Hydrogen bonding in 2-carboxyanilinium dihydrogenphosphate

Article *in* Acta Crystallographica Section E Structure Reports Online · May 2007

DOI: 10.1107/S1600536807016303/pv2008lsup2.hkl

electronic reprint

Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368
Editors: **W. Clegg and D. G. Watson**

Hydrogen bonding in 2-carboxyanilinium dihydrogenphosphate

Nourredine Benali-Cherif, Fatima Allouche, Amani Direm, Lila Boukli-H-Benmenni and Kawther Soudani

Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Hydrogen bonding in 2-carboxyanilinium dihydrogenphosphate

Nourredine Benali-Cherif,[a]* Fatima Allouche,[a] Amani Direm,[a] Lila Boukli-H-Benmenni[b] and Kawther Soudani[a]

[a]Laboratoire des Structures, Propriétés et Interactions Inter Atomiques (LASPI^{2}A), Centre Universitaire de Khenchela, 40000 Khenchela, Algeria, and [b]Département de Chimie, Université Aboubakr Belkaid, Telemcen, Algeria

Correspondence e-mail: benalicherif@hotmail.com

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.037
wR factor = 0.090
Data-to-parameter ratio = 19.4

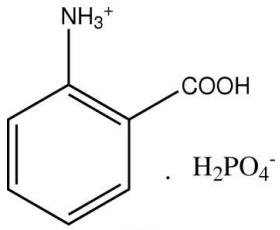
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 14 March 2007
Accepted 2 April 2007

The structure of the title compound, $C_7H_8NO_2^+\cdot H_2PO_4^-$, shows that a single proton transfer occurs. The anions and cations are held together *via* strong and short O—H···O hydrogen bonds, in addition to N—H···O interactions. The three-dimensional complex network of hydrogen bonds ensures the cohesion of the ionic structure.

Comment

This work is part of our research on intermolecular interactions in hydrogen-bonded molecular and ionic crystals. In recent years investigations of hybrid materials have attracted a great deal of attention; in addition to their interesting structural topologies and potential application in the field of new materials science, such as ion-exchange, adsorption, molecular recognition, catalysis and magnetism, hybrid compounds have very interesting electrical, magnetic and optical properties (Kagan *et al.*, 1999; Mazeaud *et al.*, 2000; Ravikumar *et al.*, 2002; Aakeroy *et al.*, 1999; Siegel *et al.*, 1998). The kind of hydrogen bonding in hybrid compounds is also present in the active sites of several biological systems.



(I)

The structure of the title compound, (I) (Fig. 1), is composed of cationic HOO—C_6H_4—NH_3^+ and anionic $H_2PO_4^-$ layers alternating along the *a* axis with a spacing of 5.239 (3) Å. All bond lengths and angles in (I) are within normal ranges and in good agreement with those observed in similar compounds (In *et al.*, 1997; Slouf, 2000).

The phosphate anion is stabilized by strong interactions with its environment; there are two types of P—O bonds and three types of O—P—O angles. The bond lengths and angles of the phosphate anions are similar to those observed in *p*-carboxyphenylammonium dihydrogenmonophosphate monohydrate (Benali-Cherif *et al.*, 2002), in accord with a tetrahedral configuration (Table 1).

There are two types of hydrogen bonds that are observed in (I): cation–anion and anion–anion interactions (Table 2). Each of the cations is bonded to the anions *via* hydrogen bonds as shown in Fig. 2. The protonated N atoms are involved in the

strongest hydrogen bonds *via* intermolecular interactions to phosphate. Another strong interaction involving the carboxylic acid group is observed between anions and cations.

The dihydrogenmonophosphate anions, with their four O atoms and two H atoms, are of great importance in the crystal cohesion; an intricate three-dimensional network of hydrogen bonding is observed. The crystal packing is estabilished by the arrangement of parallel layers of anions and cations.

Experimental

Single crystals of (I) were prepared by slow evaporation at room temperature of an equimolar aqueous solution of 2-aminobenzoic acid (*o*-ABA) and orthophosphoric acid (H_3PO_4).

Crystal data

$C_7H_8O_2N^+\cdot H_2PO_4^-$
M_r = 235.13
Triclinic, $P\overline{1}$
a = 4.8541 (8) Å
b = 9.9845 (9) Å
c = 10.4849 (2) Å
α = 108.383 (5)°
β = 97.816 (8)°
γ = 96.071 (6)°
V = 471.74 (9) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.30 mm^{-1}
T = 293 (2) K
0.2 × 0.15 × 0.1 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: none
8460 measured reflections
2713 independent reflections
2363 reflections with $I > 2\sigma(I)$
R_{int} = 0.044

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.090
S = 1.08
2713 reflections
140 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

P—O1	1.502 (1)	O5—C1	1.203 (2)
P—O2	1.504 (2)	N—C3	1.460 (1)
P—O4	1.562 (1)	C1—O6	1.323 (1)
P—O3	1.579 (2)		
O1—P—O2	115.84 (6)	O1—P—O3	108.21 (6)
O1—P—O4	109.74 (7)	O2—P—O3	108.92 (6)
O2—P—O4	106.23 (6)	O4—P—O3	107.61 (6)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N—H3*N*···O1	0.89	1.98	2.856 (2)	167
N—H2*N*···O1^{i}	0.89	2.01	2.888 (1)	170
N—H1*N*···O1^{ii}	0.89	1.97	2.852 (2)	173
O3—H03···O2^{iii}	0.82	1.77	2.584 (1)	173
O4—H04···O2^{iv}	0.82	1.78	2.564 (2)	159
O6—H1···O3^{v}	0.82	1.98	2.794 (2)	174
C6—H6···O2^{vi}	0.93	2.67	3.399 (2)	135
C7—H7···O6	0.93	2.44	2.759 (2)	100

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

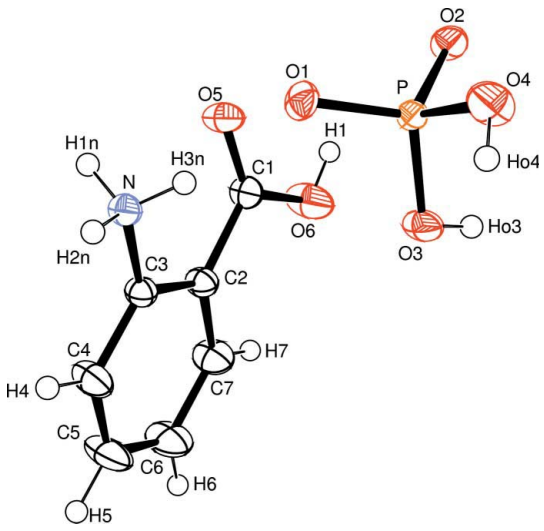


Figure 1
The molecular structure of (I). Displacement ellipsoids are drawn at the 50% probability level.

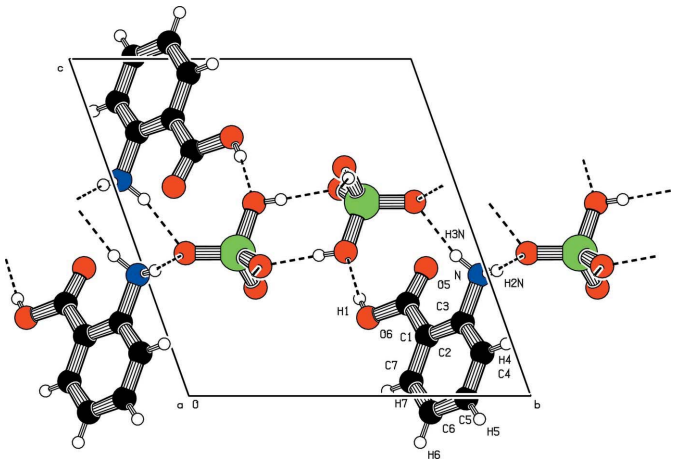


Figure 2
A unit-cell projection down the *a* axis, showing the hydrogen-bonding (dashed lines) network and the alternating layers of $C_7H_8NO_2^+$ and $H_2PO_4^-$.

H atoms were located in difference Fourier syntheses and included as riding atoms with distance constraints of N—H = 0.89, O—H = 0.82 and C—H = 0.93 Å [U_{iso}(H) = 1.5U_{eq}(N,O) and 1.2U_{eq}(C)].

Data collection: *KappaCCD Server Software* (Nonius, 1998); cell refinement: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK*; program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

We thank Dr M. Giorgi from LBS-UMR 6517, Faculté des Sciences et Techniques de Saint Jérôme, Marseille, France, for providing diffraction facilities and le Centre Universitaire de Khenchela for financial support.

References

Aakeroy, C. B., Beatty, A. M. & Leinen, D. S. (1999). *Angew. Chem. Int. Ed.* **38**, 1815–1819.

Benali-Cherif, N., Abouimrane, A., Sbai, K., Merazig, H., Cherouana, A. & Bendjeddou, L. (2002). *Acta Cryst.* E**58**, o160–o161.

Burla, M. C., Caliandro, R., Camalli, M., Carrozzini, B., Cascarano, G. L., De Caro, L., Giacovazzo, C., Polidori, G. & Spagna, R. (2005). *J. Appl. Cryst.* **38**, 381–388.

Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.

Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.

In, Y., Nagata, H., Doi, M., Ishida, T. & Wakahara, A. (1997). *Acta Cryst.* C**53**, 646–648.

Kagan, C. R., Mitzi, D. B. & Dimitrakopoulos, C. D. (1999). *Science*, **286**, 945–947.

Mazeaud, A., Dromzee, Y. & Thouvenot, R. (2000). *Inorg. Chem.* **39**, 4735–4740.

Nonius (1998). *KappaCCD Server Software*. Nonius BV, Delft, The Netherlands.

Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.

Ravikumar, B. S., Sridhar, B. & Rajaram, R. K. (2002). *Acta Cryst.* E**58**, o879–o881.

Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.

Siegel, R. K. O., Freisinger, E., Metzger, S. & Lippert, B. (1998). *J. Am. Chem. Soc.* **120**, 12000–12007.

Slouf, M. (2000). *Acta Cryst.* C**56**, e353.

Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.