Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

cis-Aquabis(di-2-pyridylamine-κ^2N,N')-iodidomanganese(II) iodide

Kwang Ha

School of Applied Chemical Engineering, The Research Institute of Catalysis, Chonnam National University, Gwangju 500-757, Republic of Korea
Correspondence e-mail: hakwang@chonnam.ac.kr

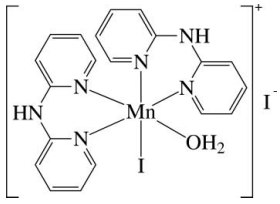
Received 7 November 2011; accepted 9 November 2011

Key indicators: single-crystal X-ray study; T = 200 K; mean σ(C–C) = 0.013 Å; R factor = 0.050; wR factor = 0.134; data-to-parameter ratio = 16.6.

The asymmetric unit of the title compound, $[MnI(C_{10}H_9N_3)_2(H_2O)]I$, contains a cationic Mn^{II} complex and an I^- anion. In the complex, the Mn^{II} ion is six-coordinated in a considerably distorted *cis*-N_4IO octahedral environment defined by four N atoms of the two chelating di-2-pyridylamine (dpa) ligands, one I^- anion and one O atom of a water ligand. As a result of the different *trans* effects of the I, N and O atoms, the Mn—N bond *trans* to the I atom is slightly longer than the Mn—N bond *trans* to the N or O atoms. The dpa ligands are not planar, with dihedral angles between the two pyridine rings of 26.2 (4) and 26.5 (4)°. The complex cations are stacked in columns along the *a* axis and are linked to the anions by intermolecular O—H···I and N—H···I hydrogen bonds.

Related literature

For the crystal structures of related Mn^{II} complexes with dpa, see: Bose *et al.* (2005).



Experimental

Crystal data

$[MnI(C_{10}H_9N_3)_2(H_2O)]I$
M_r = 669.16
Triclinic, $P\overline{1}$
a = 8.598 (3) Å
b = 10.156 (3) Å
c = 13.909 (4) Å
α = 93.091 (6)°
β = 104.402 (6)°
γ = 98.262 (6)°
V = 1159.0 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 3.26 mm^{-1}
T = 200 K
0.28 × 0.23 × 0.19 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.725, T_{max} = 1.000
7310 measured reflections
4509 independent reflections
3069 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.134
S = 1.06
4509 reflections
271 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.01 e Å^{-3}
$\Delta\rho_{min}$ = −1.13 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Mn1—O1	2.164 (6)	Mn1—N6	2.249 (6)
Mn1—N4	2.215 (6)	Mn1—N1	2.312 (6)
Mn1—N3	2.238 (6)	Mn1—I1	2.8785 (15)
N4—Mn1—N6	81.0 (2)	N3—Mn1—N1	78.8 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···I2^{i}	0.84	2.76	3.500 (6)	148
O1—H1B···I1^{ii}	0.84	2.73	3.490 (6)	152
N2—H2N···I2^{iii}	0.92	2.77	3.681 (7)	172
N5—H5N···I2^{iv}	0.92	2.80	3.710 (6)	173

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

This work was supported by the Priority Research Centers Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science and Technology (2010–0029626).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2558).

References

Bose, D., Mostafa, G., Fun, H.-K. & Ghosh, B. K. (2005). *Polyhedron*, **24**, 747–758.
Bruker (2000). *SADABS*, *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

supplementary materials

Acta Cryst. (2011). E**67**, m1751 [**doi:10.1107/S1600536811047349**]

cis-Aquabis(di-2-pyridylamine-κ^2N,N')iodidomanganese(II) iodide

K. Ha

Comment

Cationic Mn^{II} complexes with the di-2-pyridylamine (dpa; $C_{10}H_9N_3$) ligand, such as $[MnX(dpa)_2(H_2O)]ClO_4$ ($X = N_3^-$, NCO^-), have been investigated previously (Bose *et al.*, 2005).

The asymmetric unit of the title compound, $[MnI(dpa)_2(H_2O)]I$, consists of a cationic Mn^{II} complex and an I^- anion (Fig. 1). In the complex, the Mn^{II} ion is six-coordinated in a considerably distorted *cis*-N_4IO octahedral environment defined by four N atoms of the two chelating dpa ligands, one I^- anion and one O atom of a water ligand. The main contribution to the distortion is the tight N—Mn—N chelating angles (Table 1), which results in non-linear *trans* axes [N3—Mn1—N4 = 165.7 (2)° and O1—Mn1—N6 = 171.7 (2)°]. However, the apical I1—Mn1—N1 bond is almost linear with a bond angle of 177.61 (17)°. The Mn—N(dpa) bond lengths are somewhat different and longer than the Mn—O(H_2O) bond (Table 1). As a result of the different *trans* effects of the I, N and O atoms, the Mn1—N1 bond *trans* to the I atom is slightly longer than the Mn—N bond *trans* to the N or O atoms. In the crystal structure, the dpa ligands are not planar. The dihedral angles between the two pyridyl rings of dpa are 26.2 (4)° and 26.5 (4)°.

The complexes are stacked in columns along the *a* axis, and the component cations and anions are linked by intermolecular O—H···I and N—H···I hydrogen bonds (Fig. 2, Table 2). In the column, numerous inter- and intramolecular π-π interactions between the pyridyl rings are present, the shortest centroid-centroid distance being 3.728 (5) Å.

Experimental

To a solution of di-2-pyridylamine (0.3432 g, 2.005 mmol) in acetone (50 ml) was added MnI_2 (0.3108 g, 1.007 mmol) and refluxed for 7 h. The formed precipitate was separated by filtration and washed with acetone, and dried at 323 K, to give a white powder (0.1571 g). Crystals suitable for X-ray analysis were obtained by slow evaporation from an MeOH solution.

Refinement

Carbon-bound H atoms were positioned geometrically and allowed to ride on their respective parent atoms [C—H = 0.95 Å and $U_{iso}(H) = 1.2U_{eq}(C)$]. Nitrogen- and oxygen-bound H atoms were located from Fourier difference maps then allowed to ride on their parent atoms in the final cycles of refinement with N—H = 0.92 Å, O—H = 0.84 Å and $U_{iso}(H) = 1.5\ U_{eq}$(N, O). The highest peak (1.01 e $Å^{-3}$) and the deepest hole (-1.13 e $Å^{-3}$) in the difference Fourier map are located 1.01 Å and 0.79 Å from the atoms C8 and I1, respectively.

Figures

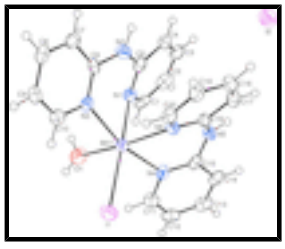


Fig. 1. The molecular structure the title compound, with displacement ellipsoids drawn at the 40% probability level for non-H atoms.

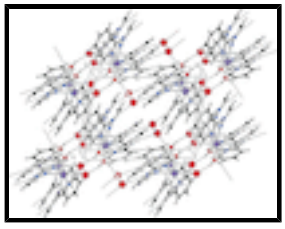


Fig. 2. View of the unit-cell contents of the title compound. Hydrogen-bond interactions are drawn with dashed lines.

cis-Aquabis(di-2-pyridylamine-κ^2N,N')iodidomanganese(II) iodide

Crystal data

$[MnI(C_{10}H_9N_3)_2(H_2O)]I$	$Z = 2$
$M_r = 669.16$	$F(000) = 642$
Triclinic, $P\overline{1}$	$D_x = 1.917$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 8.598$ (3) Å	Cell parameters from 2534 reflections
$b = 10.156$ (3) Å	$\theta = 2.5$–$25.7°$
$c = 13.909$ (4) Å	$\mu = 3.26$ mm^{-1}
$\alpha = 93.091$ (6)°	$T = 200$ K
$\beta = 104.402$ (6)°	Block, colorless
$\gamma = 98.262$ (6)°	0.28 × 0.23 × 0.19 mm
$V = 1159.0$ (6) Å^3	

Data collection

Bruker SMART 1000 CCD diffractometer	4509 independent reflections
Radiation source: fine-focus sealed tube	3069 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.041$
φ and ω scans	$\theta_{max} = 26.0°$, $\theta_{min} = 2.0°$
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)	$h = -9 \rightarrow 10$
$T_{min} = 0.725$, $T_{max} = 1.000$	$k = -12 \rightarrow 12$
7310 measured reflections	$l = -17 \rightarrow 15$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.050$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.134$	H-atom parameters constrained
$S = 1.06$	$w = 1/[\sigma^2(F_o^2) + (0.0448P)^2 + 2.3714P]$ where $P = (F_o^2 + 2F_c^2)/3$
4509 reflections	$(\Delta/\sigma)_{max} < 0.001$
271 parameters	$\Delta\rho_{max} = 1.01$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -1.13$ e Å^{-3}

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	0.92450 (15)	0.83226 (11)	0.17727 (9)	0.0334 (3)
I1	0.70020 (7)	0.84510 (6)	−0.01259 (4)	0.0439 (2)
O1	1.0782 (8)	1.0190 (6)	0.1727 (5)	0.0597 (19)
H1A	1.1370	1.0566	0.2276	0.090*
H1B	1.1097	1.0741	0.1359	0.090*
N1	1.0972 (8)	0.8255 (6)	0.3329 (5)	0.0330 (15)
N2	0.8918 (8)	0.8161 (7)	0.4170 (5)	0.0399 (17)
H2N	0.8627	0.7822	0.4712	0.060*
N3	0.7974 (8)	0.9327 (6)	0.2754 (5)	0.0362 (16)
N4	1.0645 (8)	0.7020 (6)	0.1115 (5)	0.0320 (15)
N5	1.0185 (8)	0.5213 (6)	0.2056 (5)	0.0348 (16)
H5N	1.0725	0.4583	0.2387	0.052*
N6	0.7948 (8)	0.6322 (6)	0.1996 (5)	0.0318 (15)
C1	1.2452 (10)	0.7983 (8)	0.3321 (6)	0.040 (2)
H1	1.2943	0.8345	0.2831	0.048*
C2	1.3298 (11)	0.7210 (10)	0.3981 (7)	0.051 (3)
H2	1.4363	0.7076	0.3966	0.061*
C3	1.2553 (12)	0.6636 (9)	0.4664 (7)	0.048 (2)

H3	1.3062	0.6038	0.5094	0.057*
C4	1.1086 (11)	0.6936 (8)	0.4715 (6)	0.040 (2)
H4	1.0567	0.6577	0.5194	0.048*
C5	1.0354 (10)	0.7785 (8)	0.4046 (6)	0.0348 (19)
C6	0.7953 (9)	0.9056 (7)	0.3694 (6)	0.0304 (18)
C7	0.6994 (10)	0.9603 (8)	0.4199 (6)	0.0371 (19)
H7	0.7061	0.9430	0.4872	0.045*
C8	0.5937 (10)	1.0399 (8)	0.3740 (7)	0.040 (2)
H8	0.5243	1.0762	0.4082	0.048*
C9	0.5890 (11)	1.0668 (8)	0.2771 (6)	0.042 (2)
H9	0.5148	1.1198	0.2424	0.051*
C10	0.6939 (11)	1.0151 (8)	0.2330 (6)	0.042 (2)
H10	0.6950	1.0382	0.1679	0.050*
C11	1.1421 (10)	0.7549 (9)	0.0432 (6)	0.038 (2)
H11	1.1232	0.8405	0.0232	0.046*
C12	1.2430 (10)	0.6932 (10)	0.0028 (6)	0.046 (2)
H12	1.2942	0.7343	−0.0436	0.055*
C13	1.2698 (10)	0.5664 (10)	0.0317 (6)	0.046 (2)
H13	1.3415	0.5209	0.0055	0.055*
C14	1.1937 (10)	0.5088 (9)	0.0966 (6)	0.041 (2)
H14	1.2095	0.4222	0.1155	0.050*
C15	1.0906 (9)	0.5798 (7)	0.1355 (6)	0.0314 (18)
C16	0.8692 (9)	0.5266 (7)	0.2229 (6)	0.0303 (18)
C17	0.7977 (11)	0.4190 (8)	0.2649 (6)	0.042 (2)
H17	0.8529	0.3454	0.2814	0.050*
C18	0.6502 (12)	0.4210 (8)	0.2814 (6)	0.046 (2)
H18	0.6030	0.3504	0.3125	0.055*
C19	0.5665 (10)	0.5270 (8)	0.2529 (6)	0.038 (2)
H19	0.4609	0.5288	0.2620	0.046*
C20	0.6419 (9)	0.6271 (8)	0.2117 (6)	0.0312 (18)
H20	0.5845	0.6979	0.1900	0.037*
I2	0.23491 (7)	0.28327 (5)	0.35974 (4)	0.03842 (18)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0398 (7)	0.0302 (6)	0.0334 (7)	0.0067 (6)	0.0144 (6)	0.0048 (5)
I1	0.0482 (4)	0.0497 (4)	0.0375 (3)	0.0134 (3)	0.0131 (3)	0.0129 (3)
O1	0.084 (5)	0.040 (3)	0.054 (4)	−0.021 (3)	0.034 (4)	−0.003 (3)
N1	0.034 (4)	0.031 (4)	0.033 (4)	−0.001 (3)	0.012 (3)	0.000 (3)
N2	0.043 (4)	0.047 (4)	0.036 (4)	0.015 (3)	0.016 (3)	0.011 (3)
N3	0.045 (4)	0.031 (4)	0.040 (4)	0.017 (3)	0.018 (3)	0.002 (3)
N4	0.030 (4)	0.026 (3)	0.042 (4)	0.003 (3)	0.014 (3)	−0.001 (3)
N5	0.034 (4)	0.033 (4)	0.042 (4)	0.013 (3)	0.013 (3)	0.011 (3)
N6	0.035 (4)	0.028 (3)	0.029 (4)	0.002 (3)	0.005 (3)	0.005 (3)
C1	0.031 (5)	0.051 (5)	0.032 (5)	−0.003 (4)	0.008 (4)	−0.017 (4)
C2	0.032 (5)	0.064 (6)	0.051 (6)	0.013 (5)	0.003 (4)	−0.014 (5)
C3	0.057 (6)	0.048 (5)	0.037 (5)	0.021 (5)	0.002 (5)	−0.003 (4)

C4	0.054 (6)	0.030 (4)	0.033 (5)	0.002 (4)	0.009 (4)	0.001 (4)
C5	0.032 (5)	0.031 (4)	0.037 (5)	0.003 (4)	0.004 (4)	−0.004 (4)
C6	0.031 (4)	0.019 (4)	0.040 (5)	−0.002 (3)	0.009 (4)	0.005 (3)
C7	0.039 (5)	0.036 (5)	0.039 (5)	0.005 (4)	0.018 (4)	−0.002 (4)
C8	0.037 (5)	0.031 (4)	0.055 (6)	0.010 (4)	0.015 (4)	−0.005 (4)
C9	0.056 (6)	0.030 (4)	0.043 (5)	0.018 (4)	0.011 (4)	0.008 (4)
C10	0.053 (6)	0.039 (5)	0.038 (5)	0.011 (4)	0.019 (4)	0.005 (4)
C11	0.031 (5)	0.047 (5)	0.041 (5)	0.006 (4)	0.015 (4)	0.005 (4)
C12	0.036 (5)	0.070 (6)	0.034 (5)	0.000 (5)	0.015 (4)	0.005 (5)
C13	0.027 (5)	0.073 (7)	0.040 (5)	0.016 (4)	0.011 (4)	−0.008 (5)
C14	0.033 (5)	0.047 (5)	0.039 (5)	0.011 (4)	−0.001 (4)	−0.011 (4)
C15	0.019 (4)	0.031 (4)	0.036 (4)	−0.003 (3)	0.000 (3)	−0.011 (4)
C16	0.035 (4)	0.023 (4)	0.029 (4)	0.001 (3)	0.002 (3)	0.002 (3)
C17	0.042 (5)	0.032 (4)	0.051 (5)	0.013 (4)	0.007 (4)	0.005 (4)
C18	0.062 (6)	0.034 (5)	0.040 (5)	−0.006 (4)	0.017 (5)	0.006 (4)
C19	0.038 (5)	0.035 (5)	0.042 (5)	0.004 (4)	0.014 (4)	−0.002 (4)
C20	0.025 (4)	0.038 (4)	0.034 (4)	0.014 (4)	0.007 (3)	0.003 (4)
I2	0.0426 (3)	0.0392 (3)	0.0373 (3)	0.0124 (3)	0.0130 (2)	0.0094 (2)

Geometric parameters (Å, °)

Mn1—O1	2.164 (6)	C3—H3	0.9500
Mn1—N4	2.215 (6)	C4—C5	1.399 (11)
Mn1—N3	2.238 (6)	C4—H4	0.9500
Mn1—N6	2.249 (6)	C6—C7	1.364 (10)
Mn1—N1	2.312 (6)	C7—C8	1.366 (11)
Mn1—I1	2.8785 (15)	C7—H7	0.9500
O1—H1A	0.8400	C8—C9	1.383 (12)
O1—H1B	0.8400	C8—H8	0.9500
N1—C5	1.321 (10)	C9—C10	1.356 (11)
N1—C1	1.343 (9)	C9—H9	0.9500
N2—C5	1.391 (10)	C10—H10	0.9500
N2—C6	1.401 (9)	C11—C12	1.349 (11)
N2—H2N	0.9200	C11—H11	0.9500
N3—C6	1.355 (10)	C12—C13	1.403 (13)
N3—C10	1.359 (10)	C12—H12	0.9500
N4—C15	1.338 (10)	C13—C14	1.351 (12)
N4—C11	1.381 (10)	C13—H13	0.9500
N5—C16	1.371 (10)	C14—C15	1.407 (11)
N5—C15	1.395 (10)	C14—H14	0.9500
N5—H5N	0.9200	C16—C17	1.403 (11)
N6—C16	1.339 (9)	C17—C18	1.347 (12)
N6—C20	1.361 (9)	C17—H17	0.9500
C1—C2	1.378 (12)	C18—C19	1.401 (11)
C1—H1	0.9500	C18—H18	0.9500
C2—C3	1.382 (13)	C19—C20	1.356 (11)
C2—H2	0.9500	C19—H19	0.9500
C3—C4	1.358 (12)	C20—H20	0.9500
O1—Mn1—N4	96.3 (2)	N1—C5—N2	119.4 (7)

O1—Mn1—N3	91.1 (2)	N1—C5—C4	123.5 (8)
N4—Mn1—N3	165.7 (2)	N2—C5—C4	117.1 (8)
O1—Mn1—N6	171.7 (2)	N3—C6—C7	122.5 (7)
N4—Mn1—N6	81.0 (2)	N3—C6—N2	119.7 (7)
N3—Mn1—N6	89.9 (2)	C7—C6—N2	117.8 (7)
O1—Mn1—N1	85.5 (2)	C6—C7—C8	120.1 (8)
N4—Mn1—N1	89.6 (2)	C6—C7—H7	120.0
N3—Mn1—N1	78.8 (2)	C8—C7—H7	120.0
N6—Mn1—N1	86.7 (2)	C7—C8—C9	119.0 (8)
O1—Mn1—I1	94.82 (18)	C7—C8—H8	120.5
N4—Mn1—I1	92.68 (17)	C9—C8—H8	120.5
N3—Mn1—I1	98.81 (18)	C10—C9—C8	117.8 (8)
N6—Mn1—I1	93.11 (16)	C10—C9—H9	121.1
N1—Mn1—I1	177.61 (17)	C8—C9—H9	121.1
Mn1—O1—H1A	116.6	C9—C10—N3	124.7 (8)
Mn1—O1—H1B	145.6	C9—C10—H10	117.6
H1A—O1—H1B	97.7	N3—C10—H10	117.6
C5—N1—C1	116.5 (7)	C12—C11—N4	124.4 (8)
C5—N1—Mn1	118.9 (5)	C12—C11—H11	117.8
C1—N1—Mn1	114.9 (5)	N4—C11—H11	117.8
C5—N2—C6	131.9 (7)	C11—C12—C13	117.8 (8)
C5—N2—H2N	112.5	C11—C12—H12	121.1
C6—N2—H2N	115.2	C13—C12—H12	121.1
C6—N3—C10	115.7 (7)	C14—C13—C12	120.1 (8)
C6—N3—Mn1	126.3 (5)	C14—C13—H13	119.9
C10—N3—Mn1	117.4 (5)	C12—C13—H13	119.9
C15—N4—C11	115.9 (7)	C13—C14—C15	118.6 (8)
C15—N4—Mn1	126.9 (5)	C13—C14—H14	120.7
C11—N4—Mn1	117.1 (5)	C15—C14—H14	120.7
C16—N5—C15	130.6 (6)	N4—C15—N5	119.0 (7)
C16—N5—H5N	114.2	N4—C15—C14	123.1 (8)
C15—N5—H5N	114.4	N5—C15—C14	117.8 (7)
C16—N6—C20	117.4 (7)	N6—C16—N5	120.3 (7)
C16—N6—Mn1	123.8 (5)	N6—C16—C17	121.6 (8)
C20—N6—Mn1	117.2 (5)	N5—C16—C17	118.2 (7)
N1—C1—C2	123.8 (8)	C18—C17—C16	119.3 (8)
N1—C1—H1	118.1	C18—C17—H17	120.3
C2—C1—H1	118.1	C16—C17—H17	120.3
C1—C2—C3	118.1 (9)	C17—C18—C19	120.1 (8)
C1—C2—H2	121.0	C17—C18—H18	120.0
C3—C2—H2	121.0	C19—C18—H18	120.0
C4—C3—C2	119.2 (8)	C20—C19—C18	117.5 (8)
C4—C3—H3	120.4	C20—C19—H19	121.3
C2—C3—H3	120.4	C18—C19—H19	121.3
C3—C4—C5	118.5 (8)	C19—C20—N6	124.0 (7)
C3—C4—H4	120.8	C19—C20—H20	118.0
C5—C4—H4	120.8	N6—C20—H20	118.0
O1—Mn1—N1—C5	142.6 (6)	Mn1—N1—C5—C4	138.1 (6)
N4—Mn1—N1—C5	−121.0 (6)	C6—N2—C5—N1	−4.3 (12)

N3—Mn1—N1—C5	50.6 (6)	C6—N2—C5—C4	174.6 (7)
N6—Mn1—N1—C5	−40.0 (6)	C3—C4—C5—N1	3.9 (12)
O1—Mn1—N1—C1	−72.4 (6)	C3—C4—C5—N2	−174.9 (7)
N4—Mn1—N1—C1	23.9 (6)	C10—N3—C6—C7	−1.9 (11)
N3—Mn1—N1—C1	−164.5 (6)	Mn1—N3—C6—C7	−172.1 (6)
N6—Mn1—N1—C1	105.0 (6)	C10—N3—C6—N2	176.7 (7)
O1—Mn1—N3—C6	−117.8 (6)	Mn1—N3—C6—N2	6.5 (10)
N4—Mn1—N3—C6	3.7 (14)	C5—N2—C6—N3	26.0 (12)
N6—Mn1—N3—C6	54.0 (6)	C5—N2—C6—C7	−155.4 (8)
N1—Mn1—N3—C6	−32.6 (6)	N3—C6—C7—C8	3.7 (12)
I1—Mn1—N3—C6	147.1 (6)	N2—C6—C7—C8	−174.9 (7)
O1—Mn1—N3—C10	72.1 (6)	C6—C7—C8—C9	−1.8 (12)
N4—Mn1—N3—C10	−166.3 (8)	C7—C8—C9—C10	−1.7 (12)
N6—Mn1—N3—C10	−116.1 (6)	C8—C9—C10—N3	3.7 (13)
N1—Mn1—N3—C10	157.3 (6)	C6—N3—C10—C9	−1.9 (12)
I1—Mn1—N3—C10	−22.9 (6)	Mn1—N3—C10—C9	169.2 (7)
O1—Mn1—N4—C15	143.8 (6)	C15—N4—C11—C12	−1.9 (12)
N3—Mn1—N4—C15	22.8 (14)	Mn1—N4—C11—C12	174.1 (7)
N6—Mn1—N4—C15	−28.3 (6)	N4—C11—C12—C13	0.6 (13)
N1—Mn1—N4—C15	58.4 (6)	C11—C12—C13—C14	1.1 (13)
I1—Mn1—N4—C15	−121.0 (6)	C12—C13—C14—C15	−1.2 (12)
O1—Mn1—N4—C11	−31.7 (6)	C11—N4—C15—N5	178.8 (7)
N3—Mn1—N4—C11	−152.7 (9)	Mn1—N4—C15—N5	3.2 (10)
N6—Mn1—N4—C11	156.2 (6)	C11—N4—C15—C14	1.6 (11)
N1—Mn1—N4—C11	−117.1 (6)	Mn1—N4—C15—C14	−173.9 (5)
I1—Mn1—N4—C11	63.4 (5)	C16—N5—C15—N4	36.6 (11)
N4—Mn1—N6—C16	36.5 (6)	C16—N5—C15—C14	−146.2 (8)
N3—Mn1—N6—C16	−132.5 (6)	C13—C14—C15—N4	−0.2 (12)
N1—Mn1—N6—C16	−53.7 (6)	C13—C14—C15—N5	−177.3 (7)
I1—Mn1—N6—C16	128.7 (6)	C20—N6—C16—N5	175.3 (7)
N4—Mn1—N6—C20	−158.5 (6)	Mn1—N6—C16—N5	−19.7 (9)
N3—Mn1—N6—C20	32.5 (5)	C20—N6—C16—C17	−4.4 (10)
N1—Mn1—N6—C20	111.3 (5)	Mn1—N6—C16—C17	160.5 (6)
I1—Mn1—N6—C20	−66.3 (5)	C15—N5—C16—N6	−27.0 (12)
C5—N1—C1—C2	2.9 (11)	C15—N5—C16—C17	152.7 (8)
Mn1—N1—C1—C2	−142.9 (7)	N6—C16—C17—C18	0.6 (12)
N1—C1—C2—C3	2.8 (12)	N5—C16—C17—C18	−179.2 (8)
C1—C2—C3—C4	−5.2 (13)	C16—C17—C18—C19	2.7 (12)
C2—C3—C4—C5	2.1 (12)	C17—C18—C19—C20	−2.0 (12)
C1—N1—C5—N2	172.5 (6)	C18—C19—C20—N6	−2.1 (12)
Mn1—N1—C5—N2	−43.2 (9)	C16—N6—C20—C19	5.3 (11)
C1—N1—C5—C4	−6.3 (11)	Mn1—N6—C20—C19	−160.7 (6)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1A···I2^{i}	0.84	2.76	3.500 (6)	148.
O1—H1B···I1^{ii}	0.84	2.73	3.490 (6)	152.

N2—H2N···I2^{iii}	0.92	2.77	3.681 (7)	172.
N5—H5N···I2^{iv}	0.92	2.80	3.710 (6)	173.

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

Fig. 1

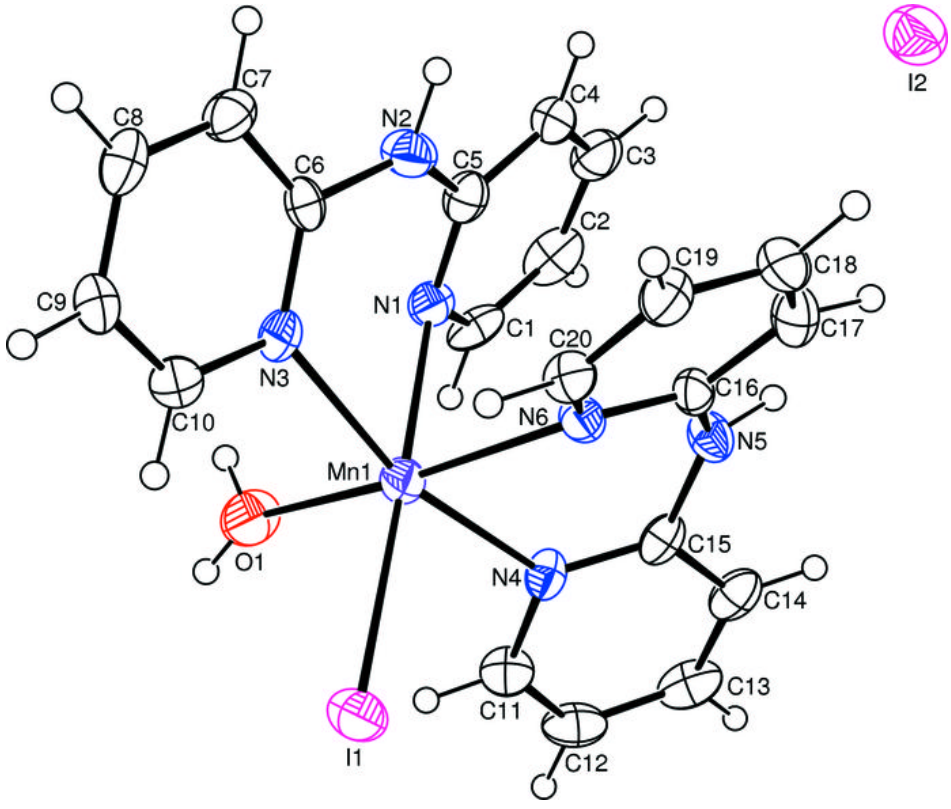

I2
C7
C8
N2
C4
C6
C5
C3
C2
C19
C18
C9
N1
C1
C17
C20
N3
C16
N6
C10
N5
Mn1
O1
C15
N4
C14
C13
C11
I1
C12

Fig. 2