

The importance of hydrogen bond in a new hybrids compound

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Abstract. Organic inorganic compounds constitute a vast family of hybrid materials of considerable technological importance. Indeed, due to the nature (molecular, ionic, hydrogen bonding, etc...) of organic and inorganic components, many combinations may be achieved to elaborate suitable materials, so as to exhibit some interesting crystal structure and some special properties in several areas, such as nonlinear optical (NLO), magnetism, luminescence, photography and drug delivery, etc [1]. Moreover, hydrogen bonding is of intense interest because of their widespread occurrence in biological systems. So, it is very helpful to search simple molecules allowing to understanding the configuration and the function of some complex molecules.

The hybrid compounds are rich in H-bonds and they could be used to this effect because of their potential importance in constructing sophisticated assemblies from discrete ionic or molecular building blocks due to its strength and directionality [2]. In order to enrich the varieties in such kinds of hybrid materials and to investigate the influence of hydrogen bonds on the on the structural features, they have synthesized a new compound, This kind of hydrogen bonding appears in the active sites of several biological systems and is observed in similar previously studied hybrid compounds [3, 4, 5]. The combination of the organic matrix and the mineral anions allowed us to obtain original structures [6,7].

Our current domain of research consists the study of the hydrogen connections in a series of hybrids compound, To do it, we are going to use the potentialities which offers the ADF software (Amsterdam Density Functional) to study this type chap of compounds under solid (determination of gaps, level of fermi etc.....).

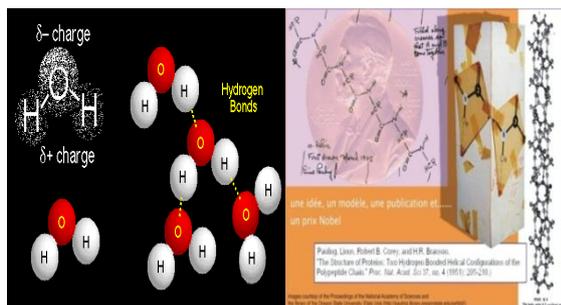
1. Introduction

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.

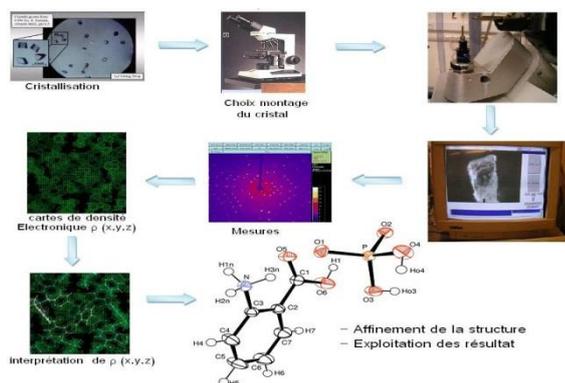
The hybrid compounds are rich in H-bonds and they could be used to this effect because of their potential importance in constructing sophisticated assemblies from discrete ionic or molecular building blocks due to its strength and directionality .The combination of the organic matrix and the mineral anions allowed us to obtain original structures.

We were able to isolate two new compounds:

- o-Carboxyanilinium dihydrogen phosphate (o-CADP)
Acta Cryst. E63, o2054--o2056, (2007).
- o-Carboxyanilinium dihydrogen phosphite (o-CADPx)
Acta Cryst. E65, o664—o665, (2009).



2. Acquisition of the results made by the kappa CCD:



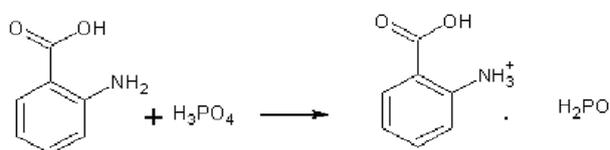
3. Results and Discussion

3.1. Hydrogen bonding in 2-carboxyanilinium dihydrogen phosphate (o-CADP):

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

3.1.1. 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).



The structure (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.

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 $H_2PO_4^-$.

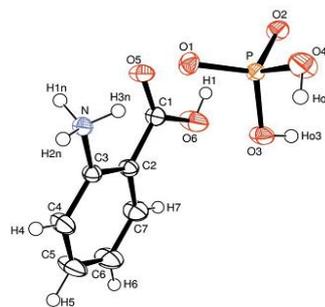


Figure 1.

There are two types of hydrogen bonds that are observed in (I): cation–anion and anion–anion interactions. Each of the cations is bonded to the anions via hydrogen bonds as shown in Fig. 2-3. 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 crystal packing is established by the arrangement of parallel layers of anions and cations.

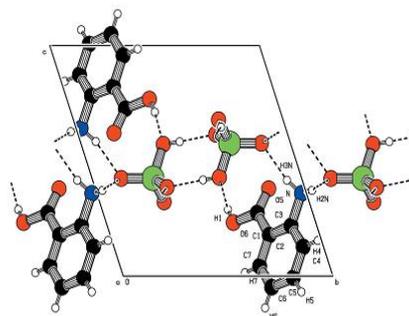


Figure 2: A unit-cell projection down the **a** axis, showing the hydrogen-bonding

(dashed lines) network and the alternating layers of $C_7H_8NO_2^+$ and $H_2PO_4^-$

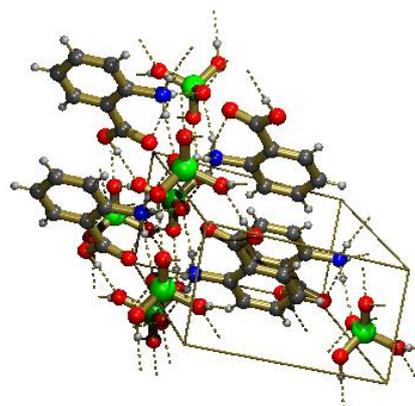


Figure 3

The table 1 showing the different hydrogen bonding in the structure.

D: Donneur H: Hydrogène et A: Accepteur.

Table 1 : The hydrogen bond of (o-CADP).

D—H...A	D—H (Å°)	H...A (Å°)	D...A (Å°)	D—H...A (°)
N-H3N...O1	0,89	1,98	2,856(2)	166,7
N-H2N...O1	0,89	2,01	2,8880(10)	170,3
N-H1N...O1	0,89	1,97	2,852(2)	172,8
O3-HO3...O2	0,82	1,77	2,584(10)	173,1
O4-HO4...O2	0,82	1,78	2,564(2)	159,1
O6-H1...O3	0,82	1,98	2,794(2)	173,6
C6-H6...O2	0,93	2,67	3,399(2)	135,3
C7-H7...O6	0,93	2,44	2,759(2)	100,0

3.2. Hydrogen bonding in 2-carboxyanilinium dihydrogen phosphite (o-CADPx):

3.2.1. Experimental

Crystals of anthranilicium phosphate are prepared by slow evaporation at room temperature of an aqueous solution of 2-aminobenzoic acid and H_3PO_3 in a 1:1 stoichiometric ratio.

The structure (I) (Fig. 4), is composed of cationic $\text{HOO---C}_6\text{H}_4\text{---NH}_3^+$ and anionic H_2PO_3^-

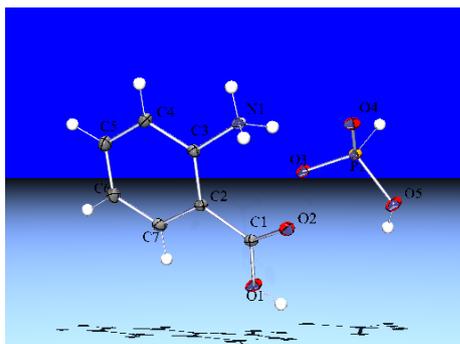
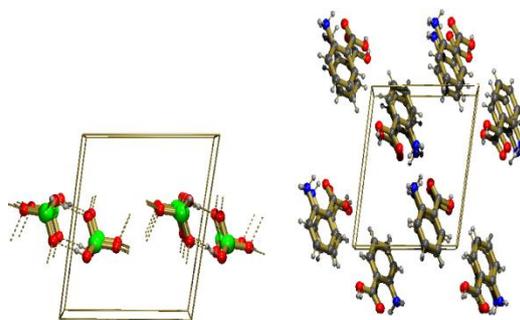


Figure 4

The title compound, $\text{C}_7\text{H}_8\text{NO}_2^+ \cdot \text{H}_2\text{PO}_3^-$, is formed from alternating layers of organic cations and inorganic anions stacked along the *a*-axis. They are associated via O—HO, N—HO and C—HO hydrogen bonding, giving rise to two different $\text{R}_2^2(8)$ graph-set motifs and generating a three-dimensional network.



The organic cations are placed between dimères $[(\text{H}_4\text{P}_2\text{O}_6)]^{2-}$ formed by the grouping of H_2PO_3^-

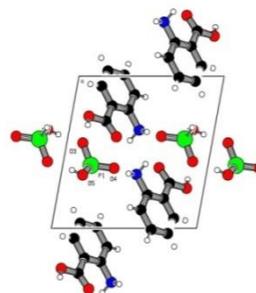
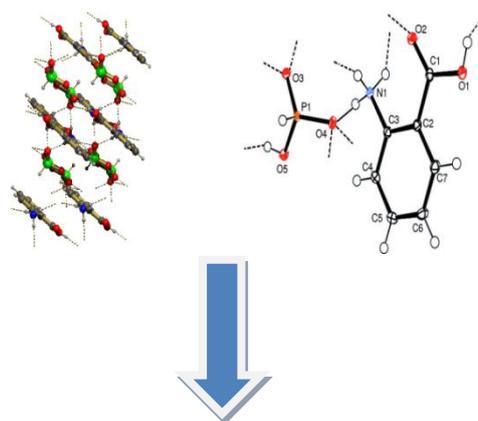
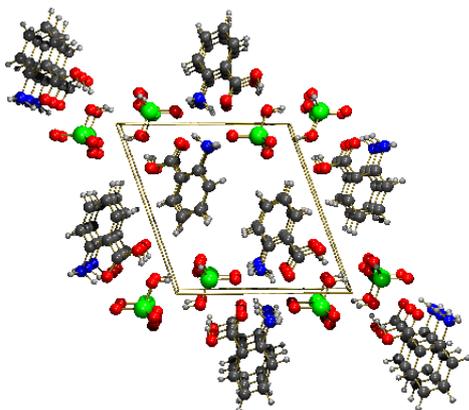


Figure 5

The three H atoms of the anilinium group are subsequently involved in extensive N—H...O hydrogen-bonding (table 2) interactions with O4 being a multiple acceptor of three different phosphate anions, while O3 behaves as double acceptor of hydrogen bonds from one cation, via O1 in the carboxylic group, and one anion, via O5 in the phosphite anion. These interactions give rise to two different $\text{R}_2^2(8)$ graph set motifs (Bernstein et al. 1995), shown in Fig 5. In addition, there are intramolecular interactions involving the benzene ring and the carboxylic group ensuring cohesion and stability of the crystal structure.



**Table 2 : The hydrogen bonding**

D—H...A	D—H (Å°)	H...A (Å°)	D...A (Å°)	D—H...A (°)
O1-H1...O3 ⁱ	0,84	1,77	2,6085(13)	178
N1-H1A...O4	0,91	1,96	2,8589(14)	169
N1-H1B...O4 ⁱⁱ	0,91	2,02	2,9160(13)	169
N1-H1C...O4 ⁱⁱⁱ	0,91	1,97	2,8740(14)	173
O5-H5O...O3 ^{iv}	0,84	1,78	2,6059(13)	167
O6-H6...O5	0,95	2,55	2,8542(15)	132

we can see that the two compounds have the same geometrical characteristics in both structures.

o-CADP	o-CADPx
a = 4,8541(8) Å.	a = 4.876 Å.
b = 9,9845(9) Å.	b = 9,460 Å.
c = 10,4849(2) Å.	c = 10,080 Å.
α = 108,383(5)°.	α = 78,93°.
β = 97,816(8)°.	β = 76,06°.
γ = 96,816(6)°.	γ = 86,81°.
V = 471,74(9) Å ³ .	V = 442,8 Å ³ .
Z = 2,	Z = 2,
Triclinique : P-1.	Triclinique : P-1.
V/Z = 235,87	V/Z = 221,4

4. Conclusions

The combination of the organic matrix and anions minerals allowed us to obtain original structures [I, II]. Presenting connections hydrogens strong, average or low (weak). Actually, several crystals of this type were isolated in our laboratory.

The objective of our researches consists in studying the influence on the geometry of the agglomerate formed by the organic matrix given in the presence of a series of

anions generating the three-dimensional network of hydrogen bonds.

References

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