13—C12	121.2 (3)
N5—N4—Mn1	136.93 (17)	O2—C13—C12	117.8 (3)
C11—N5—N4	110.9 (2)	C13—O1—Mn1	85.49 (18)
C11—N5—H5B	124.6	C13—O2—Mn1	97.79 (17)
N4—N5—H5B	124.6	C15—C14—H14A	109.5
N1—C1—C2	108.3 (2)	C15—C14—H14B	109.5
N1—C1—H1A	125.8	H14A—C14—H14B	109.5
C2—C1—H1A	125.8	C15—C14—H14C	109.5
C1—C2—C3	103.0 (3)	H14A—C14—H14C	109.5
C1—C2—H2A	128.5	H14B—C14—H14C	109.5
C3—C2—H2A	128.5	O3—C15—O4	121.3 (3)
N2—C3—C2	112.1 (2)	O3—C15—C14	120.6 (3)
N2—C3—C4	118.0 (2)	O4—C15—C14	118.1 (2)
C2—C3—C4	129.8 (3)	C15—O4—Mn1	101.76 (17)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N1—H1B...O4 <sup>i</sup>	0.86	1.91	2.751 (3)	165
N5—H5B...O2 <sup>ii</sup>	0.86	1.85	2.712 (3)	180

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

Fig. 1

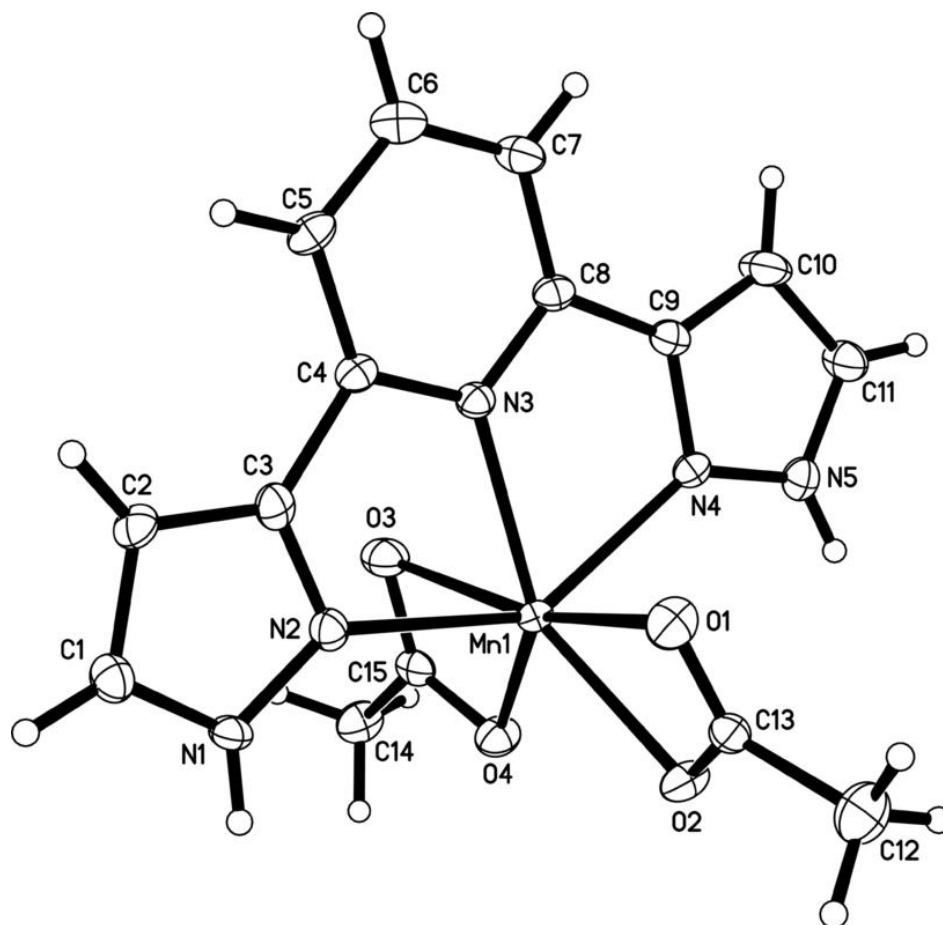




Fig. 2

