

Diaquabis[[1-hydroxy-2-(1*H*-imidazol-3-ium-1-yl)ethane-1,1-diyl]bis(hydrogen phosphonato)]manganese(II)

Zai-Chao Zhang,* Rong-Qing Li and Yu Zhang

Jiangsu Key Laboratory for the Chemistry of Low-dimensional Materials, Department of Chemistry, Huaiyin Teachers College, 111 West Changjiang Road, Huaian 223300, Jiangsu, People's Republic of China

Correspondence e-mail: overloadzz@hotmail.com

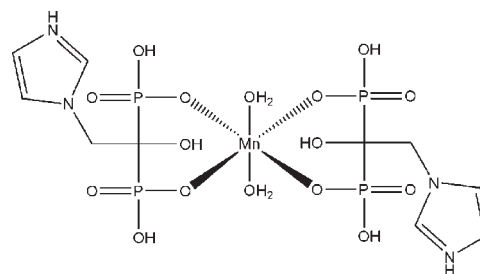
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 Key indicators: single-crystal X-ray study; $T = 153$ K; mean $\sigma(\text{C}-\text{C}) = 0.007$ Å; R factor = 0.052; wR factor = 0.135; data-to-parameter ratio = 10.5.

In the title compound, $[\text{Mn}(\text{C}_5\text{H}_9\text{N}_2\text{O}_7\text{P}_2)_2(\text{H}_2\text{O})_2]$, the Mn^{II} atom (site symmetry $\bar{1}$) is coordinated by four phosphonate O atoms from a pair of partially deprotonated 1-hydroxy-2-(imidazol-3-yl)ethane-1,1-bisphosphonic acid ligands (imhedpH₃[−]) and two water molecules, resulting in a slightly distorted *trans*- MnO_6 octahedral geometry for the metal ion. In the ligands, the imidazole units are protonated and two of the hydroxy O atoms of the phosphonate groups are deprotonated and chelate the Mn^{II} , thus forming the neutral molecule of the title compound. The two protonated O atoms within the phosphonate groups of one imhedpH₃[−] ligand act as hydrogen-bond acceptors for a bifurcated hydrogen bond originating from the coordinated water molecule. The phosphonate units of neighboring molecules are connected with their equivalents in neighboring molecules *via* two types of inversion-symmetric hydrogen-bonding arrangements with four and two strong O—H...O hydrogen bonds, respectively. The two interactions connect molecules into infinite chains along [111] and [110], in combination forming a tightly hydrogen-bonded three-dimensional supramolecular network. This network is further stabilized by additional hydrogen bonds between the protonated imidazole units and one of the coordinated P—O O atoms and by additional O—H...O hydrogen bonds between the water molecules and the P=O O atoms of neighboring molecules.

Related literature

For a review of the structures and applications of lanthanide phosphonates, see: Mao (2007). For other complexes based on the imhedpH₄ ligand, see: Cao *et al.* (2007, 2008). For the structures and properties of some metal organophosphonates, see: Rao *et al.* (2004); Yang *et al.* (2009).



Experimental

Crystal data

$[\text{Mn}(\text{C}_5\text{H}_9\text{N}_2\text{O}_7\text{P}_2)_2(\text{H}_2\text{O})_2]$
 $M_r = 633.14$
 Triclinic, $P\bar{1}$
 $a = 7.4408$ (17) Å
 $b = 8.566$ (2) Å
 $c = 9.680$ (2) Å
 $\alpha = 105.366$ (4)°
 $\beta = 110.865$ (4)°

$\gamma = 97.461$ (4)°
 $V = 538.4$ (2) Å³
 $Z = 1$
 Mo $K\alpha$ radiation
 $\mu = 1.00$ mm^{−1}
 $T = 153$ K
 $0.25 \times 0.20 \times 0.20$ mm

Data collection

Bruker SMART APEXII diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2000)
 $T_{\text{min}} = 0.788$, $T_{\text{max}} = 0.825$

2637 measured reflections
 1829 independent reflections
 1543 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.029$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.052$
 $wR(F^2) = 0.135$
 $S = 0.99$
 1829 reflections
 175 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.49$ e Å^{−3}
 $\Delta\rho_{\text{min}} = -0.46$ e Å^{−3}

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N2}-\text{H2A}\cdots\text{O4}^{\text{i}}$	0.88	1.85	2.718 (5)	167
$\text{O7}-\text{H7A}\cdots\text{O5}^{\text{ii}}$	0.85 (5)	2.07 (5)	2.889 (4)	162 (5)
$\text{O6}-\text{H6A}\cdots\text{O5}^{\text{ii}}$	0.84 (5)	1.82 (5)	2.653 (4)	167 (5)
$\text{O3}-\text{H3A}\cdots\text{O2}^{\text{iii}}$	0.85 (5)	1.74 (5)	2.573 (4)	167 (5)
$\text{O8}-\text{H8A}\cdots\text{O2}^{\text{iv}}$	0.86 (6)	1.88 (6)	2.707 (5)	162 (5)
$\text{O8}-\text{H8B}\cdots\text{O3}$	0.85 (6)	2.32 (6)	3.042 (5)	143 (5)
$\text{O8}-\text{H8B}\cdots\text{O6}$	0.85 (6)	2.59 (6)	3.124 (5)	122 (5)

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

Data collection: APEX2 (Bruker, 2004); cell refinement: SAINT (Bruker, 2004); 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 for Windows (Farrugia, 1997); software used to prepare material for publication: SHELXL97 and PLATON (Spek, 2009).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZL2255).

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supporting information

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Diaquabis{[1-hydroxy-2-(1*H*-imidazol-3-ium-1-yl)ethane-1,1-diyl]bis(hydrogen phosphonato)}manganese(II)

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S1. Comment

Organophosphonic acids have attracted much attention in the field of organic-inorganic hybrid materials because of their flexible coordination modes and strong coordination ability (Mao 2007; Rao *et al.* 2008; Yang *et al.* 2009). Compared to other organophosphonic acid derivatives, there are only few complexes of metal-organic compounds with 1-hydroxy-2-(imidazol-3-yl)ethane-1,1-bisphosphonic acid (imhedpH₄) and its anions as the ligand (Cao *et al.* 2007; Cao *et al.* 2008). Herein, we thus report the synthesis and structure of the title compound, a manganese complex of the monoanion of the aforementioned acid.

The title compound crystallizes in the triclinic system with the space group $P\bar{1}$. The Mn^{II} ion adopts a slightly distorted octahedral geometry and is located on a crystallographic inversion center. Two pairs of phosphonate oxygen atoms (O1, O4, O1ⁱ, O4ⁱ; symmetry code: *i*, $-x$, $-y$, $-z$) from two equivalent imhedpH₃⁻ ligands define the equatorial plane, while two equivalent water molecules (O8 and O8ⁱ) occupy the axial sites. The Mn–O bond lengths are in the range of 2.118 (3)–2.218 (3) Å. In the equatorial plane, the O—Mn—O bond angles are 88.35 (11)–91.65 (11)°. The two imhedpH₃⁻ ligands act as bidentate chelating ligands towards the Mn cation via the two deprotonated phosphonate oxygen atoms O1 and O4, while two of the remaining four phosphonate oxygens are protonated [P1—O3 = 1.565 (3) Å and P2—O6 = 1.572 (3) Å]. These two protonated O atoms O3 and O6 act as a hydrogen bond acceptors for a bifurcated H bond from the coordinated water molecule (O8, see Table 1 for numerical values).

The phosphonate units are connected with their equivalents in neighboring molecules via two types of inversion symmetric hydrogen bonding arrangements (Fig. 2). Phosphonate units of P atom P1 are connecting neighboring molecules along the diagonal of the unit cell by means of four strong O—H \cdots O hydrogen bonds between the P—O—H (O6), C—O—H (O7) and P=O units (O5) of the imhedpH₃⁻ ligands (Table 1). Dimeric P—O—H \cdots O=P connections are formed between the phosphonate units of P2 in neighboring molecules involving O2 and O3. This second interaction connects molecules along the {1 1 0} direction, and both of these strong hydrogen bonding interactions lead to the formation of infinite chains, and in combination to a tightly hydrogen bonded three-dimensional supramolecular network (Fig. 3). This network is further stabilized by additional hydrogen bonds between the protonated imidazole units towards one of the coordinated P–O oxygen atoms (O4) and by additional O—H \cdots O hydrogen bonds between the water molecule and P=O oxygen atoms (O2) of neighboring molecules (Table 1).

S2. Experimental

The title compound was prepared by the hydrothermal reaction of a mixture of MnSO₄ (0.1 mmol), imhedpH₄ (0.1 mmol) and H₂O (8.0 mL) in a Teflon-lined stainless steel autoclave (25 ml), which was heated to 413 K for 48 h. Block-shaped light-pink crystals were collected (yield: 48%, based on imhedpH₄). Anal. calcd for C₁₀H₂₂MnN₄O₁₆P₄ (633.13): C 18.97, H 3.50, N 8.85%; found: C 19.06, H 3.71, N 8.90%.

S3. Refinement

All non-hydrogen atoms were found in Fourier maps and were refined anisotropically. Hydrogen atoms attached to C and N atoms were positioned geometrically with bond distances of 0.95 or 0.99 Å for C—H and 0.88 Å for N—H. Water and hydroxy H atoms were located in a difference Fourier map and refined with distance restraints on all O—H bond lengths with distances of 0.85 (1) Å, and the H···H distance within the water molecule was restrained to 1.55 (2) Å. The isotropic displacement parameters of H atoms are related to the non-H atom to which they are bonded, *viz.* $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{parent})$.

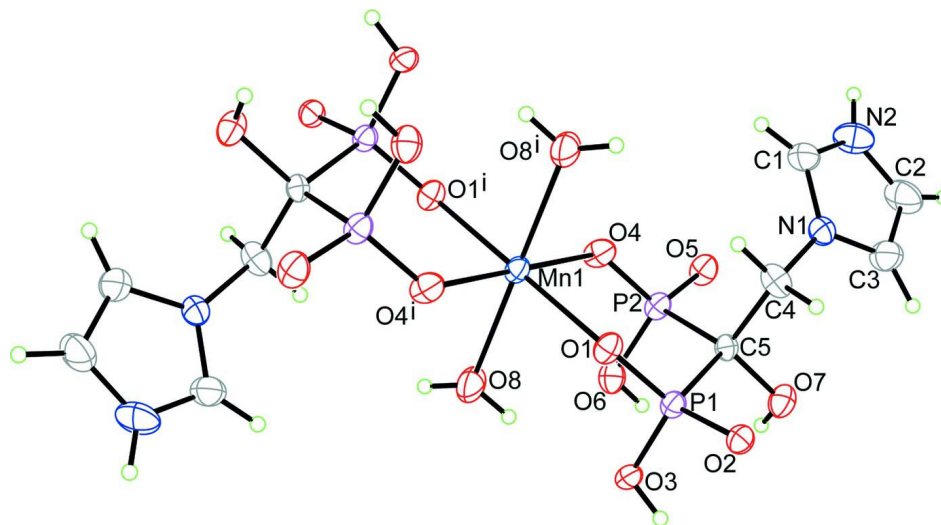


Figure 1

The molecular view of the title compound with atomic labeling scheme (50% probability, symmetry code: i, -x, -y, -z).

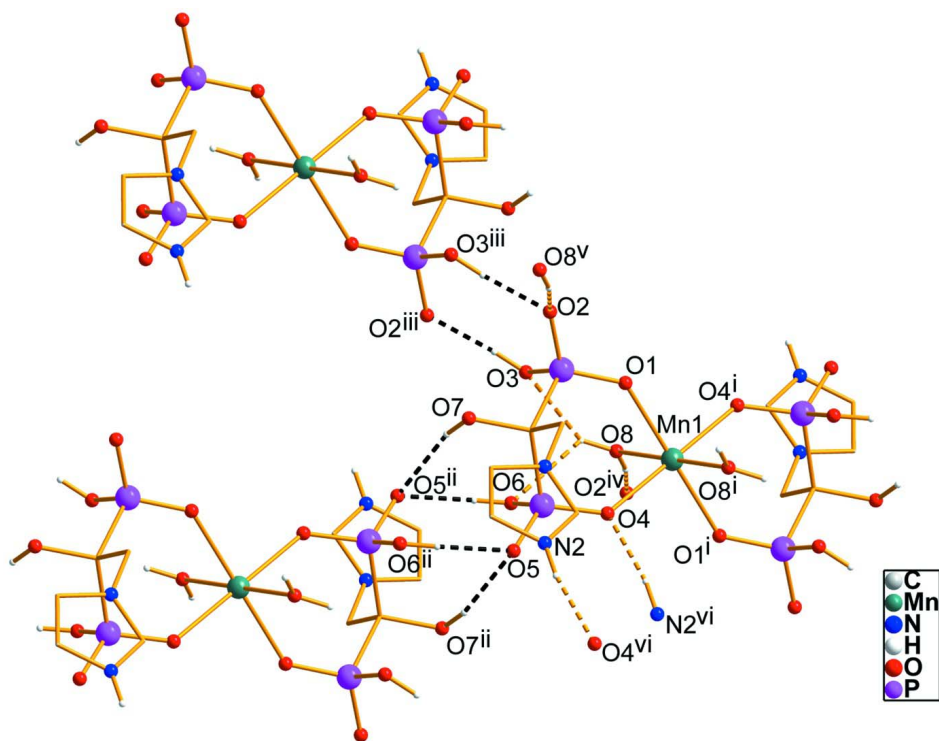
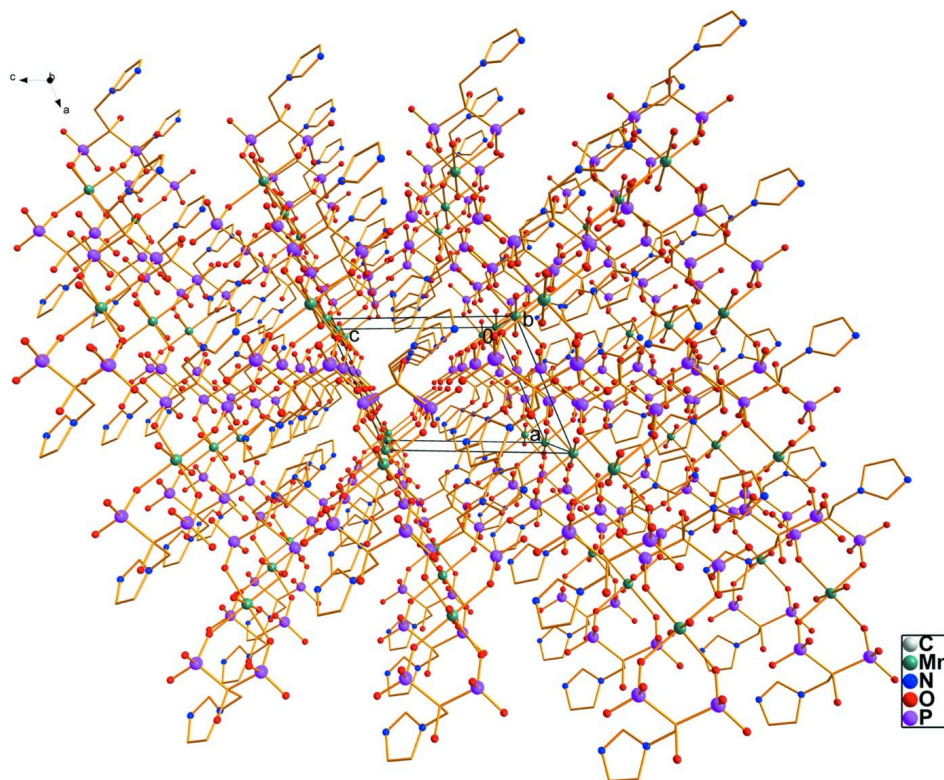


Figure 2

A view of the hydrogen bonding interactions in the structure of the title compound based on its asymmetric unit.

Hydrogen bonding interactions within the centrosymmetric units (see comment) are represented by black dashed lines, other as dashed yellow lines (symmetry codes: i, $-x, -y, -z$; ii, $1-x, 1-y, 1-z$; iii, $1-x, 1-y, -z$; iv, $-1+x, y, z$; v, $1+x, y, z$; vi, $1-x, -y, 1-z$).

**Figure 3**

Packing diagram of the title compound.

Diaquabis{[1-hydroxy-2-(1*H*-imidazol-3-ium-1-yl)ethane-1,1- diyl]bis(hydrogen phosphonato)}manganese(II)*Crystal data*[Mn(C₅H₉N₂O₇P₂)(H₂O)₂] $M_r = 633.14$ Triclinic, $P\bar{1}$

Hall symbol: -P 1

 $a = 7.4408 (17) \text{ \AA}$ $b = 8.566 (2) \text{ \AA}$ $c = 9.680 (2) \text{ \AA}$ $\alpha = 105.366 (4)^\circ$ $\beta = 110.865 (4)^\circ$ $\gamma = 97.461 (4)^\circ$ $V = 538.4 (2) \text{ \AA}^3$ $Z = 1$ $F(000) = 323$ $D_x = 1.953 \text{ Mg m}^{-3}$ Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 584 reflections

 $\theta = 2.4\text{--}24.6^\circ$ $\mu = 1.00 \text{ mm}^{-1}$ $T = 153 \text{ K}$

Block, light pink

 $0.25 \times 0.20 \times 0.20 \text{ mm}$ *Data collection*Bruker SMART APEXII
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

 ω scansAbsorption correction: multi-scan
(*SADABS*; Bruker, 2000) $T_{\min} = 0.788$, $T_{\max} = 0.825$

2637 measured reflections

1829 independent reflections

1543 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.029$ $\theta_{\text{max}} = 25.0^\circ$, $\theta_{\text{min}} = 2.4^\circ$ $h = -8 \rightarrow 4$ $k = -10 \rightarrow 10$ $l = -9 \rightarrow 11$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.052$
 $wR(F^2) = 0.135$
 $S = 0.99$
 1829 reflections
 175 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 atoms treated by a mixture of independent
 and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0806P)^2 + 0.0364P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.49 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\min} = -0.46 \text{ e } \text{Å}^{-3}$

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\sigma(F^2)$ 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)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.7059 (7)	0.0407 (6)	0.4433 (6)	0.0313 (11)
H1	0.5957	-0.0541	0.3933	0.038*
C2	0.9765 (8)	0.2242 (6)	0.6170 (6)	0.0411 (13)
H2	1.0898	0.2812	0.7125	0.049*
C3	0.9192 (7)	0.2695 (6)	0.4880 (5)	0.0330 (12)
H3	0.9850	0.3632	0.4743	0.040*
C4	0.6265 (7)	0.1604 (6)	0.2269 (5)	0.0263 (10)
H4A	0.5289	0.0511	0.1646	0.032*
H4B	0.7133	0.1768	0.1719	0.032*
C5	0.5147 (6)	0.2977 (5)	0.2313 (5)	0.0186 (9)
Mn1	0.0000	0.0000	0.0000	0.0188 (3)
N1	0.7483 (5)	0.1543 (4)	0.3809 (4)	0.0231 (8)
N2	0.8436 (7)	0.0832 (5)	0.5856 (5)	0.0393 (11)
H2A	0.8485	0.0279	0.6511	0.047*
O1	0.2208 (4)	0.1161 (3)	-0.0561 (3)	0.0218 (7)
O2	0.5292 (4)	0.2914 (3)	-0.0465 (3)	0.0212 (7)
O3	0.2772 (4)	0.4247 (4)	0.0239 (4)	0.0236 (7)
H3A	0.355 (7)	0.511 (6)	0.031 (5)	0.028*
O4	0.1983 (4)	0.1153 (4)	0.2449 (3)	0.0256 (7)
O5	0.4729 (4)	0.3069 (4)	0.5030 (3)	0.0258 (7)
O6	0.2356 (5)	0.4203 (4)	0.3166 (3)	0.0258 (7)
H6A	0.316 (7)	0.515 (6)	0.369 (6)	0.031*
O7	0.6604 (5)	0.4552 (4)	0.3074 (4)	0.0274 (8)
H7A	0.616 (7)	0.534 (6)	0.347 (6)	0.033*

O8	-0.1140 (6)	0.2247 (5)	-0.0097 (5)	0.0421 (10)
H8A	-0.232 (9)	0.226 (7)	-0.018 (7)	0.051*
H8B	-0.021 (9)	0.314 (7)	0.028 (7)	0.051*
P1	0.37848 (16)	0.27554 (13)	0.02248 (13)	0.0187 (3)
P2	0.34950 (16)	0.27977 (13)	0.33400 (12)	0.0203 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.032 (3)	0.032 (3)	0.038 (3)	0.011 (2)	0.017 (2)	0.020 (2)
C2	0.041 (3)	0.036 (3)	0.030 (3)	0.008 (3)	-0.003 (2)	0.011 (2)
C3	0.031 (3)	0.029 (3)	0.030 (3)	0.001 (2)	0.004 (2)	0.011 (2)
C4	0.027 (3)	0.030 (3)	0.020 (2)	0.013 (2)	0.008 (2)	0.006 (2)
C5	0.015 (2)	0.020 (2)	0.016 (2)	0.0023 (18)	0.0028 (18)	0.0052 (17)
Mn1	0.0177 (5)	0.0178 (5)	0.0178 (5)	0.0005 (4)	0.0058 (4)	0.0047 (4)
N1	0.021 (2)	0.025 (2)	0.022 (2)	0.0057 (16)	0.0065 (17)	0.0092 (16)
N2	0.052 (3)	0.045 (3)	0.031 (2)	0.016 (2)	0.017 (2)	0.026 (2)
O1	0.0219 (17)	0.0240 (17)	0.0183 (16)	0.0013 (13)	0.0098 (13)	0.0051 (13)
O2	0.0197 (16)	0.0242 (16)	0.0232 (16)	0.0056 (13)	0.0111 (13)	0.0099 (13)
O3	0.0211 (17)	0.0222 (17)	0.0342 (18)	0.0055 (13)	0.0143 (15)	0.0155 (14)
O4	0.0316 (18)	0.0241 (17)	0.0153 (16)	-0.0009 (14)	0.0062 (14)	0.0061 (13)
O5	0.0251 (17)	0.0299 (18)	0.0168 (16)	0.0001 (14)	0.0063 (14)	0.0057 (13)
O6	0.0223 (18)	0.0273 (18)	0.0225 (17)	0.0041 (14)	0.0080 (14)	0.0027 (14)
O7	0.0222 (17)	0.0244 (18)	0.0294 (18)	0.0004 (14)	0.0095 (15)	0.0035 (14)
O8	0.023 (2)	0.026 (2)	0.077 (3)	0.0073 (16)	0.021 (2)	0.0163 (19)
P1	0.0175 (6)	0.0197 (6)	0.0188 (6)	0.0028 (5)	0.0078 (5)	0.0065 (5)
P2	0.0211 (6)	0.0205 (6)	0.0162 (6)	0.0009 (5)	0.0073 (5)	0.0038 (5)

Geometric parameters (Å, °)

C1—N2	1.309 (6)	Mn1—O4	2.159 (3)
C1—N1	1.334 (6)	Mn1—O4 ⁱ	2.159 (3)
C1—H1	0.9500	Mn1—O8 ⁱ	2.213 (4)
C2—N2	1.345 (6)	Mn1—O8	2.213 (4)
C2—C3	1.347 (6)	N2—H2A	0.8800
C2—H2	0.9500	O1—P1	1.489 (3)
C3—N1	1.363 (6)	O2—P1	1.505 (3)
C3—H3	0.9500	O3—P1	1.565 (3)
C4—N1	1.462 (5)	O3—H3A	0.85 (5)
C4—C5	1.526 (6)	O4—P2	1.499 (3)
C4—H4A	0.9900	O5—P2	1.499 (3)
C4—H4B	0.9900	O6—P2	1.571 (3)
C5—O7	1.437 (5)	O6—H6A	0.84 (5)
C5—P2	1.850 (4)	O7—H7A	0.85 (5)
C5—P1	1.854 (4)	O8—H8A	0.86 (6)
Mn1—O1	2.116 (3)	O8—H8B	0.85 (6)
Mn1—O1 ⁱ	2.116 (3)		

N2—C1—N1	107.7 (4)	O1—Mn1—O8	84.33 (13)
N2—C1—H1	126.2	O1 ⁱ —Mn1—O8	95.67 (13)
N1—C1—H1	126.2	O4—Mn1—O8	93.01 (13)
N2—C2—C3	107.3 (4)	O4 ⁱ —Mn1—O8	86.99 (13)
N2—C2—H2	126.3	O8 ⁱ —Mn1—O8	180.0
C3—C2—H2	126.3	C1—N1—C3	108.7 (4)
C2—C3—N1	106.5 (4)	C1—N1—C4	125.9 (4)
C2—C3—H3	126.8	C3—N1—C4	125.4 (4)
N1—C3—H3	126.8	C1—N2—C2	109.9 (4)
N1—C4—C5	114.6 (3)	C1—N2—H2A	125.1
N1—C4—H4A	108.6	C2—N2—H2A	125.1
C5—C4—H4A	108.6	P1—O1—Mn1	134.48 (17)
N1—C4—H4B	108.6	P1—O3—H3A	111 (3)
C5—C4—H4B	108.6	P2—O4—Mn1	132.06 (17)
H4A—C4—H4B	107.6	P2—O6—H6A	110 (3)
O7—C5—C4	107.3 (3)	C5—O7—H7A	113 (3)
O7—C5—P2	111.1 (3)	Mn1—O8—H8A	121 (4)
C4—C5—P2	112.1 (3)	Mn1—O8—H8B	113 (4)
O7—C5—P1	108.2 (3)	H8A—O8—H8B	123 (5)
C4—C5—P1	104.7 (3)	O1—P1—O2	115.48 (17)
P2—C5—P1	113.0 (2)	O1—P1—O3	108.67 (17)
O1—Mn1—O1 ⁱ	180.00 (17)	O2—P1—O3	110.18 (16)
O1—Mn1—O4	88.32 (11)	O1—P1—C5	108.75 (17)
O1 ⁱ —Mn1—O4	91.68 (11)	O2—P1—C5	107.50 (18)
O1—Mn1—O4 ⁱ	91.68 (11)	O3—P1—C5	105.82 (18)
O1 ⁱ —Mn1—O4 ⁱ	88.32 (11)	O5—P2—O4	115.53 (17)
O4—Mn1—O4 ⁱ	180.00 (17)	O5—P2—O6	111.28 (17)
O1—Mn1—O8 ⁱ	95.67 (13)	O4—P2—O6	107.09 (18)
O1 ⁱ —Mn1—O8 ⁱ	84.33 (13)	O5—P2—C5	109.22 (18)
O4—Mn1—O8 ⁱ	86.99 (13)	O4—P2—C5	107.87 (18)
O4 ⁱ —Mn1—O8 ⁱ	93.01 (13)	O6—P2—C5	105.31 (18)

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

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N2—H2A \cdots O4 ⁱⁱ	0.88	1.85	2.718 (5)	167
O7—H7A \cdots O5 ⁱⁱⁱ	0.85 (5)	2.07 (5)	2.889 (4)	162 (5)
O6—H6A \cdots O5 ⁱⁱⁱ	0.84 (5)	1.82 (5)	2.653 (4)	167 (5)
O3—H3A \cdots O2 ^{iv}	0.85 (5)	1.74 (5)	2.573 (4)	167 (5)
O8—H8A \cdots O2 ^v	0.86 (6)	1.88 (6)	2.707 (5)	162 (5)
O8—H8B \cdots O3	0.85 (6)	2.32 (6)	3.042 (5)	143 (5)
O8—H8B \cdots O6	0.85 (6)	2.59 (6)	3.124 (5)	122 (5)

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