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p-Carboxyphenylammonium dihydrogenmonophosphate monohydrate

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.039
wR factor = 0.058
Data-to-parameter ratio = 10.4

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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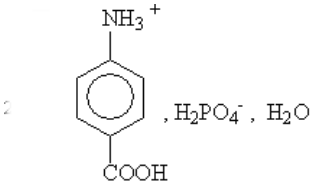
The title compound, $C_7H_8NO_2^+\cdot H_2PO_4^-\cdot H_2O$, is an ionic compound consisting of dihydrogenmonophosphate anions, water molecules and *p*-carboxyphenylammonium cations. The asymmetric unit contains two independent entities, *i.e.* $2(HOOC–C_6H_4–NH_3^+\cdot H_2PO_4^-\cdot H_2O)$. Anions and cations are linked to each other through strong hydrogen bonds, formed by all H atoms covalently bonded to anions, nitrogen, carboxylic groups and water molecules. A three-dimensional complex network of hydrogen bonds ensures the cohesion of the ionic structure.

Comment

The ionic crystal structure of the title compound consists of dihydrogenmonophosphate anions, water molecules and *p*-carboxyphenylammonium cations linked to each other through hydrogen bonds. In the $H_2PO_4^-$ anions, there are two types of P—O bonds, similar to those observed in other ionic compounds (Fabry *et al.*, 1997; Trojette *et al.*, 1998). The shortest mean bond length of 1.505 Å corresponds to the terminal bonds and the P—O bond with the largest mean distance of 1.565 Å corresponds to the P—OH bonds. The independent $[PO_4]$ tetrahedra have three types of O—P—O angles: (i) the smallest bond angles (106.84°) are observed for non-terminal O atoms; (ii) the intermediate mean value (108.62°) corresponds to the angles between terminal and non-terminal O atoms; (iii) bond angles involving only terminal O atoms are the largest (115.1°).



(I)

The average C—C distance of 1.382 Å and the average C—C—C bond angle of 119.96° in the organic $(HOOC–C_6H_4–NH_3)^+$ cations are normal. The phenyl rings are planar, with mean deviations from planarity of less than 0.0027. The ammonium H atoms are involved in hydrogen bonds with water molecules and dihydrogenmonophosphate anions. The water molecules ensure the cohesion between the anions and cations. The tetrahedral $H_2PO_4^-$ anions are linked through hydrogen bonds, giving rise to infinite chains. In turn, phos-

phate groups are linked to the organic cation, first, *via* the carboxylic acid group and, secondly, *via* the ammonium group.

The exceptional shortness [O···O 2.704 (2), 2.563 (2) and 2.577 (2) Å] of the anion–anion (Philippot & Lindqvist, 1971; Calleri & Speakman, 1964) and anion–cation (Blessing & McGandy, 1972) hydrogen bonds is probably due to strong interactions between neighbouring anions and cations. Intra- and intermolecular water–anion and water–cation hydrogen bonds consolidate the ionic packing of this structure.

Experimental

The title compound is formed in the reaction of H_3PO_4 with $HOOC(C_6H_4)NH_2$. Orange plate-like single crystals were obtained after one week by slow evaporation of the solution.

Crystal data

$C_7H_8NO_2^+\cdot H_2PO_4^-\cdot H_2O$	$Z = 4$
$M_r = 253.15$	$D_x = 1.596$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 8.517$ (2) Å	Cell parameters from 25 reflections
$b = 8.902$ (4) Å	$\theta = 1.4$–$30.0°$
$c = 14.513$ (4) Å	$\mu = 0.28$ mm^{-1}
$\alpha = 106.49$ (4)°	$T = 294$ K
$\beta = 90.17$ (5)°	Plate, orange
$\gamma = 92.76$ (4)°	0.6 × 0.3 × 0.2 mm
$V = 1053.6$ (5) Å^3	

Data collection

Enraf–Nonius MACH3 diffractometer	$\theta_{max} = 30.0°$
$\theta/2\theta$ scans	$h = -11 \rightarrow 11$
6146 measured reflections	$k = -12 \rightarrow 12$
6146 independent reflections	$l = -20 \rightarrow 0$
3740 reflections with $I > 3\sigma(I)$	3 standard reflections every 200 reflections
$R_{int} = 0.015$	intensity decay: 1.2%

Refinement

Refinement on F	Only coordinates of H atoms refined
$R = 0.039$	$w = 4F_o^2/[\sigma^2(F_o^2) + 0.0016\ F_o^4]$
$wR = 0.058$	$(\Delta/\sigma)_{max} = 0.014$
$S = 1.14$	$\Delta\rho_{max} = 0.24$ e Å^{-3}
3740 reflections	$\Delta\rho_{min} = -0.37$ e Å^{-3}
361 parameters	

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

D—H···A	D—H	H···A	D···A	D—H···A
O3*a*—H03*a*···O1*b*	0.77 (3)	1.96 (3)	2.720 (2)	171 (3)
O3*b*—H03*b*···O2*a*^{i}	1.02 (3)	1.69 (3)	2.704 (2)	171 (3)
O1*w*—H2*w*1···O1*b*^{ii}	0.79 (3)	1.97 (3)	2.723 (2)	159 (3)
O2*w*—H2*w*2···O2*b*	0.77 (3)	1.99 (3)	2.724 (2)	160 (3)
O2*w*—H1*w*2···O2*a*^{iii}	0.86 (3)	1.89 (3)	2.722 (2)	162 (3)
O1*w*—H1*w*1···O1*a*	0.96 (3)	1.86 (3)	2.797 (2)	165 (2)
N1*a*—H3*na*···O1*b*^{iv}	0.87 (3)	1.96 (3)	2.819 (2)	169 (3)
N1*b*—H1*nb*···O2a	0.96 (3)	1.85 (3)	2.803 (2)	173 (2)
O6*b*—H1*b*···O1*a*^{v}	0.91 (3)	1.67 (3)	2.563 (2)	166 (3)
O6*a*—H1*a*···O2*b*^{vi}	0.98 (3)	1.63 (3)	2.577 (2)	161 (3)
O4*b*—H04*b*···O5*a*^{vi}	0.80 (3)	1.88 (3)	2.643 (2)	160 (3)
O4*a*—H04*a*···O5*b*^{v}	0.75 (3)	1.89 (3)	2.641 (2)	177 (3)
N1*a*—H2*na*···O2*w*	0.92 (3)	1.91 (3)	2.770 (2)	154 (2)
N1*a*—H1*na*···O1*w*^{iv}	0.77 (3)	2.13 (3)	2.862 (3)	158 (3)
N1*b*—H2*nb*···O2*w*^{vii}	0.93 (3)	1.90 (3)	2.802 (3)	163 (2)
N1*b*—H3*nb*···O1*w*^{iv}	0.94 (3)	1.84 (3)	2.778 (2)	173 (2)

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

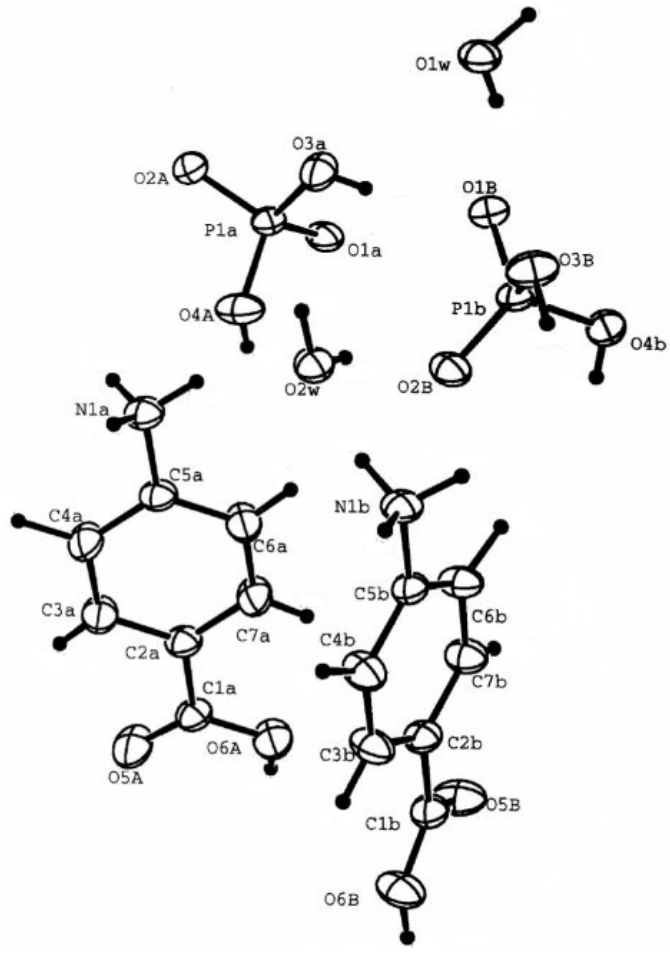


Figure 1
*ORTEP*II (Johnson, 1976) view of the title compound with the atomic labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

Data collection: *CAD*-4 *Operations Manual* (Enraf–Nonius, 1994); cell refinement: *CAD*-4 *Operations Manual*; data reduction: *OpenMoleN* (Nonius, 1997); program(s) used to solve structure: *SIR* (Burla *et al.*, 1989); program(s) used to refine structure: *OpenMoleN*; software used to prepare material for publication: *OpenMoleN*.

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supporting information

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p-Carboxyphenylammonium dihydrogenmonophosphate monohydrate

Nourredine Benali-Cherif, Ali Abouimrane, Kacem Sbai, Hocine Merazig, Aouatef Cherouana and Lamia Bendjeddou

_p_-Carboxyphenyl ammonium dihydrogenmonophosphate hydrate

Crystal data

$C_7H_8NO_2^+·H_2PO_4^-·H_2O$
$M_r = 253.15$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 8.517$ (2) Å
$b = 8.902$ (4) Å
$c = 14.513$ (4) Å
$\alpha = 106.49$ (4)°
$\beta = 90.17$ (5)°
$\gamma = 92.76$ (4)°
$V = 1053.6$ (5) Å^3
$Z = 4.0$
$F(000) = 528$
$D_x = 1.596$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 1.4$–$30.0°$
$\mu = 0.28$ mm^{-1}
$T = 294$ K
Plate, orange
0.6 × 0.3 × 0.2 mm

Data collection

MACH3 diffractometer
Radiation source: X-ray_tube
$\theta/2\theta$ scans
6146 measured reflections
6146 independent reflections
3740 reflections with $I > 3\sigma(I)$
$R_{int} = 0.015$
$\theta_{max} = 30.0°$
$h = -11 \rightarrow 11$
$k = -12 \rightarrow 12$
$l = -20 \rightarrow 0$
3 standard reflections every 200 reflections
intensity decay: −1,2%

Refinement

Refinement on F
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.058$
$S = 1.14$
3740 reflections
361 parameters
24 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
Only H-atom coordinates refined
$w = 4F_o^2/[\sigma^2(F_o^2) + 0.0016\,F_o^4]$
$(\Delta/\sigma)_{max} = 0.014$
$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.37$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1w	1.0978 (2)	0.7401 (2)	0.1100 (1)	0.0332 (7)
O2w	0.4062 (2)	0.2456 (2)	0.1063 (1)	0.0320 (7)

P1b	0.82631 (7)	0.23331 (7)	0.13409 (4)	0.0275 (2)
P1a	0.67246 (7)	0.72132 (7)	0.13677 (4)	0.0270 (2)
O1a	0.8105 (2)	0.7791 (2)	0.2046 (1)	0.0317 (7)
O1B	0.8950 (2)	0.3495 (2)	0.0855 (1)	0.0327 (7)
O2A	0.6136 (2)	0.8385 (2)	0.0891 (1)	0.0327 (7)
O2B	0.6908 (2)	0.2895 (2)	0.1987 (1)	0.0336 (7)
O3a	0.7172 (2)	0.5756 (2)	0.0530 (1)	0.0378 (8)
O3B	0.7738 (2)	0.0831 (2)	0.0511 (1)	0.0383 (8)
O4A	0.5324 (2)	0.6653 (2)	0.1901 (1)	0.0384 (8)
O4b	0.9609 (2)	0.1855 (2)	0.1921 (1)	0.0390 (8)
O5A	0.0942 (2)	0.7385 (2)	0.6217 (1)	0.0453 (9)
O5B	0.4348 (2)	1.2418 (2)	0.6208 (1)	0.0400 (8)
O6B	0.1993 (2)	1.1160 (2)	0.6119 (1)	0.0379 (8)
O6A	0.2891 (2)	0.5790 (2)	0.6187 (1)	0.0395 (8)
N1a	0.1904 (2)	0.4749 (2)	0.1676 (1)	0.0298 (8)
N1b	0.3345 (2)	0.9755 (2)	0.1638 (1)	0.0285 (8)
C1a	0.1852 (3)	0.6433 (3)	0.5775 (1)	0.0307 (9)
C1b	0.3247 (3)	1.1625 (3)	0.5741 (1)	0.0313 (9)
C2a	0.1866 (3)	0.5934 (3)	0.4706 (1)	0.0288 (9)
C2b	0.3248 (3)	1.1106 (2)	0.4670 (1)	0.0281 (9)
C3b	0.1903 (3)	1.0467 (3)	0.4140 (2)	0.034 (1)
C3a	0.0716 (3)	0.6441 (3)	0.4203 (2)	0.037 (1)
C4a	0.0714 (3)	0.6032 (3)	0.3207 (1)	0.037 (1)
C4b	0.1934 (3)	1.0028 (3)	0.3142 (1)	0.032 (1)
C5a	0.1887 (3)	0.5147 (2)	0.2727 (1)	0.0268 (9)
C5b	0.3318 (3)	1.0216 (2)	0.2687 (1)	0.0267 (8)
C6b	0.4673 (3)	1.0842 (3)	0.3208 (1)	0.033 (1)
C6a	0.3029 (3)	0.4606 (3)	0.3207 (2)	0.033 (1)
C7a	0.3007 (3)	0.5004 (3)	0.4203 (2)	0.034 (1)
C7b	0.4636 (3)	1.1290 (3)	0.4200 (1)	0.032 (1)
H1nb	0.431 (3)	0.927 (3)	0.143 (2)	0.0399*
H1b	0.196 (3)	1.137 (3)	0.677 (2)	0.0573*
H1na	0.191 (3)	0.551 (3)	0.152 (2)	0.0404*
H1a	0.303 (3)	0.649 (3)	0.684 (2)	0.0559*
H2na	0.277 (3)	0.422 (3)	0.140 (2)	0.0404*
H2nb	0.338 (3)	1.062 (3)	0.140 (2)	0.0399*
H3b	0.099 (3)	1.033 (3)	0.445 (2)	0.0482*
H03a	0.763 (3)	0.514 (3)	0.068 (2)	0.0522*
H03b	0.716 (3)	−0.004 (3)	0.072 (2)	0.0535*
H3nb	0.249 (3)	0.902 (3)	0.144 (2)	0.0399*
H3na	0.104 (3)	0.424 (3)	0.142 (2)	0.0404*
H3a	0.009 (3)	0.706 (3)	0.456 (2)	0.0511*
H04a	0.539 (3)	0.693 (3)	0.244 (2)	0.0532*
H04b	0.923 (3)	0.200 (3)	0.244 (2)	0.0538*
H4a	−0.020 (3)	0.642 (3)	0.282 (2)	0.0502*
H4b	0.103 (3)	0.971 (3)	0.276 (2)	0.0465*
H6b	0.580 (3)	1.092 (3)	0.292 (2)	0.0453*
H6a	0.377 (3)	0.397 (3)	0.283 (2)	0.0448*

H7a	0.370 (3)	0.465 (3)	0.453 (2)	0.0450*
H7b	0.557 (3)	1.187 (3)	0.458 (2)	0.0452*
H1w1	0.999 (3)	0.771 (3)	0.140 (2)	0.0459*
H1w2	0.410 (3)	0.239 (3)	0.046 (2)	0.0441*
H2w1	1.082 (3)	0.730 (3)	0.055 (2)	0.0459*
H2w2	0.487 (3)	0.278 (3)	0.129 (2)	0.0441*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1w	0.0360 (8)	0.0484 (8)	0.0210 (6)	0.0013 (7)	0.0021 (6)	0.0093 (6)
O2w	0.0335 (7)	0.0461 (8)	0.0212 (6)	0.0039 (7)	−0.0007 (6)	0.0085 (6)
P1b	0.0323 (3)	0.0362 (2)	0.0177 (2)	−0.0006 (2)	−0.0004 (2)	0.0090 (2)
P1a	0.0313 (2)	0.0352 (2)	0.0179 (2)	0.0035 (2)	0.0011 (2)	0.0084 (2)
O1a	0.0290 (7)	0.0560 (9)	0.0195 (6)	0.0024 (7)	0.0003 (6)	0.0105 (6)
O1b	0.0381 (8)	0.0372 (7)	0.0246 (6)	−0.0001 (6)	0.0016 (6)	0.0118 (5)
O2a	0.0367 (8)	0.0368 (7)	0.0260 (6)	0.0061 (6)	0.0010 (6)	0.0118 (5)
O2b	0.0309 (7)	0.0575 (9)	0.0213 (6)	0.0027 (7)	−0.0003 (6)	0.0095 (6)
O3a	0.0556 (9)	0.0400 (8)	0.0242 (7)	0.0169 (7)	−0.0010 (7)	0.0062 (6)
O3b	0.056 (1)	0.0402 (8)	0.0247 (7)	−0.0100 (8)	−0.0014 (7)	0.0076 (6)
O4a	0.0423 (9)	0.0574 (9)	0.0233 (6)	−0.0119 (8)	−0.0000 (6)	0.0128 (6)
O4b	0.0440 (9)	0.0588 (9)	0.0228 (6)	0.0140 (7)	−0.0003 (6)	0.0137 (6)
O5a	0.067 (1)	0.0611 (9)	0.0226 (7)	0.0279 (8)	0.0030 (7)	0.0103 (6)
O5b	0.052 (1)	0.060 (1)	0.0207 (6)	−0.0143 (8)	−0.0020 (7)	0.0088 (6)
O6b	0.0376 (8)	0.071 (1)	0.0204 (6)	−0.0008 (8)	0.0036 (6)	0.0095 (7)
O6a	0.0451 (9)	0.0600 (9)	0.0227 (6)	0.0122 (8)	−0.0027 (7)	0.0086 (6)
N1a	0.0360 (9)	0.0363 (8)	0.0202 (7)	0.0011 (8)	0.0002 (7)	0.0076 (6)
N1b	0.0360 (9)	0.0392 (9)	0.0165 (6)	0.0024 (8)	0.0020 (7)	0.0061 (6)
C1a	0.035 (1)	0.038 (1)	0.0218 (8)	0.0015 (9)	−0.0024 (8)	0.0100 (7)
C1b	0.038 (1)	0.037 (1)	0.0222 (8)	0.0055 (9)	0.0025 (8)	0.0100 (7)
C2a	0.032 (1)	0.0369 (9)	0.0200 (7)	0.0001 (8)	−0.0007 (7)	0.0088 (7)
C2b	0.038 (1)	0.0324 (9)	0.0181 (7)	0.0040 (8)	0.0021 (8)	0.0065 (7)
C3b	0.031 (1)	0.053 (1)	0.0234 (8)	0.001 (1)	0.0056 (8)	0.0072 (8)
C3a	0.046 (1)	0.051 (1)	0.0223 (8)	0.021 (1)	0.0058 (9)	0.0096 (8)
C4a	0.044 (1)	0.051 (1)	0.0229 (8)	0.018 (1)	0.0005 (9)	0.0110 (8)
C4b	0.032 (1)	0.049 (1)	0.0217 (9)	0.002 (1)	−0.0002 (8)	0.0031 (8)
C5a	0.031 (1)	0.0335 (9)	0.0183 (7)	−0.0008 (8)	−0.0014 (7)	0.0067 (7)
C5b	0.033 (1)	0.0316 (9)	0.0183 (7)	0.0047 (8)	0.0015 (7)	0.0087 (6)
C6b	0.035 (1)	0.045 (1)	0.0222 (8)	−0.0039 (9)	0.0031 (8)	0.0105 (7)
C6a	0.034 (1)	0.044 (1)	0.0247 (9)	0.0098 (9)	−0.0014 (8)	0.0048 (8)
C7a	0.035 (1)	0.046 (1)	0.0248 (9)	0.0085 (9)	−0.0054 (8)	0.0074 (8)
C7b	0.034 (1)	0.043 (1)	0.0234 (8)	−0.0036 (9)	−0.0006 (8)	0.0084 (8)

Geometric parameters (Å, º)

O1w—H1w1	0.97 (3)	N1b—C5b	1.460 (2)
O1w—H2w1	0.78 (3)	N1b—H1nb	0.96 (3)
O2w—H1w2	0.87 (3)	N1b—H2nb	0.93 (3)

O2w—H2w2	0.77 (2)	N1b—H3nb	0.94 (2)
P1b—O1b	1.506 (2)	C1a—C2a	1.488 (3)
P1b—O2b	1.502 (2)	C1b—C2b	1.491 (3)
P1b—O3b	1.569 (1)	C2a—C3a	1.386 (4)
P1b—O4b	1.564 (2)	C2a—C7a	1.379 (3)
P1a—O1a	1.505 (1)	C2b—C3b	1.382 (3)
P1a—O2a	1.509 (2)	C2b—C7b	1.393 (3)
P1a—O3a	1.568 (1)	C3b—C4b	1.390 (3)
P1a—O4a	1.561 (2)	C3b—H3b	0.92 (3)
O3a—H03a	0.77 (3)	C3a—C4a	1.387 (3)
O3b—H03b	1.02 (3)	C3a—H3a	0.86 (2)
O4a—H04a	0.75 (3)	C4a—C5a	1.368 (3)
O4b—H04b	0.80 (3)	C4a—H4a	1.08 (3)
O5a—C1a	1.220 (3)	C4b—C5b	1.379 (3)
O5b—C1b	1.224 (3)	C4b—H4b	0.93 (3)
O6b—C1b	1.305 (3)	C5a—C6a	1.376 (3)
O6b—H1b	0.92 (3)	C5b—C6b	1.381 (3)
O6a—C1a	1.307 (3)	C6b—C7b	1.381 (3)
O6a—H1a	0.98 (2)	C6b—H6b	1.06 (3)
N1a—C5a	1.465 (3)	C6a—C7a	1.388 (3)
N1a—H1na	0.78 (3)	C6a—H6a	0.93 (2)
N1a—H2na	0.92 (2)	C7a—H7a	0.89 (3)
N1a—H3na	0.87 (2)	C7b—H7b	1.00 (2)

H1w1—O1w—H2w1	104 (2)	O6b—C1b—C2b	114.3 (2)
H1w2—O2w—H2w2	107 (2)	C1a—C2a—C3a	119.1 (2)
O1b—P1b—O2b	115.0 (1)	C1a—C2a—C7a	121.8 (2)
O1b—P1b—O3b	105.92 (9)	C3a—C2a—C7a	119.1 (2)
O1b—P1b—O4b	108.3 (1)	C1b—C2b—C3b	121.4 (2)
O2b—P1b—O3b	110.42 (9)	C1b—C2b—C7b	118.8 (2)
O2b—P1b—O4b	110.00 (9)	C3b—C2b—C7b	119.7 (2)
O3b—P1b—O4b	106.9 (1)	C2b—C3b—C4b	120.0 (2)
O1a—P1a—O2a	115.2 (1)	C2b—C3b—H3b	119 (1)
O1a—P1a—O3a	110.06 (9)	C4b—C3b—H3b	120 (1)
O1a—P1a—O4a	110.22 (9)	C2a—C3a—C4a	120.7 (2)
O2a—P1a—O3a	105.90 (9)	C2a—C3a—H3a	113 (1)
O2a—P1a—O4a	108.2 (1)	C4a—C3a—H3a	125 (1)
O3a—P1a—O4a	106.78 (9)	C3a—C4a—C5a	118.9 (2)
P1a—O3a—H03a	115 (1)	C3a—C4a—H4a	120 (1)
P1b—O3b—H03b	115 (1)	C5a—C4a—H4a	120 (1)
P1a—O4a—H04a	115 (2)	C3b—C4b—C5b	119.5 (2)
P1b—O4b—H04b	101 (2)	C3b—C4b—H4b	122 (1)
C1b—O6b—H1b	118 (1)	C5b—C4b—H4b	117 (1)
C1a—O6a—H1a	105 (1)	N1a—C5a—C4a	118.9 (2)
C5a—N1a—H1na	109 (1)	N1a—C5a—C6a	119.5 (2)
C5a—N1a—H2na	114 (1)	C4a—C5a—C6a	121.6 (2)
C5a—N1a—H3na	111 (1)	N1b—C5b—C4b	119.4 (2)
H1na—N1a—H2na	106 (2)	N1b—C5b—C6b	119.6 (2)

H1na—N1a—H3na	104 (2)	C4b—C5b—C6b	121.0 (2)
H2na—N1a—H3na	110 (2)	C5b—C6b—C7b	119.3 (2)
C5b—N1b—H1nb	109 (1)	C5b—C6b—H6b	125 (1)
C5b—N1b—H2nb	111 (1)	C7b—C6b—H6b	114 (1)
C5b—N1b—H3nb	105 (1)	C5a—C6a—C7a	118.9 (2)
H1nb—N1b—H2nb	103 (2)	C5a—C6a—H6a	117 (1)
H1nb—N1b—H3nb	110 (2)	C7a—C6a—H6a	123 (1)
H2nb—N1b—H3nb	116 (2)	C2a—C7a—C6a	120.6 (2)
O5a—C1a—O6a	123.8 (2)	C2a—C7a—H7a	117 (1)
O5a—C1a—C2a	121.4 (2)	C6a—C7a—H7a	121 (1)
O6a—C1a—C2a	114.8 (2)	C2b—C7b—C6b	120.3 (2)
O5b—C1b—O6b	124.1 (2)	C2b—C7b—H7b	119 (1)
O5b—C1b—C2b	121.5 (2)	C6b—C7b—H7b	119 (1)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3a—H03a···O1b	0.77 (3)	1.96 (3)	2.720 (2)	171 (3)
O3b—H03b···O2a^{i}	1.02 (3)	1.69 (3)	2.704 (2)	171 (3)
O1w—H2w1···O1b^{ii}	0.79 (3)	1.97 (3)	2.723 (2)	159 (3)
O2w—H2w2···O2b	0.77 (3)	1.99 (3)	2.724 (2)	160 (3)
O2w—H1w2···O2a^{iii}	0.86 (3)	1.89 (3)	2.722 (2)	162 (3)
O1w—H1w1···O1a	0.96 (3)	1.86 (3)	2.797 (2)	165 (2)
N1a—H3na···O1b^{iv}	0.87 (3)	1.96 (3)	2.819 (2)	169 (3)
N1b—H1nb···O2a	0.96 (3)	1.85 (3)	2.803 (2)	173 (2)
O6b—H1b···O1a^{v}	0.91 (3)	1.67 (3)	2.563 (2)	166 (3)
O6a—H1a···O2b^{vi}	0.98 (3)	1.63 (3)	2.577 (2)	161 (3)
O4b—H04b···O5a^{vi}	0.80 (3)	1.88 (3)	2.643 (2)	160 (3)
O4a—H04a···O5b^{v}	0.75 (3)	1.89 (3)	2.641 (2)	177 (3)
N1a—H2na···O2w	0.92 (3)	1.91 (3)	2.770 (2)	154 (2)
N1a—H1na···O1w^{iv}	0.77 (3)	2.13 (3)	2.862 (3)	158 (3)
N1b—H2nb···O2w^{vii}	0.93 (3)	1.90 (3)	2.802 (3)	163 (2)
N1b—H3nb···O1w^{iv}	0.94 (3)	1.84 (3)	2.778 (2)	173 (2)

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