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p-Carboxyphenylammonium dihydrogenmonophosphate monohydrate

Nourredine Benali-Cherif,[a]* Ali Abouimrane,[b] Kacem Sbai,[b] Hocine Merazig,[a] Aouatef Cherouana[a] and Lamia Bendjeddou[a]

[a]Laboratoire de Chimie Moléculaire, du Contrôle, de l'Environnement et de Mesures Physico-Chimiques, Faculté des Sciences, Département de Chimie, Université Mentouri de Constantine, 25000 Constantine, Algeria, and [b]Laboratoire de Recherche de Chimie-Physique Générale, Faculté des Sciences Ben M'sik, Université HassanII-Mohammedia, BP 7955 Casablanca, Morroco

Correspondence e-mail: benalicherif@hotmail.com

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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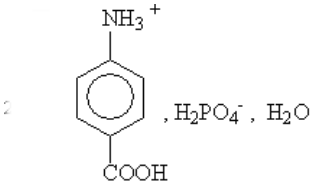
The title compound, $C_7H_8NO_2^+\cdot H_2PO_4^-\cdot H_2O$, is an ionic compound consisting of dihydrogenmonophosphate anions, water molecules and *p*-carboxyphenylammonium cations. The asymmetric unit contains two independent entities, *i.e.* $2(HOOC–C_6H_4–NH_3^+\cdot H_2PO_4^-\cdot H_2O)$. Anions 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) $x, 1+y, z$.

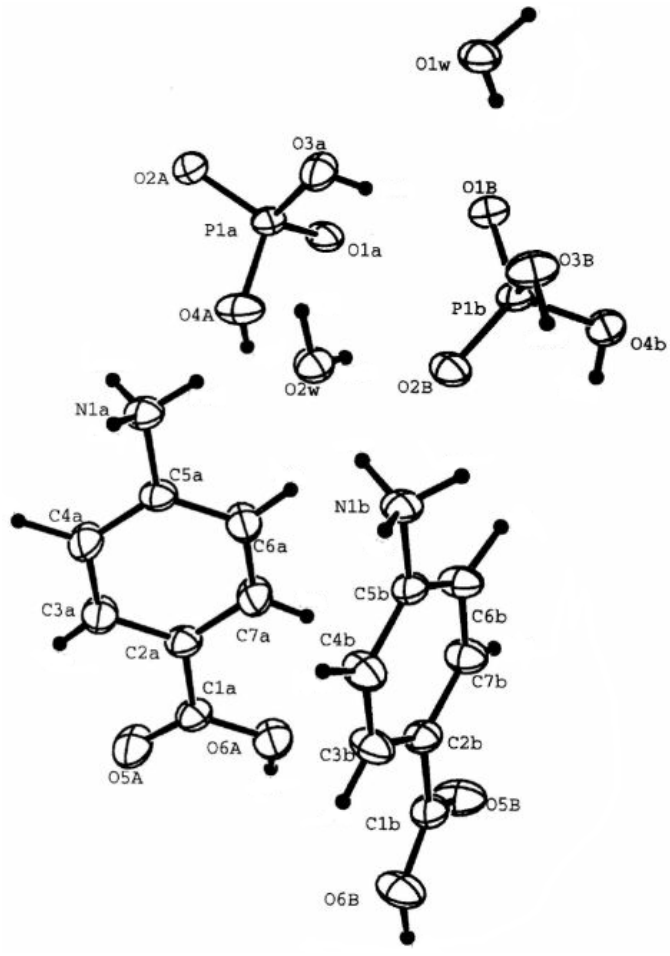


Figure 1
*ORTEP*II (Johnson, 1976) view of the title compound with the atomic labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

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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