

1,10-Phenanthroline-1-ium hydrogen D,L-tartrate dihydrate

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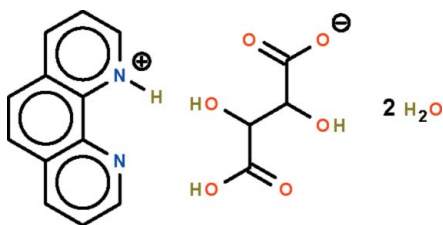
Received 27 April 2011; accepted 27 April 2011

 Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å;
 R factor = 0.047; wR factor = 0.160; data-to-parameter ratio = 13.6.

In the title hydrated molecular salt, $\text{C}_{12}\text{H}_9\text{N}_2^+ \cdot \text{C}_4\text{H}_5\text{O}_6^- \cdot 2\text{H}_2\text{O}$, the cation is almost planar (r.m.s. deviation = 0.014 Å); the carbon skeleton of the anion assumes a *trans* conformation [$\text{C}-\text{C}-\text{C}-\text{C}$ torsion angle = -179.86 (14)°]. The carboxyl end of one hydrogen tartrate anion forms a short hydrogen bond to the carboxylate end of another anion [$\text{O} \cdots \text{O} = 2.508$ (2) Å] in a head-to-tail manner, forming a chain; the chains and water molecules interact, generating an $\text{O}-\text{H} \cdots \text{O}$ hydrogen-bonded layer. The cation binds to the layer by an $\text{N}-\text{H} \cdots \text{O}$ hydrogen bond.

Related literature

For the trihydrated 1,10-phenanthroline-1-ium salts of D- and L-tartaric acid, see: Derikvand & Olmstead (2010); Wang *et al.* (2006).



Experimental

Crystal data

 $\text{C}_{12}\text{H}_9\text{N}_2^+ \cdot \text{C}_4\text{H}_5\text{O}_6^- \cdot 2\text{H}_2\text{O}$
 $M_r = 366.32$
 Triclinic, $P\bar{1}$
 $a = 7.0933$ (7) Å
 $b = 10.5849$ (11) Å
 $c = 11.4694$ (11) Å

 $\alpha = 98.081$ (1)°
 $\beta = 100.350$ (1)°
 $\gamma = 103.903$ (1)°
 $V = 806.95$ (14) Å³
 $Z = 2$

 Mo $K\alpha$ radiation
 $\mu = 0.12$ mm⁻¹
 $T = 100$ K
 $0.40 \times 0.10 \times 0.10$ mm

Data collection

 Bruker SMART APEX
 diffractometer
 7610 measured reflections

 3635 independent reflections
 2880 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.028$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.047$
 $wR(F^2) = 0.160$
 $S = 1.04$
 3635 reflections
 267 parameters

 H atoms treated by a mixture of
 independent and constrained
 refinement
 $\Delta\rho_{\text{max}} = 0.35$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.31$ e Å⁻³
Table 1

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$\text{O3}-\text{H3} \cdots \text{O1w}^{\text{i}}$	0.89 (3)	1.82 (3)	2.709 (2)	175 (3)
$\text{O4}-\text{H4} \cdots \text{O2w}^{\text{ii}}$	0.90 (3)	1.84 (3)	2.739 (2)	172 (3)
$\text{O5}-\text{H5} \cdots \text{O2}^{\text{iii}}$	0.99 (3)	1.52 (3)	2.508 (2)	169 (3)
$\text{O1w}-\text{H12} \cdots \text{O1}$	0.93 (3)	1.97 (3)	2.846 (2)	157 (3)
$\text{O1w}-\text{H11} \cdots \text{O1}^{\text{iv}}$	0.90 (4)	1.86 (4)	2.753 (2)	173 (4)
$\text{O2w}-\text{H21} \cdots \text{O2}$	0.84 (4)	1.93 (4)	2.764 (2)	168 (3)
$\text{O2w}-\text{H22} \cdots \text{O6}^{\text{v}}$	0.87 (3)	1.97 (3)	2.835 (2)	176 (3)
$\text{N1}-\text{H1} \cdots \text{O1w}$	0.93 (3)	1.89 (3)	2.753 (2)	153 (3)

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINTE* (Bruker, 2009); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *pubCIF* (Westrip, 2010).

We thank the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5536).

References

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supplementary materials

Acta Cryst. (2011). E67, o1306 [doi:10.1107/S1600536811015972]

1,10-Phenanthroline-1-ium hydrogen D,L-tartrate dihydrate

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Comment

D-tartaric acid transfers one proton to 1,10-phenanthroline to yield 1,10-phenanthroline hydrogen D-tartrate, which separates from solution as a trihydrate. The hydrogen D-tartrate anions are connected in a head-to-tail fashion by an $O-H_{\text{carboxylic acid}} \cdots O_{\text{carboxyl}}$ hydrogen bond [$O \cdots O$ 2.455 (1) Å] (Derikvand & Olmstead, 2010). The identical feature should be presented in the L analog (Wang *et al.*, 2006). The anion and water molecules are linked by extensive $O-H \cdots O$ hydrogen bonds into a three-dimensional network, with the cations occupying the cavities. Racemic tartaric furnishes the corresponding dihydrate. In $C_{12}H_9N_2^+ C_4H_5O_4^- \cdot 2H_2O$ (Scheme I, Fig. 1), the carboxylic acid $-CO_2H$ end of one hydrogen (D,L)-tartrate anion forms a short hydrogen bond to the carboxylate $-CO_2^-$ end of another anion [$O \cdots O$ 2.508 (2) Å] in a head-to-tail manner to form a chain; the chains and water molecules interact to generate an $O-H \cdots O$ hydrogen-bonded layer. The cation binds to the layer by an $N-H \cdots O$ hydrogen bond (Table 1).

Experimental

D,L-Tartaric acid (2 mmol, 0.30 g) and 1,10-phenanthroline (0.33 mmol, 0.06 g) were dissolved in water (5 ml). The solution was heated briefly to dissolve the reactants. The solution was set aside for the growth of colorless crystals, which were isolated after 10 days. The bulk crystals were faintly tinted a shade of pink.

Refinement

Carbon-bound H-atoms were placed in calculated positions ($C-H$ 0.95 to 1.00 Å) and were included in the refinement in the riding model approximation, with $U(H)$ set to 1.2 $U(C)$.

The ammonium and water H-atoms were located in a difference Fourier map, and were freely refined.

Omitted from the refinement owing to bad disagreements were these reflections: (-2 - 3 1), (-8 8 2), (2 2 4), (-7 6 7) and (3 - 3 4).

Figures

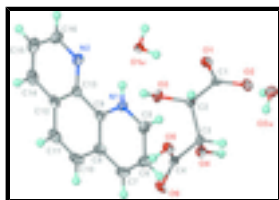


Fig. 1. Anisotropic displacement ellipsoid plot (Barbour, 2001) of $C_{12}H_9N_2^+ C_4H_5O_6^- \cdot 2H_2O$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

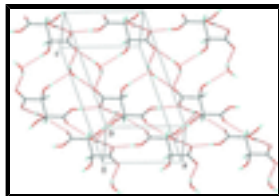


Fig. 2. Hydrogen-bonded layer structure arising from tartrate–water interactions.

1,10-Phenanthroline-1-ium hydrogen D,L-tartrate dihydrate

Crystal data

$C_{12}H_9N_2^+ \cdot C_4H_5O_6^- \cdot 2H_2O$

$M_r = 366.32$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 7.0933\ (7)\ \text{\AA}$

$b = 10.5849\ (11)\ \text{\AA}$

$c = 11.4694\ (11)\ \text{\AA}$

$\alpha = 98.081\ (1)^\circ$

$\beta = 100.350\ (1)^\circ$

$\gamma = 103.903\ (1)^\circ$

$V = 806.95\ (14)\ \text{\AA}^3$

$Z = 2$

$F(000) = 384$

$D_x = 1.508\ \text{Mg m}^{-3}$

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

Cell parameters from 2722 reflections

$\theta = 2.5\text{--}28.2^\circ$

$\mu = 0.12\ \text{mm}^{-1}$

$T = 100\ \text{K}$

Prism, colorless

$0.40 \times 0.10 \times 0.10\ \text{mm}$

Data collection

Bruker SMART APEX
diffractometer

Radiation source: fine-focus sealed tube
graphite

ω scans

7610 measured reflections

3635 independent reflections

2880 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.028$

$\theta_{\text{max}} = 27.5^\circ$, $\theta_{\text{min}} = 1.8^\circ$

$h = -9 \rightarrow 9$

$k = -13 \rightarrow 13$

$l = -14 \rightarrow 14$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.047$

$wR(F^2) = 0.160$

$S = 1.04$

3635 reflections

267 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

$w = 1/[\sigma^2(F_o^2) + (0.1012P)^2 + 0.1854P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} = 0.001$

$\Delta\rho_{\text{max}} = 0.35\ \text{e \AA}^{-3}$

$\Delta\rho_{\text{min}} = -0.31\ \text{e \AA}^{-3}$

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.0272 (2)	0.97612 (14)	0.33939 (12)	0.0172 (3)
O2	0.00294 (19)	1.04199 (14)	0.16223 (12)	0.0167 (3)
O3	0.3922 (2)	0.95680 (14)	0.34847 (12)	0.0163 (3)
O4	0.1832 (2)	0.78094 (13)	0.12086 (12)	0.0154 (3)
O5	0.6410 (2)	1.02428 (13)	0.15147 (12)	0.0153 (3)
O6	0.5609 (2)	0.80301 (14)	0.09605 (13)	0.0192 (3)
O1W	0.2228 (2)	0.90933 (13)	0.55174 (12)	0.0145 (3)
O2W	0.1595 (2)	1.23818 (15)	0.04324 (13)	0.0174 (3)
N1	0.2289 (2)	0.65380 (16)	0.46822 (15)	0.0143 (3)
N2	0.2713 (2)	0.66417 (16)	0.71074 (15)	0.0171 (4)
C1	0.0952 (3)	1.00580 (17)	0.25142 (16)	0.0125 (4)
C2	0.3085 (3)	1.00188 (18)	0.24666 (16)	0.0124 (4)
H2A	0.3902	1.0934	0.2475	0.015*
C3	0.3050 (3)	0.91028 (18)	0.12952 (16)	0.0115 (4)
H3A	0.2505	0.9473	0.0594	0.014*
C4	0.5161 (3)	0.90552 (18)	0.12418 (16)	0.0122 (4)
C5	0.2130 (3)	0.6578 (2)	0.35202 (18)	0.0184 (4)
H5A	0.2027	0.7366	0.3240	0.022*
C6	0.2114 (3)	0.5459 (2)	0.27087 (19)	0.0220 (5)
H6	0.2015	0.5487	0.1876	0.026*
C7	0.2243 (3)	0.4319 (2)	0.31181 (19)	0.0213 (4)
H7	0.2216	0.3552	0.2567	0.026*
C8	0.2417 (3)	0.42852 (19)	0.43589 (19)	0.0178 (4)
C9	0.2446 (3)	0.54419 (18)	0.51418 (17)	0.0138 (4)
C10	0.2550 (3)	0.3129 (2)	0.4856 (2)	0.0220 (5)
H10	0.2530	0.2340	0.4337	0.026*
C11	0.2704 (3)	0.3145 (2)	0.6049 (2)	0.0224 (5)
H11A	0.2778	0.2366	0.6356	0.027*
C12	0.2757 (3)	0.43249 (19)	0.68601 (19)	0.0173 (4)
C13	0.2645 (3)	0.54791 (18)	0.64134 (18)	0.0149 (4)
C14	0.2935 (3)	0.4390 (2)	0.8110 (2)	0.0227 (5)
H14	0.3004	0.3633	0.8456	0.027*
C15	0.3006 (3)	0.5558 (2)	0.8818 (2)	0.0236 (5)
H15	0.3135	0.5626	0.9665	0.028*
C16	0.2888 (3)	0.6661 (2)	0.82806 (18)	0.0210 (4)
H16	0.2936	0.7464	0.8787	0.025*
H3	0.517 (5)	1.006 (3)	0.381 (3)	0.048 (9)*
H4	0.066 (4)	0.767 (3)	0.067 (3)	0.032 (7)*
H5	0.781 (5)	1.020 (3)	0.156 (3)	0.057 (10)*
H11	0.145 (5)	0.944 (4)	0.593 (4)	0.067 (11)*
H12	0.195 (4)	0.938 (3)	0.480 (3)	0.039 (8)*
H21	0.120 (5)	1.172 (4)	0.074 (3)	0.052 (10)*
H22	0.247 (5)	1.223 (3)	0.003 (3)	0.037 (8)*
H1	0.233 (5)	0.731 (3)	0.520 (3)	0.046 (8)*

supplementary materials

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0162 (7)	0.0231 (7)	0.0161 (7)	0.0078 (6)	0.0087 (5)	0.0054 (5)
O2	0.0131 (7)	0.0224 (7)	0.0178 (7)	0.0070 (5)	0.0060 (5)	0.0070 (6)
O3	0.0120 (7)	0.0243 (7)	0.0118 (7)	0.0032 (6)	0.0015 (5)	0.0055 (5)
O4	0.0139 (7)	0.0137 (7)	0.0165 (7)	0.0017 (5)	0.0018 (5)	0.0020 (5)
O5	0.0123 (7)	0.0156 (7)	0.0197 (7)	0.0047 (5)	0.0058 (5)	0.0036 (5)
O6	0.0187 (7)	0.0173 (7)	0.0250 (8)	0.0097 (6)	0.0070 (6)	0.0042 (6)
O1W	0.0160 (7)	0.0181 (7)	0.0111 (7)	0.0070 (5)	0.0038 (5)	0.0037 (5)
O2W	0.0167 (7)	0.0191 (7)	0.0168 (7)	0.0047 (6)	0.0053 (6)	0.0034 (6)
N1	0.0141 (8)	0.0146 (8)	0.0132 (8)	0.0028 (6)	0.0023 (6)	0.0017 (6)
N2	0.0195 (8)	0.0153 (8)	0.0154 (8)	0.0040 (6)	0.0017 (7)	0.0033 (6)
C1	0.0139 (9)	0.0108 (8)	0.0123 (9)	0.0027 (7)	0.0044 (7)	-0.0003 (7)
C2	0.0105 (8)	0.0153 (9)	0.0120 (9)	0.0034 (7)	0.0039 (7)	0.0027 (7)
C3	0.0115 (8)	0.0142 (8)	0.0101 (8)	0.0042 (7)	0.0035 (7)	0.0041 (7)
C4	0.0146 (9)	0.0153 (8)	0.0083 (8)	0.0053 (7)	0.0036 (7)	0.0041 (7)
C5	0.0159 (9)	0.0225 (10)	0.0166 (10)	0.0039 (8)	0.0040 (7)	0.0051 (8)
C6	0.0196 (10)	0.0278 (11)	0.0169 (10)	0.0038 (8)	0.0059 (8)	0.0009 (8)
C7	0.0148 (9)	0.0226 (10)	0.0229 (11)	0.0041 (8)	0.0051 (8)	-0.0062 (8)
C8	0.0110 (9)	0.0167 (9)	0.0230 (10)	0.0016 (7)	0.0039 (7)	-0.0015 (8)
C9	0.0107 (8)	0.0125 (8)	0.0178 (10)	0.0037 (7)	0.0020 (7)	0.0015 (7)
C10	0.0184 (10)	0.0128 (9)	0.0330 (12)	0.0042 (8)	0.0063 (9)	-0.0019 (8)
C11	0.0201 (10)	0.0122 (9)	0.0354 (12)	0.0058 (8)	0.0042 (9)	0.0065 (8)
C12	0.0131 (9)	0.0145 (9)	0.0239 (11)	0.0038 (7)	0.0020 (8)	0.0050 (8)
C13	0.0113 (8)	0.0134 (9)	0.0189 (10)	0.0029 (7)	0.0016 (7)	0.0031 (7)
C14	0.0227 (10)	0.0194 (10)	0.0282 (11)	0.0068 (8)	0.0026 (9)	0.0137 (9)
C15	0.0270 (11)	0.0248 (11)	0.0188 (10)	0.0056 (9)	0.0016 (8)	0.0105 (8)
C16	0.0262 (11)	0.0180 (10)	0.0164 (10)	0.0047 (8)	0.0016 (8)	0.0017 (8)

Geometric parameters (\AA , $^\circ$)

O1—C1	1.241 (2)	C3—H3A	1.0000
O2—C1	1.269 (2)	C5—C6	1.395 (3)
O3—C2	1.410 (2)	C5—H5A	0.9500
O3—H3	0.89 (3)	C6—C7	1.372 (3)
O4—C3	1.412 (2)	C6—H6	0.9500
O4—H4	0.91 (3)	C7—C8	1.412 (3)
O5—C4	1.311 (2)	C7—H7	0.9500
O5—H5	1.00 (3)	C8—C9	1.406 (3)
O6—C4	1.219 (2)	C8—C10	1.437 (3)
O1W—H11	0.90 (4)	C9—C13	1.434 (3)
O1W—H12	0.92 (3)	C10—C11	1.350 (3)
O2W—H21	0.84 (4)	C10—H10	0.9500
O2W—H22	0.87 (3)	C11—C12	1.437 (3)
N1—C5	1.325 (3)	C11—H11A	0.9500
N1—C9	1.360 (3)	C12—C13	1.403 (3)
N1—H1	0.93 (3)	C12—C14	1.407 (3)

N2—C16	1.326 (3)	C14—C15	1.365 (3)
N2—C13	1.354 (2)	C14—H14	0.9500
C1—C2	1.534 (2)	C15—C16	1.407 (3)
C2—C3	1.535 (2)	C15—H15	0.9500
C2—H2A	1.0000	C16—H16	0.9500
C3—C4	1.522 (2)		
C2—O3—H3	111 (2)	C5—C6—H6	120.1
C3—O4—H4	110.2 (17)	C6—C7—C8	119.99 (19)
C4—O5—H5	111.6 (19)	C6—C7—H7	120.0
H11—O1W—H12	101 (3)	C8—C7—H7	120.0
H21—O2W—H22	109 (3)	C9—C8—C7	118.09 (19)
C5—N1—C9	122.93 (18)	C9—C8—C10	118.62 (19)
C5—N1—H1	117.6 (19)	C7—C8—C10	123.30 (19)
C9—N1—H1	119.4 (19)	N1—C9—C8	119.30 (18)
C16—N2—C13	116.48 (17)	N1—C9—C13	119.82 (17)
O1—C1—O2	125.36 (18)	C8—C9—C13	120.88 (18)
O1—C1—C2	119.50 (17)	C11—C10—C8	121.05 (19)
O2—C1—C2	115.13 (16)	C11—C10—H10	119.5
O3—C2—C1	109.60 (14)	C8—C10—H10	119.5
O3—C2—C3	110.78 (15)	C10—C11—C12	120.86 (19)
C1—C2—C3	109.30 (14)	C10—C11—H11A	119.6
O3—C2—H2A	109.0	C12—C11—H11A	119.6
C1—C2—H2A	109.0	C13—C12—C14	117.29 (18)
C3—C2—H2A	109.0	C13—C12—C11	119.93 (19)
O4—C3—C4	109.91 (14)	C14—C12—C11	122.78 (18)
O4—C3—C2	111.42 (14)	N2—C13—C12	124.24 (18)
C4—C3—C2	109.66 (14)	N2—C13—C9	117.11 (17)
O4—C3—H3A	108.6	C12—C13—C9	118.65 (18)
C4—C3—H3A	108.6	C15—C14—C12	118.92 (19)
C2—C3—H3A	108.6	C15—C14—H14	120.5
O6—C4—O5	124.72 (17)	C12—C14—H14	120.5
O6—C4—C3	123.46 (17)	C14—C15—C16	119.4 (2)
O5—C4—C3	111.81 (15)	C14—C15—H15	120.3
N1—C5—C6	119.94 (19)	C16—C15—H15	120.3
N1—C5—H5A	120.0	N2—C16—C15	123.7 (2)
C6—C5—H5A	120.0	N2—C16—H16	118.1
C7—C6—C5	119.74 (19)	C15—C16—H16	118.1
C7—C6—H6	120.1		
O1—C1—C2—O3	2.5 (2)	C10—C8—C9—C13	1.3 (3)
O2—C1—C2—O3	-178.33 (15)	C9—C8—C10—C11	-0.1 (3)
O1—C1—C2—C3	124.08 (18)	C7—C8—C10—C11	-179.65 (19)
O2—C1—C2—C3	-56.7 (2)	C8—C10—C11—C12	-0.6 (3)
O3—C2—C3—O4	62.92 (19)	C10—C11—C12—C13	0.1 (3)
C1—C2—C3—O4	-57.94 (19)	C10—C11—C12—C14	-179.4 (2)
O3—C2—C3—C4	-58.99 (19)	C16—N2—C13—C12	-0.3 (3)
C1—C2—C3—C4	-179.86 (14)	C16—N2—C13—C9	179.70 (17)
O4—C3—C4—O6	11.4 (2)	C14—C12—C13—N2	0.6 (3)
C2—C3—C4—O6	134.17 (19)	C11—C12—C13—N2	-178.96 (18)

supplementary materials

O4—C3—C4—O5	-169.64 (14)	C14—C12—C13—C9	-179.49 (17)
C2—C3—C4—O5	-46.8 (2)	C11—C12—C13—C9	1.0 (3)
C9—N1—C5—C6	0.1 (3)	N1—C9—C13—N2	-1.5 (3)
N1—C5—C6—C7	0.7 (3)	C8—C9—C13—N2	178.28 (17)
C5—C6—C7—C8	-0.8 (3)	N1—C9—C13—C12	178.54 (17)
C6—C7—C8—C9	0.2 (3)	C8—C9—C13—C12	-1.7 (3)
C6—C7—C8—C10	179.72 (19)	C13—C12—C14—C15	-0.6 (3)
C5—N1—C9—C8	-0.8 (3)	C11—C12—C14—C15	178.92 (19)
C5—N1—C9—C13	179.01 (18)	C12—C14—C15—C16	0.4 (3)
C7—C8—C9—N1	0.6 (3)	C13—N2—C16—C15	0.1 (3)
C10—C8—C9—N1	-178.97 (17)	C14—C15—C16—N2	-0.2 (3)
C7—C8—C9—C13	-179.19 (17)		

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

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O3—H3 \cdots O1w ⁱ	0.89 (3)	1.82 (3)	2.709 (2)	175 (3)
O4—H4 \cdots O2w ⁱⁱ	0.90 (3)	1.84 (3)	2.739 (2)	172 (3)
O5—H5 \cdots O2 ⁱⁱⁱ	0.99 (3)	1.52 (3)	2.508 (2)	169 (3)
O1w—H12 \cdots O1	0.93 (3)	1.97 (3)	2.846 (2)	157 (3)
O1w—H11 \cdots O1 ^{iv}	0.90 (4)	1.86 (4)	2.753 (2)	173 (4)
O2w—H21 \cdots O2	0.84 (4)	1.93 (4)	2.764 (2)	168 (3)
O2w—H22 \cdots O6 ^v	0.87 (3)	1.97 (3)	2.835 (2)	176 (3)
N1—H1 \cdots O1w	0.93 (3)	1.89 (3)	2.753 (2)	153 (3)

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

Fig. 1

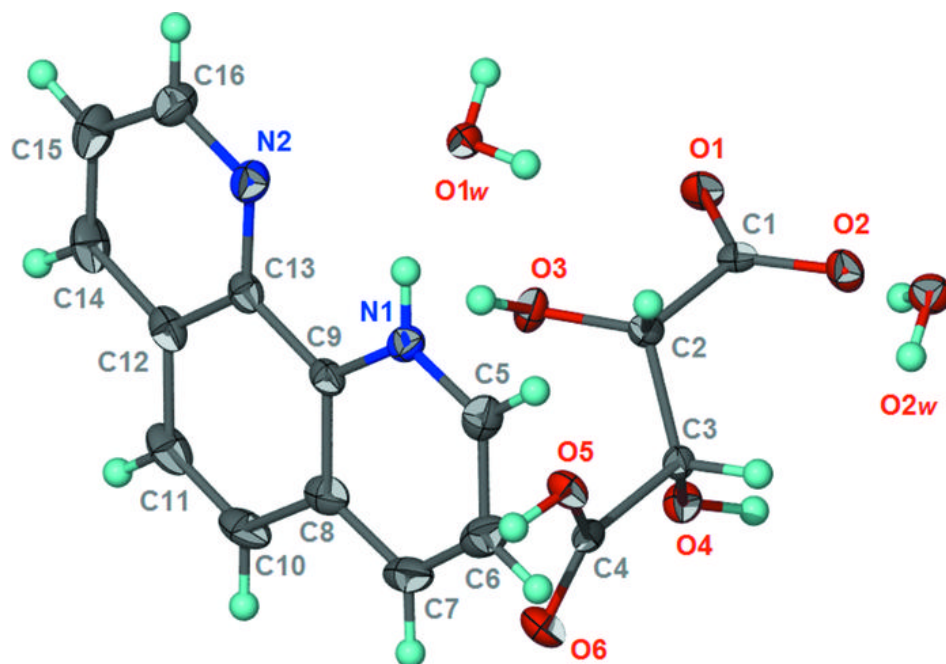


Fig. 2

