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Hexaaquamanganese(II) bis[hydrogen (4-aminophenyl)arsonate] tetrahydrate

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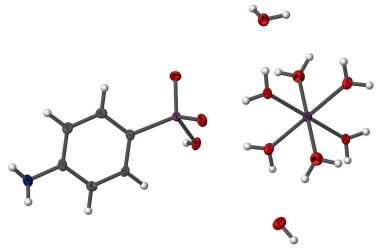
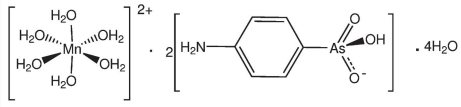
In the structure of the complex salt formed from the reaction of manganese(II) acetate with (4-aminophenyl)arsonic acid (*p*-arsanilic acid), $[Mn(H_2O)_6](C_6H_7AsNO_3)_2\cdot 4H_2O$, the centrosymmetric $Mn(H_2O)_6$ coordination polyhedron has slightly distorted octahedral stereochemistry, with the two hydrogen (4-aminophenyl)arsonate anions and the four water molecules of solvation related by inversion. Extensive O—H···O, O—H···N and N—H···O hydrogen bonds link all species, giving an overall three-dimensional supramolecular structure, which also has weak π–π ring interactions [minimum ring-centroid separation = 3.7304 (15) Å]. The structure is isotypic with that of the Mg salt.

3D view



Chemical scheme



Structure description

The arsenical (4-aminophenyl)arsonic acid (*p*-arsanilic acid) has biological significance as an anti-helminth in veterinary applications (Steverding, 2010) and its crystal structure (Shimada, 1961; Nuttall & Hunter, 1996) has shown that it exists as a zwitterion. The hydrated monosodium salt had early usage as an anti-syphilitic (atoxyl) (Ehrlich & Bertheim, 1907). We have reported the crystal structure of this salt (a dihydrate) and the NH_4^+ salt (Smith & Wermuth, 2014), together with the structures of the K, Rb and Cs salts (Smith & Wermuth, 2017*a*), as well as the alkaline-earth metal salts Mg, Ca, Sr and Ba (Smith & Wermuth, 2017*b*). Other single-metal complex structures are known, *e.g.* with Ag, Pb, Cd, Zn (Lesikar-Parrish *et al.*, 2013), but no structures of single-metal first transition series compounds of hydrogen *p*-arsanilic acid have been reported. Our reaction of this acid with manganese(II) acetate in aqueous ethanol gave the title complex salt, $[Mn(H_2O)_6](C_6H_7AsNO_3)_2\cdot 4H_2O$, and the structure is reported herein.

In the structure (Fig. 1), the cations exist as the common centrosymmetric octahedral $[Mn(H_2O)_6]^{2+}$ species with the hydrogen *p*-arsanilate counter-anions and the water

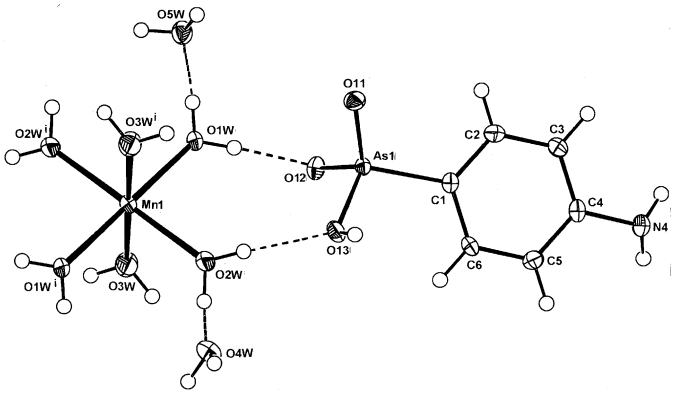


Figure 1
The molecular configuration and atom-numbering scheme for the centrosymmetric complex cation, the hydrogen *p*-arsanilate anion and the water molecules of solvation (O4*W* and O5*W*) in the asymmetric unit of the title compound. [Symmetry code: (i) $-x+1, -y+1, -z+1$.] Non-H atoms are shown as 40% probability displacement ellipsoids and hydrogen-bonding interactions are shown as dashed lines

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

D—H···A	D—H	H···A	D···A	D—H···A
O13—H13···N4^{i}	0.84 (2)	1.90 (2)	2.734 (3)	174 (4)
N4—H41···O4W^{ii}	0.87 (2)	2.09 (3)	2.911 (3)	158 (3)
N4—H42···O12^{ii}	0.87 (3)	2.13 (3)	2.982 (3)	169 (3)
O1W—H11W···O5W	0.82 (2)	1.90 (2)	2.715 (3)	173 (3)
O1W—H12W···O12	0.84 (2)	1.79 (2)	2.626 (3)	176 (4)
O2W—H21W···O13	0.83 (3)	1.99 (3)	2.811 (3)	175 (4)
O2W—H22W···O11^{iii}	0.85 (2)	1.88 (2)	2.704 (3)	164 (3)
O3W—H31W···O5W^{iv}	0.84 (3)	1.96 (3)	2.791 (3)	171 (3)
O3W—H32W···O4W	0.86 (3)	1.91 (3)	2.773 (3)	174 (3)
O4W—H41W···O12^{iv}	0.84 (3)	1.88 (3)	2.725 (3)	177 (3)
O4W—H42W···O11^{iii}	0.85 (2)	1.90 (2)	2.720 (3)	164 (3)
O5W—H51W···O11^{v}	0.86 (3)	1.90 (3)	2.749 (3)	170 (4)
O5W—H52W···O1W^{vi}	0.85 (2)	2.07 (2)	2.895 (3)	164 (3)

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

molecules of solvation (O4*W*, (O4*W*^{i}, and O5*W*, O5*W*^{i}) inversion related [symmetry code (i): $-x+1, -y+1, -z+1$]. The Mn—O bond length range is 2.170 (2)–2.180 (2) Å. Structures having the $[Mn(H_2O)_6]^{2+}$ cation are quite common, but no examples involving arsonate anions are known and phosphonate examples are few, *e.g.* hexaaquamanganese(II) bis(hydrogen *t*-butylphosphonate)·6H_2O (Wang *et al.*, 2009). The structure of the title compound is isotypic with that of the Mg hydrogen *p*-arsanilate complex, $[Mg(H_2O)_6](C_6H_7AsNO_3)_2{\cdot}4H_2O$ (Smith & Wermuth, 2017*b*), with cell data: a = 15.1693 (6), b = 6.7367 (2), c = 12.9532 (4) Å, β = 108.033 (4), V = 1258.63 (7)°, Z = 4, space group $P2_1/c$.

In the crystal, extensive inter-species O—H···O, O—H···N and N—H···O hydrogen-bonding interactions (Table 1) are present with the *p*-arsanilate anions linking the hydrogen-bonded layers of associated cations and water molecules across [010], generating a three-dimensional supramolecular structure (Fig. 2). Weak π–π associations are also present between inversion-related anions [minimum ring-centroid separation = 3.7304 (15) Å].

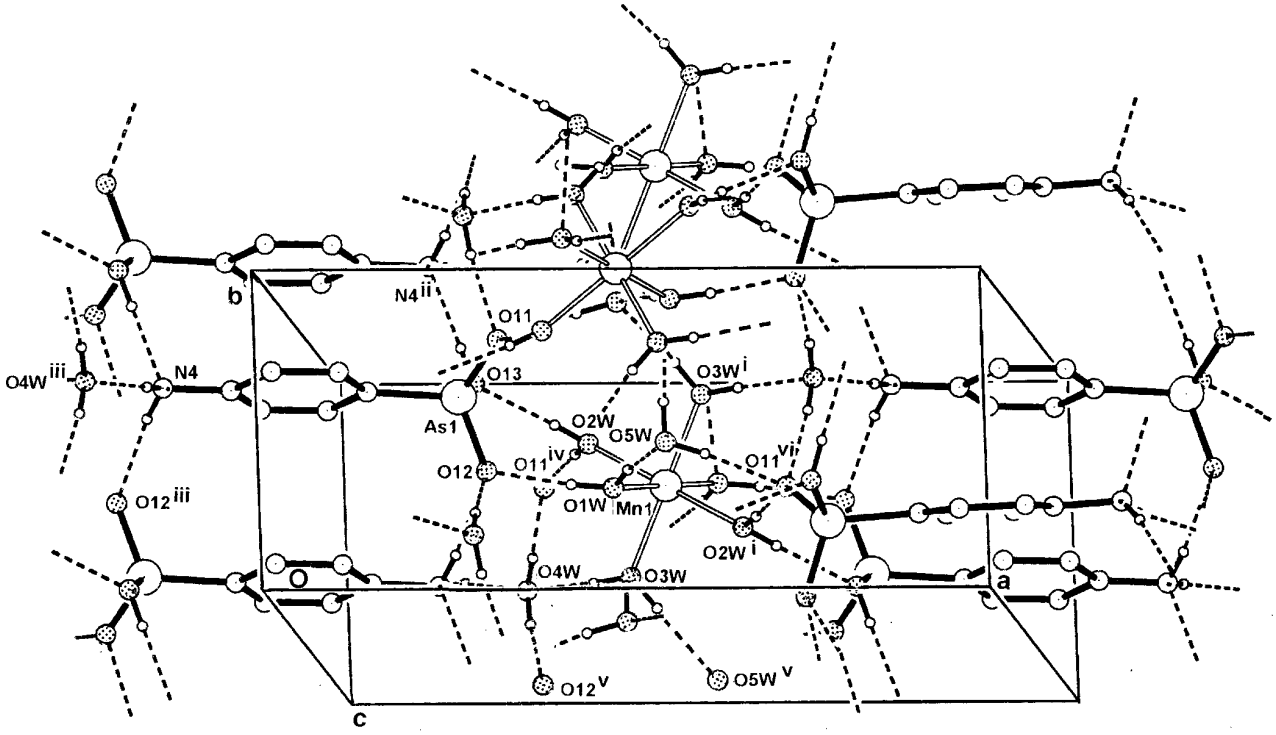


Figure 2
The packing in the unit cell, viewed along the *c*-axis direction, showing the associated $[Mn(H_2O)_6]^{2+}$ cation layers linked peripherally across *a* by hydrogen bonds involving the anions and the water molecules of solvation. Hydrogen-bonding interactions are shown as dashed lines and aromatic H atoms have been omitted.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Mn(H_2O)_6](C_6H_7AsNO_3)_2{\cdot}4H_2O$
M_r	667.19
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	200
a, b, c (Å)	15.2040 (9), 6.7388 (3), 13.0699 (8)
β (°)	107.951 (7)
V (Å^3)	1273.91 (13)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	3.17
Crystal size (mm)	0.35 × 0.26 × 0.18
Data collection	
Diffractometer	Oxford Diffraction Gemini-S CCD detector
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2015)
T_{min}, T_{max}	0.662, 0.980
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	5155, 2496, 2128
R_{int}	0.025
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.027, 0.068, 1.02
No. of reflections	2496
No. of parameters	190
No. of restraints	13
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.32, −0.46

Computer programs: *CrysAlis PRO* (Rigaku OD, 2015), *SHELXS97* (Sheldrick, 2008), *SHELXL97* (Sheldrick, 2008) within *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

Synthesis and crystallization

The title compound was synthesized by heating together for 5 min, 1 mmol quantities of (4-aminophenyl)arsonic acid and manganese(II) acetate in 20 ml of 50% ethanol/water. Room temperature evaporation of the solution gave thin colourless crystal blocks suitable for the X-ray analysis.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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full crystallographic data

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Crystal data

$[Mn(H_2O)_6](C_6H_7AsNO_3)_2·4H_2O$
M_r = 667.19
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 15.2040 (9) Å
b = 6.7388 (3) Å
c = 13.0699 (8) Å
β = 107.951 (7)°
V = 1273.91 (13) Å^3
Z = 2
$F(000)$ = 678
D_x = 1.739 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1801 reflections
θ = 3.9–29.2°
μ = 3.17 mm^{-1}
T = 200 K
Block, colourless
0.35 × 0.26 × 0.18 mm

Data collection

Oxford Diffraction Gemini-S CCD-detector diffractometer
Radiation source: Enhance (Mo) X-ray source
Graphite monochromator
Detector resolution: 16.077 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis PRO; Rigaku OD, 2015)
T_{min} = 0.662, T_{max} = 0.980
5155 measured reflections
2496 independent reflections
2128 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 26.0°, θ_{min} = 3.3°
h = −18→11
k = −8→8
l = −12→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.068
S = 1.02
2496 reflections
190 parameters
13 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
$w = 1/[\sigma^2(F_o^2) + (0.0288P)^2 + 0.7443P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
As1	0.22953 (2)	0.74539 (4)	0.59945 (2)	0.0134 (1)
O11	0.29612 (12)	0.8896 (3)	0.69561 (14)	0.0193 (6)
O12	0.26527 (12)	0.5118 (3)	0.60584 (15)	0.0193 (5)
O13	0.23649 (13)	0.8281 (3)	0.47601 (15)	0.0200 (6)
N4	−0.17885 (16)	0.7872 (3)	0.5635 (2)	0.0196 (7)
C1	0.10328 (18)	0.7644 (3)	0.5914 (2)	0.0157 (8)
C2	0.07608 (19)	0.7936 (4)	0.6825 (2)	0.0228 (8)
C3	−0.01696 (19)	0.7990 (4)	0.6739 (2)	0.0229 (9)
C4	−0.08400 (18)	0.7749 (4)	0.5742 (2)	0.0170 (8)
C5	−0.05619 (19)	0.7490 (4)	0.4827 (2)	0.0184 (8)
C6	0.03656 (18)	0.7431 (3)	0.4914 (2)	0.0167 (8)
Mn1	0.50000	0.50000	0.50000	0.0164 (2)
O1W	0.44009 (13)	0.4411 (3)	0.62823 (15)	0.0203 (6)
O2W	0.38051 (15)	0.6723 (3)	0.40765 (16)	0.0293 (7)
O3W	0.43599 (15)	0.2291 (3)	0.42193 (18)	0.0281 (7)
O4W	0.26434 (15)	0.2457 (3)	0.26621 (17)	0.0244 (7)
O5W	0.54204 (13)	0.5174 (3)	0.83471 (16)	0.0228 (6)
H2	0.12130	0.80990	0.75080	0.0270*
H3	−0.03530	0.81930	0.73630	0.0280*
H5	−0.10130	0.73540	0.41410	0.0220*
H6	0.05500	0.72450	0.42890	0.0200*
H13	0.223 (2)	0.948 (3)	0.465 (3)	0.0300*
H41	−0.190 (2)	0.764 (4)	0.6237 (18)	0.0230*
H42	−0.2109 (19)	0.704 (4)	0.516 (2)	0.0230*
H11W	0.470 (2)	0.474 (5)	0.6899 (16)	0.0300*
H12W	0.3851 (13)	0.467 (4)	0.624 (3)	0.0300*
H21W	0.340 (2)	0.724 (5)	0.429 (3)	0.0440*
H22W	0.359 (2)	0.674 (5)	0.3397 (15)	0.0440*
H31W	0.469 (2)	0.147 (4)	0.402 (3)	0.0420*
H32W	0.3817 (16)	0.226 (5)	0.375 (2)	0.0420*
H41W	0.266 (2)	0.164 (4)	0.218 (2)	0.0370*
H42W	0.263 (2)	0.359 (3)	0.238 (2)	0.0370*
H51W	0.5943 (15)	0.473 (4)	0.833 (3)	0.0340*
H52W	0.546 (2)	0.636 (3)	0.858 (3)	0.0340*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
As1	0.0117 (2)	0.0153 (2)	0.0139 (2)	0.0010 (1)	0.0052 (1)	0.0003 (1)
O11	0.0173 (10)	0.0222 (10)	0.0176 (9)	−0.0039 (8)	0.0041 (8)	−0.0026 (8)

O12	0.0162 (9)	0.0169 (9)	0.0253 (10)	0.0029 (7)	0.0073 (8)	0.0013 (8)
O13	0.0234 (10)	0.0224 (10)	0.0179 (10)	0.0081 (8)	0.0117 (8)	0.0048 (9)
N4	0.0141 (12)	0.0240 (12)	0.0221 (13)	−0.0006 (9)	0.0077 (10)	−0.0002 (11)
C1	0.0134 (13)	0.0163 (13)	0.0185 (14)	0.0010 (10)	0.0064 (11)	0.0004 (11)
C2	0.0191 (14)	0.0349 (16)	0.0136 (13)	0.0012 (12)	0.0041 (11)	−0.0003 (12)
C3	0.0209 (15)	0.0351 (16)	0.0148 (14)	0.0037 (12)	0.0085 (12)	0.0026 (12)
C4	0.0153 (13)	0.0149 (13)	0.0230 (14)	0.0012 (10)	0.0091 (11)	0.0019 (11)
C5	0.0172 (14)	0.0201 (14)	0.0163 (13)	0.0005 (10)	0.0028 (11)	0.0003 (11)
C6	0.0174 (13)	0.0196 (14)	0.0159 (13)	0.0013 (10)	0.0091 (11)	−0.0014 (11)
Mn1	0.0156 (3)	0.0203 (3)	0.0145 (3)	0.0014 (2)	0.0065 (2)	−0.0006 (2)
O1W	0.0139 (10)	0.0322 (11)	0.0164 (9)	0.0032 (8)	0.0070 (8)	−0.0001 (9)
O2W	0.0256 (12)	0.0448 (13)	0.0170 (10)	0.0168 (10)	0.0057 (9)	−0.0006 (10)
O3W	0.0240 (12)	0.0276 (12)	0.0313 (12)	0.0008 (9)	0.0064 (10)	−0.0085 (10)
O4W	0.0312 (12)	0.0238 (11)	0.0212 (11)	−0.0031 (9)	0.0126 (9)	−0.0018 (9)
O5W	0.0203 (10)	0.0216 (10)	0.0269 (11)	0.0001 (9)	0.0079 (9)	−0.0045 (9)

Geometric parameters (Å, º)

Mn1—O1W	2.177 (2)	O4W—H41W	0.84 (3)
Mn1—O1W^{i}	2.177 (2)	O4W—H42W	0.85 (2)
Mn1—O2W	2.180 (2)	O5W—H51W	0.86 (3)
Mn1—O2W^{i}	2.180 (2)	O5W—H52W	0.85 (2)
Mn1—O3W	2.170 (2)	N4—C4	1.408 (4)
Mn1—O3W^{i}	2.170 (2)	N4—H41	0.87 (2)
As1—O11	1.6627 (19)	N4—H42	0.87 (3)
As1—O12	1.659 (2)	C1—C6	1.393 (4)
As1—O13	1.7407 (19)	C1—C2	1.390 (4)
As1—C1	1.894 (3)	C2—C3	1.385 (4)
O13—H13	0.84 (2)	C3—C4	1.395 (4)
O1W—H12W	0.84 (2)	C4—C5	1.397 (4)
O1W—H11W	0.82 (2)	C5—C6	1.380 (4)
O2W—H21W	0.83 (3)	C2—H2	0.9500
O2W—H22W	0.847 (19)	C3—H3	0.9500
O3W—H32W	0.86 (3)	C5—H5	0.9500
O3W—H31W	0.84 (3)	C6—H6	0.9500
O11—As1—O12	113.76 (10)	H21W—O2W—H22W	105 (3)
O11—As1—O13	108.46 (9)	Mn1—O3W—H32W	123 (2)
O11—As1—C1	111.90 (10)	H31W—O3W—H32W	107 (3)
O12—As1—O13	103.77 (9)	Mn1—O3W—H31W	118 (2)
O12—As1—C1	112.19 (9)	H41W—O4W—H42W	105 (2)
O13—As1—C1	106.08 (10)	H51W—O5W—H52W	112 (3)
O1W^{i}—Mn1—O3W	91.42 (8)	C4—N4—H41	112 (2)
O2W^{i}—Mn1—O3W	89.35 (8)	H41—N4—H42	108 (3)
O3W—Mn1—O3W^{i}	180.00	C4—N4—H42	112 (2)
O1W^{i}—Mn1—O2W^{i}	92.77 (8)	C2—C1—C6	119.7 (3)
O1W^{i}—Mn1—O3W^{i}	88.58 (8)	As1—C1—C6	118.5 (2)
O2W^{i}—Mn1—O3W^{i}	90.65 (8)	As1—C1—C2	121.7 (2)

O1W^{i}—Mn1—O2W	87.23 (8)	C1—C2—C3	120.0 (2)
O1W—Mn1—O2W	92.77 (8)	C2—C3—C4	120.5 (2)
O1W—Mn1—O3W	88.58 (8)	N4—C4—C3	121.2 (2)
O1W—Mn1—O1W^{i}	180.00	C3—C4—C5	119.2 (3)
O1W—Mn1—O2W^{i}	87.23 (8)	N4—C4—C5	119.6 (2)
O1W—Mn1—O3W^{i}	91.42 (8)	C4—C5—C6	120.3 (2)
O2W—Mn1—O3W	90.65 (8)	C1—C6—C5	120.3 (2)
O2W—Mn1—O2W^{i}	180.00	C3—C2—H2	120.00
O2W—Mn1—O3W^{i}	89.35 (8)	C1—C2—H2	120.00
As1—O13—H13	113 (3)	C2—C3—H3	120.00
Mn1—O1W—H11W	118 (2)	C4—C3—H3	120.00
H11W—O1W—H12W	104 (3)	C6—C5—H5	120.00
Mn1—O1W—H12W	124 (2)	C4—C5—H5	120.00
Mn1—O2W—H21W	128 (3)	C1—C6—H6	120.00
Mn1—O2W—H22W	125 (2)	C5—C6—H6	120.00
O11—As1—C1—C2	−34.0 (2)	As1—C1—C6—C5	177.71 (18)
O11—As1—C1—C6	147.69 (16)	C2—C1—C6—C5	−0.6 (3)
O12—As1—C1—C2	95.2 (2)	C1—C2—C3—C4	0.1 (4)
O12—As1—C1—C6	−83.06 (18)	C2—C3—C4—N4	−177.7 (2)
O13—As1—C1—C2	−152.12 (19)	C2—C3—C4—C5	−1.2 (4)
O13—As1—C1—C6	29.59 (19)	N4—C4—C5—C6	177.9 (2)
As1—C1—C2—C3	−177.48 (19)	C3—C4—C5—C6	1.4 (4)
C6—C1—C2—C3	0.8 (4)	C4—C5—C6—C1	−0.5 (4)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O13—H13···N4^{ii}	0.84 (2)	1.90 (2)	2.734 (3)	174 (4)
N4—H41···O4*W*^{iii}	0.87 (2)	2.09 (3)	2.911 (3)	158 (3)
N4—H42···O12^{iii}	0.87 (3)	2.13 (3)	2.982 (3)	169 (3)
O1*W*—H11*W*···O5*W*	0.82 (2)	1.90 (2)	2.715 (3)	173 (3)
O1*W*—H12*W*···O12	0.84 (2)	1.79 (2)	2.626 (3)	176 (4)
O2*W*—H21*W*···O13	0.83 (3)	1.99 (3)	2.811 (3)	175 (4)
O2*W*—H22*W*···O11^{iv}	0.85 (2)	1.88 (2)	2.704 (3)	164 (3)
O3*W*—H31*W*···O5*W*^{v}	0.84 (3)	1.96 (3)	2.791 (3)	171 (3)
O3*W*—H32*W*···O4*W*	0.86 (3)	1.91 (3)	2.773 (3)	174 (3)
O4*W*—H41*W*···O12^{v}	0.84 (3)	1.88 (3)	2.725 (3)	177 (3)
O4*W*—H42*W*···O11^{iv}	0.85 (2)	1.90 (2)	2.720 (3)	164 (3)
O5*W*—H51*W*···O11^{vi}	0.86 (3)	1.90 (3)	2.749 (3)	170 (4)
O5*W*—H52*W*···O1*W*^{vii}	0.85 (2)	2.07 (2)	2.895 (3)	164 (3)

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