metal-organic compounds

Hexaaquamanganese(II) dipicrate dihydrate

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In the title compound, $[Mn(H_2O)_6](C_6H_2N_3O_7)_2 \cdot 2H_2O$, the manganese cation, on an inversion centre, is coordinated by six water molecules, but the picrate anion has no coordinative interaction with the manganese cation. The anions in the stack are linked via short intermolecular $O \cdots C$ (3.013 and 2.973 Å) and $C \cdots C$ (3.089 and 3.065 Å) contacts and hydrogen bonds.

Related literature

For related literature, see: Bibal et al. (2003); García et al. (2004); Harrowfield et al. (1995a,b); Honda et al. (2003); Ji & Chen (1996); Maartmann-Moe (1969); Olsher et al. (1996); Yang et al. (2001); Zhang et al. (2003).

$[Mn(H_2O)_6]^{2+} \cdot$

$\left[\begin{array}{c} O^- \\ O_2N \quad\quad NO_2 \\ \\ NO_2 \end{array} \right]_2$
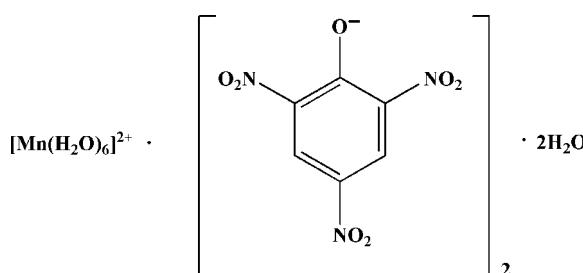
$\cdot 2H_2O$

Experimental

Crystal data

$[Mn(H_2O)_6](C_6H_2N_3O_7)_2 \cdot 2H_2O$
$M_r = 655.28$
Orthorhombic, $Pccn$
$a = 25.344$ (6) Å
$b = 7.1625$ (17) Å
$c = 13.217$ (3) Å

$V = 2399.2$ (9) Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 0.67$ mm^{-1}
$T = 294$ (2) K
$0.28 \times 0.24 \times 0.20$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.835$, $T_{max} = 0.878$

11295 measured reflections
2122 independent reflections
1643 reflections with $I > 2\sigma(I)$
$R_{int} = 0.033$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.158$
$S = 1.11$
2122 reflections
211 parameters
8 restraints

H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max} = 0.50$ e Å^{-3}
$\Delta\rho_{min} = -1.20$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Mn1—O1	2.120 (3)	Mn1—O2	2.190 (2)
Mn1—O3	2.136 (3)		
O1—Mn1—O3	91.52 (11)	O3^i—Mn1—O2^i	86.83 (11)
O1—Mn1—O3^i	88.48 (11)	O1—Mn1—O2	86.98 (11)
O1—Mn1—O2^i	93.02 (11)	O3^i—Mn1—O2	93.17 (11)

Symmetry code: (i) $-x + 1, -y, -z + 1$.

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1$A\cdots$O11^{ii}	0.846 (10)	1.938 (12)	2.780 (4)	173 (4)
O1—H1$B\cdots$O10^{iii}	0.852 (10)	2.10 (2)	2.906 (4)	157 (4)
O2—H2$A\cdots$O10^{iv}	0.848 (10)	2.048 (12)	2.889 (4)	172 (4)
O2—H2$A\cdots$O9^{iv}	0.848 (10)	2.53 (4)	2.986 (4)	115 (3)
O3—H3$A\cdots$O11^v	0.832 (10)	1.951 (12)	2.782 (4)	176 (5)
O3—H3$B\cdots$O6^{vi}	0.841 (10)	2.047 (12)	2.884 (4)	174 (5)
O11—H11$A\cdots$O2^{vii}	0.847 (10)	2.213 (19)	3.006 (4)	156 (4)
O11—H11$B\cdots$O10^{viii}	0.846 (10)	2.17 (2)	2.938 (4)	151 (4)
O11—H11$B\cdots$O4^{viii}	0.846 (10)	2.27 (3)	2.913 (4)	133 (4)
O2—H2$B\cdots$O4^{ix}	0.841 (10)	2.143 (19)	2.930 (4)	156 (4)

Symmetry codes: (ii) $x, -y + \frac{3}{2}, z - \frac{1}{2}$; (iii) $x, -y + \frac{3}{2}, z + \frac{1}{2}$; (iv) $-x + 1, y - \frac{1}{2}, -z + \frac{1}{2}$; (v) $x, y - 1, z$; (vi) $-x + \frac{1}{2}, y - 1, z + \frac{1}{2}$; (vii) $-x + 1, y + \frac{1}{2}, -z + \frac{3}{2}$; (viii) $-x + 1, -y + 2, -z + 1$; (ix) $-x + 1, -y + 1, -z + 1$.

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

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supporting information

Hexaaquamanganese(II) dipicrate dihydrate

Changying Liu, Xiufang Shi, Bin Du, Chunli Wu and Mingjie Zhang

S1. Comment

Picrate is commonly used as an accompanying ion in many systems involving extraction and transport of metal ions to improve the extractability and selectivity (Zhang *et al.*, 2003; Bibal *et al.*, 2003; García *et al.*, 2004). In many structures, picrate interacts as monodentate, bidentate and tridentate ligand (Olsher *et al.*, 1996). Besides, picrate is a penta-dentate ligand when it coordinates with sodium or potassium cation by chelating pairs of oxygen atoms from *p*-nitro groups of adjacent picrates, and with successive cation linking the array into two or three-dimensional network (Harrowfield *et al.*, 1995*a*; Maartmann-Moe, 1969). Furthermore, the picrate interacts as a heptadentate ligand through all its available oxygen donor atoms to coordinate with caesium (Harrowfield *et al.*, 1995*a*).

Fig. 1 shows the structure and the atomic numbering schemes of the crystal structure of the title manganese picrate complex (I). This situation is similar to the crystal structure of iron (II) picrate (Honda *et al.*, 2003) and Magnesium (II) picrate (Harrowfield *et al.*, 1995*b*) and the picrate anion adopts a keto form with C6—O10 bond distance of 1.257 (4) Å, C1—C6 and C5—C6 bond distance of 1.447 (5) and 1.456 (5) Å, respectively, which is longer than the other C—C bond lengths (between 1.374 (5) to 1.460 (4) Å) in the benzene ring. The Mn—O distance ranges from 2.120 (2) to 2.190 (2) Å. The bond angle C1—C6—C5 is 111.9 (3)°, which is the case in some picrate complexes, while the corresponding bond angle of picric acid is 116.4 (5)° (Yang *et al.*, 2001). Selected bond lengths and angles are given in Table 1.

In the case of planarity of picrate anion, the *ortho* nitro group are twisted relative to the plane of the benzene ring, (between 19.01 and 27.69°), while *para*-positioned nitro group is deviated 13.02° off the benzene ring. The picrate ions are stacked head-to-tail, presumably as a result of charge-transfer interactions. The anion in the stack are linked *via* short intermolecular O···C and C···C contacts of 3.013, 2.973, 3.089 and 3.065Å for O6···C1^x, O7···C5^{xi}, C2···C2^x and C4···C4^{xi} [symmetry codes: (*x*) 1/2 - *x*, 3/2 - *y*, *z*; (xi) 1/2 - *x*, 5/2 - *y*, *z*] respectively (Fig.2). The picrate anions are not parallel to one another, and the dihedral angles between neighbouring benzene planes are 25.01°, 25.25° and 3.48° respectively.

S2. Experimental

The title compound (I) was obtained by the reaction of 3.20 g (13.96 mmol) picric acid with 0.80 g (6.98 mmol) manganese carbonate in water (350 ml), according to Ji *et al.*, 1996. Heating has been continued for another 1 h and filtered while it was still hot. The filtrate was partially evaporated and left to stand in open atmosphere for a few days, during which time, yellow crystals suitable for X-Ray determination were obtained. Analysis, calculated for $C_{12}H_{20}N_6O_{22}Mn$: C 21.98, H 3.05, N 12.80, Mn 8.40%; Found: C 22.35, H 3.34, N 12.46, Mn 8.68%.

S3. Refinement

All H atoms of water were located from difference map and then refined with O—H distances restrained to 0.85 (1) Å. All other H atoms were positioned geometrically and refined using a riding mode with the C—H bond lengths of 0.93 Å and U_{iso}(H)=1.2U_{eq}(carrier atom).
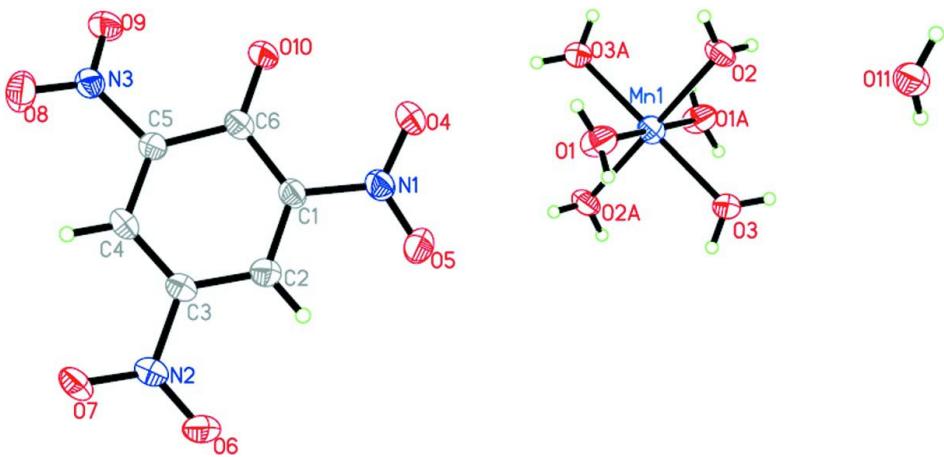
Figure 1

The molecular structure of (I), with displacement ellipsoids at the 50% probability level and the atomic labeling scheme.
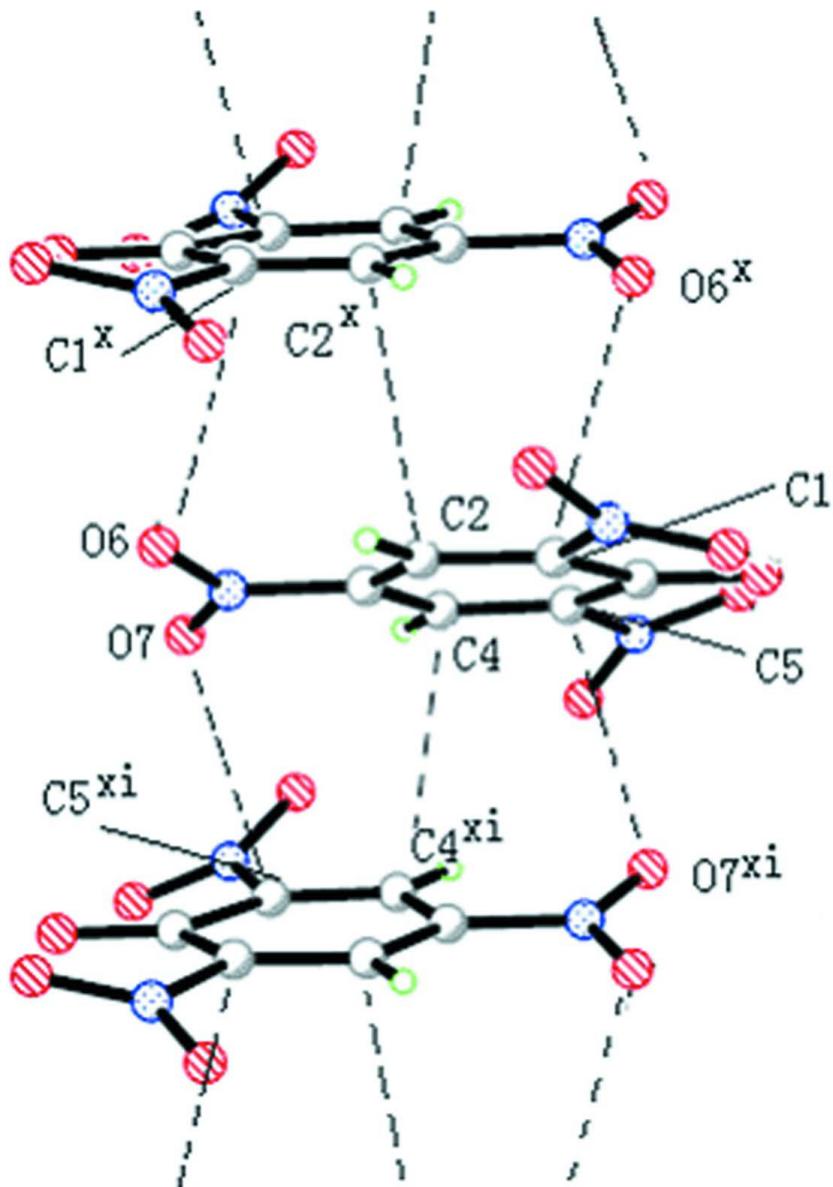
Figure 2

The crystal structure of (I), projected along the c axis. The dashed lines indicate short intermolecular contacts with N···O, C···C and O···C distances less than 3.0, 3.2 and 3.0 Å, respectively. [Symmetry mode: (x) 1/2 - x, 3/2 - y, z; (xi) 1/2 - x, 5/2 - y, z]

Hexaaquamanganese(II) dipicrate dihydrate

Crystal data

$[Mn(H_2O)_6](C_6H_2N_3O_7)_2 \cdot 2H_2O$	$V = 2399.2\ (9)$ Å^3
$M_r = 655.28$	$Z = 4$
Orthorhombic, $Pccn$	$F(000) = 1340$
Hall symbol: -P 2ab 2ac	$D_x = 1.814$ Mg m^{-3}
$a = 25.344\ (6)$ Å	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$b = 7.1625\ (17)$ Å	Cell parameters from 3819 reflections
$c = 13.217\ (3)$ Å	$\theta = 3.0–26.9°$

$\mu = 0.67$ mm^{-1}

$T = 294$ K

Prism, yellow

$0.28 \times 0.24 \times 0.20$ mm

Data collection

Bruker SMART CCD area-detector diffractometer	11295 measured reflections
Radiation source: fine-focus sealed tube	2122 independent reflections
Graphite monochromator	1643 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.033$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$\theta_{max} = 25.0°$, $\theta_{min} = 3.0°$
	$h = -30 \rightarrow 20$
$T_{min} = 0.835$, $T_{max} = 0.878$	$k = -6 \rightarrow 8$
	$l = -14 \rightarrow 15$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.047$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.158$	
$S = 1.11$	H atoms treated by a mixture of independent and constrained refinement
2122 reflections	
211 parameters	$w = 1/[\sigma^2(F_o^2) + (0.1031P)^2 + 1.8926P]$ where $P = (F_o^2 + 2F_c^2)/3$
8 restraints	
Primary atom site location: structure-invariant direct methods	$(\Delta/\sigma)_{max} = 0.002$
	$\Delta\rho_{max} = 0.50$ e Å^{-3}
	$\Delta\rho_{min} = -1.20$ 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	0.5000	0.0000	0.5000	0.0324 (3)
O1	0.46126 (10)	0.2424 (4)	0.4457 (2)	0.0421 (7)
H1A	0.4744 (16)	0.322 (5)	0.406 (3)	0.051*
H1B	0.4352 (12)	0.300 (6)	0.472 (3)	0.051*
O2	0.55826 (9)	0.1880 (4)	0.56780 (19)	0.0330 (6)
H2A	0.5744 (14)	0.275 (4)	0.537 (3)	0.040*
H2B	0.5784 (12)	0.128 (5)	0.606 (2)	0.040*
O3	0.45862 (10)	0.0148 (5)	0.6406 (2)	0.0445 (8)
H3A	0.4722 (18)	0.009 (6)	0.6979 (17)	0.053*
H3B	0.4257 (5)	0.002 (6)	0.637 (4)	0.053*
O4	0.38727 (10)	0.9511 (5)	0.2517 (2)	0.0513 (8)
O5	0.31431 (10)	0.8379 (4)	0.30495 (17)	0.0370 (6)
O6	0.15343 (9)	0.9452 (4)	0.1363 (2)	0.0377 (7)

O7	0.15241 (9)	1.0752 (4)	−0.0108 (2)	0.0394 (7)
O8	0.31310 (10)	1.1774 (4)	−0.18909 (18)	0.0380 (6)
O9	0.38129 (10)	1.0114 (4)	−0.15080 (19)	0.0366 (7)
O10	0.39594 (9)	0.9860 (4)	0.05051 (18)	0.0341 (6)
N1	0.34078 (10)	0.9135 (4)	0.2395 (2)	0.0283 (7)
N2	0.17602 (11)	1.0079 (4)	0.0613 (2)	0.0251 (7)
N3	0.33772 (10)	1.0754 (4)	−0.1311 (2)	0.0258 (6)
C1	0.31536 (13)	0.9605 (5)	0.1440 (2)	0.0242 (7)
C2	0.26072 (13)	0.9623 (5)	0.1463 (3)	0.0251 (7)
H2	0.2428	0.9370	0.2062	0.030*
C3	0.23318 (13)	1.0019 (4)	0.0588 (2)	0.0235 (7)
C4	0.25917 (13)	1.0386 (4)	−0.0315 (3)	0.0245 (7)
H4	0.2402	1.0684	−0.0895	0.029*
C5	0.31330 (13)	1.0304 (4)	−0.0340 (2)	0.0229 (7)
C6	0.34639 (13)	0.9917 (4)	0.0536 (3)	0.0246 (7)
O11	0.50741 (10)	0.9801 (4)	0.8282 (2)	0.0377 (7)
H11A	0.4971 (15)	0.878 (3)	0.854 (3)	0.045*
H11B	0.5400 (6)	0.982 (6)	0.842 (3)	0.045*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0302 (5)	0.0345 (5)	0.0324 (5)	−0.0018 (3)	−0.0020 (3)	0.0010 (3)
O1	0.0328 (14)	0.0450 (17)	0.0486 (17)	0.0143 (12)	0.0079 (12)	0.0177 (13)
O2	0.0237 (12)	0.0355 (14)	0.0398 (15)	−0.0053 (10)	−0.0081 (10)	0.0038 (11)
O3	0.0233 (14)	0.080 (2)	0.0299 (15)	−0.0049 (13)	0.0010 (11)	0.0035 (14)
O4	0.0246 (14)	0.098 (2)	0.0312 (15)	−0.0061 (14)	−0.0079 (11)	0.0097 (15)
O5	0.0351 (13)	0.0514 (17)	0.0247 (13)	0.0044 (12)	0.0019 (10)	0.0052 (12)
O6	0.0214 (13)	0.0518 (17)	0.0399 (15)	0.0010 (11)	0.0062 (11)	0.0082 (13)
O7	0.0202 (13)	0.0538 (18)	0.0443 (16)	0.0023 (12)	−0.0087 (11)	0.0137 (13)
O8	0.0415 (14)	0.0462 (16)	0.0263 (13)	0.0089 (12)	−0.0015 (11)	0.0059 (12)
O9	0.0194 (13)	0.0578 (18)	0.0325 (14)	0.0028 (11)	0.0030 (10)	−0.0004 (12)
O10	0.0160 (12)	0.0588 (18)	0.0274 (14)	0.0035 (10)	−0.0005 (9)	0.0030 (11)
N1	0.0224 (15)	0.0361 (17)	0.0265 (15)	0.0045 (12)	−0.0018 (12)	−0.0022 (13)
N2	0.0187 (14)	0.0231 (15)	0.0334 (17)	−0.0001 (11)	−0.0012 (12)	−0.0012 (12)
N3	0.0235 (14)	0.0308 (15)	0.0231 (14)	−0.0023 (12)	−0.0018 (11)	−0.0031 (12)
C1	0.0208 (16)	0.0291 (18)	0.0226 (16)	0.0028 (13)	−0.0026 (13)	−0.0010 (14)
C2	0.0218 (17)	0.0265 (18)	0.0269 (17)	0.0002 (13)	0.0015 (13)	−0.0006 (14)
C3	0.0180 (16)	0.0232 (16)	0.0294 (18)	0.0012 (12)	−0.0011 (13)	−0.0019 (13)
C4	0.0204 (17)	0.0259 (17)	0.0271 (17)	0.0018 (13)	−0.0060 (13)	−0.0009 (14)
C5	0.0200 (16)	0.0263 (18)	0.0224 (16)	−0.0011 (13)	0.0000 (13)	−0.0007 (13)
C6	0.0208 (17)	0.0265 (18)	0.0265 (19)	0.0016 (13)	−0.0029 (13)	−0.0023 (13)
O11	0.0303 (15)	0.0455 (17)	0.0374 (16)	−0.0029 (12)	−0.0032 (12)	0.0069 (12)

Geometric parameters (Å, º)

Mn1—O1	2.120 (3)	C1—C2	1.385 (5)
Mn1—O1ⁱ	2.120 (3)	C1—C6	1.447 (5)

Mn1—O3	2.136 (3)	C2—C3	1.380 (5)
Mn1—O3ⁱ	2.136 (3)	C3—C4	1.389 (5)
Mn1—O2	2.190 (2)	C4—C5	1.374 (5)
Mn1—O2	2.190 (2)	C5—C6	1.456 (5)
O4—N1	1.219 (4)	C2—H2	0.931
O5—N1	1.222 (4)	C4—H4	0.931
O6—N2	1.229 (4)	O1—H1A	0.846 (10)
O7—N2	1.225 (4)	O1—H1B	0.852 (10)
O8—N3	1.229 (4)	O2—H2A	0.848 (10)
O9—N3	1.224 (4)	O2—H2B	0.841 (10)
O10—C6	1.257 (4)	O3—H3A	0.832 (10)
N1—C1	1.456 (4)	O3—H3B	0.841 (10)
N2—C3	1.450 (4)	O11—H11A	0.847 (10)
N3—C5	1.460 (4)	O11—H11B	0.846 (10)
O1—Mn1—O1ⁱ	180.0	O9—N3—O8	123.2 (3)
O1—Mn1—O3	91.52 (11)	O9—N3—C5	119.1 (3)
O1ⁱ—Mn1—O3	88.48 (11)	O8—N3—C5	117.7 (3)
O1—Mn1—O3ⁱ	88.48 (11)	C2—C1—C6	124.1 (3)
O1ⁱ—Mn1—O3ⁱ	91.52 (11)	C2—C1—N1	115.1 (3)
O3—Mn1—O3ⁱ	180.0	C6—C1—N1	120.7 (3)
O1—Mn1—O2ⁱ	93.02 (11)	C3—C2—C1	119.3 (3)
O1ⁱ—Mn1—O2ⁱ	86.98 (11)	C2—C3—C4	121.3 (3)
O3—Mn1—O2ⁱ	93.18 (11)	C2—C3—N2	119.5 (3)
O3ⁱ—Mn1—O2ⁱ	86.83 (11)	C4—C3—N2	119.2 (3)
O1—Mn1—O2	86.98 (11)	C5—C4—C3	119.1 (3)
O1ⁱ—Mn1—O2	93.02 (11)	C4—C5—C6	124.4 (3)
O3—Mn1—O2	86.83 (11)	C4—C5—N3	115.8 (3)
O3ⁱ—Mn1—O2	93.17 (11)	C6—C5—N3	119.8 (3)
O2ⁱ—Mn1—O2	180.0	O10—C6—C1	124.4 (3)
O4—N1—O5	122.3 (3)	O10—C6—C5	123.8 (3)
O4—N1—C1	119.5 (3)	C1—C6—C5	111.9 (3)
O5—N1—C1	118.3 (3)	C3—C2—H2	120.36
O7—N2—O6	123.0 (3)	C1—C2—H2	120.37
O7—N2—C3	118.8 (3)	C3—C4—H4	120.43
O6—N2—C3	118.2 (3)	C5—C4—H4	120.41
O4—N1—C1—C2	−162.6 (3)	C3—C4—C5—C6	−2.3 (5)
O5—N1—C1—C2	17.1 (4)	C3—C4—C5—N3	−178.5 (3)
O4—N1—C1—C6	20.8 (5)	O9—N3—C5—C4	−154.6 (3)
O5—N1—C1—C6	−159.6 (3)	O8—N3—C5—C4	25.5 (4)
C6—C1—C2—C3	−2.2 (5)	O9—N3—C5—C6	29.0 (4)
N1—C1—C2—C3	−178.8 (3)	O8—N3—C5—C6	−150.8 (3)
C1—C2—C3—C4	0.5 (5)	C2—C1—C6—O10	−178.3 (3)
C1—C2—C3—N2	−178.7 (3)	N1—C1—C6—O10	−1.9 (5)
O7—N2—C3—C2	167.0 (3)	C2—C1—C6—C5	1.6 (5)
O6—N2—C3—C2	−12.8 (4)	N1—C1—C6—C5	178.0 (3)
O7—N2—C3—C4	−12.2 (4)	C4—C5—C6—O10	−179.4 (3)

O6—N2—C3—C4	168.0 (3)	N3—C5—C6—O10	−3.4 (5)
C2—C3—C4—C5	1.7 (5)	C4—C5—C6—C1	0.7 (4)
N2—C3—C4—C5	−179.1 (3)	N3—C5—C6—C1	176.7 (3)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···O11ii	0.85 (1)	1.94 (1)	2.780 (4)	173 (4)
O1—H1*B*···O10iii	0.85 (1)	2.10 (2)	2.906 (4)	157 (4)
O2—H2*A*···O10iv	0.85 (1)	2.05 (1)	2.889 (4)	172 (4)
O2—H2*A*···O9iv	0.85 (1)	2.53 (4)	2.986 (4)	115 (3)
O3—H3*A*···O11v	0.83 (1)	1.95 (1)	2.782 (4)	176 (5)
O3—H3*B*···O6vi	0.84 (1)	2.05 (1)	2.884 (4)	174 (5)
O11—H11*A*···O2vii	0.85 (1)	2.21 (2)	3.006 (4)	156 (4)
O11—H11*B*···O10viii	0.85 (1)	2.17 (2)	2.938 (4)	151 (4)
O11—H11*B*···O4viii	0.85 (1)	2.27 (3)	2.913 (4)	133 (4)
O2—H2*B*···O4ix	0.84 (1)	2.14 (2)	2.930 (4)	156 (4)

Symmetry codes: (ii) *x*, −*y*+3/2, *z*−1/2; (iii) *x*, −*y*+3/2, *z*+1/2; (iv) −*x*+1, *y*−1/2, −*z*+1/2; (v) *x*, *y*−1, *z*; (vi) −*x*+1/2, *y*−1, *z*+1/2; (vii) −*x*+1, *y*+1/2, −*z*+3/2; (viii) −*x*+1, −*y*+2, −*z*+1; (ix) −*x*+1, −*y*+1, −*z*+1.