

CHARACTERIZATION OF A NEW ORGANIC-CATION MONOHYDROGENMONOPHOSPHATE DIHYDRATE: $C_6H_{16}N_2HPO_4 \cdot 2H_2O$

L. BAOUAB, A. JOUINI

*Université du Centre, Faculté des Sciences de Monastir, Département de Chimie,
Laboratoire de Chimie du Solide, 5000 Monastir, Tunisie*

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ABSTRACT: A new organic phosphate $C_6H_{16}N_2HPO_4 \cdot 2H_2O$ (2,6DMPHP) is prepared by interaction of H_3PO_4 with the organic molecule 2,6-dimethylpiperazin. This compound crystallizes in the monoclinic system $P2_1/c$, $Z=8$ with the parameters: $a=13.271(3)$, $b=11.855(4)$, $c=15.748(4)\text{Å}$, $\beta=105.22(3)^\circ$, $\rho_c=1.379$, $\rho_m=1.367\text{g/cm}^3$, $\mu=0.243\text{mm}^{-1}$. The structural matrix is made up of a three dimensional network of $O(W)-H\cdots O$, $O(P)-H\cdots O$ and $N-H\cdots O$ hydrogen bonds. The thermal decomposition of 2,6DMPHP shows two large endothermic effects at 127 and 152°C, corresponding to the elimination of water molecules and a set of endotherms, from 170 to 300°C, probably due to the evolution of ammonia from the structure. The overall ΔH of the dehydration, deduced from the DSC thermogram, is 82.61 kJ/mol. The IR study, based on theoretical analyses and on in the literature data, allows interpretation of the IR spectrum.

RÉSUMÉ: Un nouveau phosphate organique $C_6H_{16}N_2HPO_4 \cdot 2H_2O$ (2,6DMPHP) est obtenue par interaction de l'acide phosphorique avec le 2,6-diméthylpiperazine. Ce composé cristallise dans le système monoclinique, $P2_1/c$, $Z=8$ avec les paramètres: $a=13,271(3)$, $b=11,855(4)$, $c=15,748(4)\text{Å}$, $\beta=105,22(3)^\circ$, $\rho_c=1,379$, $\rho_m=1,367\text{g/cm}^3$, $\mu=0,243\text{mm}^{-1}$. La structure est stabilisée par un réseau tridimensionnel de liaisons hydrogène du type $O(W)-H\cdots O$, $O(P)-H\cdots O$ et $N-H\cdots O$. L'étude thermique du 2,6DMPHP montre deux effets endothermiques larges à 127 et 152°C, qui correspondent à l'élimination des molécules d'eau et un ensemble de phénomènes endothermiques, allant de 170 à 300°C, probablement dues au dégagement de l'ammoniac de la structure. La valeur de ΔH , déduite de la courbe DSC qui correspond à la déshydratation, est 82,61 kJ/mol. L'étude spectrométrique IR, basée sur une analyse théorique et utilisant les données de la littérature, permet l'interprétation du spectre IR.

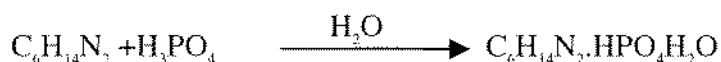
I- INTRODUCTION

The family of compounds which combine the cohesion of phosphate lattices with enhanced polarizability of organic molecules was clearly illustrated with phosphoric anions, linear $P_2O_7^{4-}$ [1] or cyclic $(P_nO_{3n})^{n-}$ ($n=3, 4, 6$) anions [2-4]. Furthermore, the structures of some centric or acentric crystals including organic cations with anionic phosphates of various shapes and charges have been determined showing the role played by the layered anionic matrices such as $(HPO_4)^{2-}$ or $(H_2PO_4)^{-}$. In our previous works, the effects of base modification and protonation, in this new field of compounds, have been mostly studied to inspect the influence of different counteranions on the conformation and the hydrogen bonding properties of organic entities and water molecules. It may be appropriate to mention, in this context, that the role of counteranions is rather efficient with small acentric ones such as $(CuCl_4)^{2-}$ [5], $(HPO_4)^{2-}$ [6] or $(H_2PO_4)^{-}$ [7]. We report here the preparation and the characterization of a new material synthesized in the system $Org^+-H_3PO_4-H_2O$ as single crystals,

where org⁺ is the 2,6-dimethylpiperazin. The compound formula C₆H₁₆N₂HPO₄·2H₂O is hereafter denoted 2,6DMPHP. Its structural properties, thermal behavior and IR spectrum are discussed.

II- CRYSTAL CHEMISTRY

Crystals of 2,6DMPHP are prepared by slow evaporation at room temperature of 200 ml of aqueous solution of H₃PO₄ (10⁻² M) neutralized by the 2,6-dimethylpiperazin. The adding, drop by drop, of the organic molecule, under vigorous stirring, is stopped when the pH of the final solution reaches the value 5 to obtain the acentric HPO₄²⁻ counteranion. The synthesis reaction is:



When the most of the solution is evaporated, large colourless and parallelepipedic crystals appear in the vessel. The chemical analysis of phosphorous and hydrogen has been carried out [8]. The cell parameters reported in table I were determined by diffraction techniques at 298 K and then refined from 25 reflections with 14° < θ < 16° using a least squares method. The observed extinction conditions: {h0l, l=2n+1; 0k0, k=2n+1} are consistent with the space group P2₁/c.

III- STRUCTURE DESCRIPTION

The structure determination was made by following the standard strategy of the SHELX programs (direct method) as reported in table I. The final atomic coordinates and the U equivalent temperature factors for the 2,6DMPHP are assigned in table II except the hydrogen atoms.

As for many hydrated monophosphates with mineral or organic cations, this structure exhibits isolated tetrahedral units [HPO₄²⁻]. By means of hydrogen-bonds via the water molecules, these units build up networks containing chains, ribbons or layers where, most of the time, polyanions of formula [HPO₄·H₂O]_n²ⁿ⁻ are encountered. The organic countercations, via hydrogen bonds, also interconnect these anionic groups and contribute to the three-dimensional building. The main feature of our structure is given on figure 1 which depicts all the hydrogen-bonds but the structure is better described from figure 2. The half contents of the cell (z=0), represented on figure 2.a, shows that two water molecules O(W1) and O(W2), both of them playing the role of acceptor and donor, link HPO₄ tetrahedra in infinite ribbons running along the **a** axis. The other two water molecules O(W3) and O(W4), assembled together via their hydrogen bonds, connect adjacent ribbons in the **b** direction to establish the infinite layer. Solvent molecules assemble HPO₄²⁻ anions through strong hydrogen bonds to form a three dimensional network as displayed in figure 2.b, viewed along the **b** direction. Meanwhile the anionic arrangement can be described as a stacking of layers centered by (**a,b**) planes and interconnected by H(1W3)···O(7) hydrogen bonds. Organic cations, as shown in figure 1 depicting the various components of the structure, are anchored onto the anionic arrangement through N—H···O hydrogen bonds originating from the organic donor groups.

TABLE I: Main crystallographic features, x-ray diffraction data and results of 2.6DMPHP.**I. Crystal data**

Formula: $(C_6H_{16}N_2)HPO_4 \cdot 2H_2O$	$F_w = 248.22$ g/mol
Crystal system: Monoclinic	Space group: $P2_1/c$
$a = 13.271(3)$ Å, $b = 11.855(4)$ Å, $c = 15.748(4)$ Å, $\beta = 105.22(3)^\circ$	$V = 2391(1)$ Å ³
$\rho_{calcd} = 1.379$, $\rho_{measd} = 1.367$ g.cm ⁻¹	$Z = 8$
Linear absorption factor	$F(000) = 1072$
Morphology	$\mu(MoK\alpha) = 0.243$ mm ⁻¹
Crystal size	parallelepiped 0.45x0.41x0.35

II. Intensity measurements

Diffraction measurement device	Kappa CCD Nonius
Monochromator:	Graphite plate
Wave length: (MoK α)	0.7107 Å
Computing data collection	Kappa CCD Nonius
Computing cell refinement	Kappa CCD Nonius
Computing data reduction	Denzo [9]
θ range and temperature:	2-25° ; 298 K
Diffraction standards number	1
Diffraction standards interval time	120 s
Measurement area: $\pm h, k, l$	$h_{max} = 16, k_{max} = 14, l_{max} = 19$
Number of scanned reflection:	4566
Intensity decay %	None

III. Structure determination

Computing structure solution	SHELXS-86 [10]
Computing structure refinement	SHELXL-93 [11]
Reflections number observed	3518
Reflections observed criterion	2 sigma(I)
Refined parameters	433
S	1.173
Secondary extinction coefficient	0.0000(4)
R_w/R	0.092/0.036
Weight	
$W = 1/[\sigma^2(F_o^2) + (0.0600P)^2 + 0.0000P]$	where $P = (F_o^2 + 2F_c^2)/3$

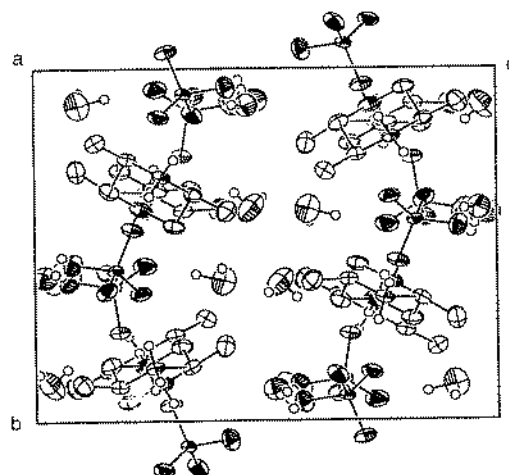
Figure 1: projection along the a direction of the atomic arrangement. The thermal ellipsoids are scaled to enclose 50% probability.

TABLE II: Final atomic coordinates and U_{eq} of 2,6DMPHP

Atoms	x(σ)	y(σ)	z(σ)	U_{eq} (\AA^2)
P(1)	0.06261(3)	0.07065(3)	0.32540(3)	0.0225(1)
P(2)	-0.55894(3)	0.61975(3)	0.16691(3)	0.0246(1)
O(1)	0.1467(1)	0.0530(2)	0.4178(1)	0.0450(4)
O(2)	-0.0298(1)	0.1299(1)	0.34411(9)	0.0435(4)
O(3)	0.1191(1)	0.1370(1)	0.27111(9)	0.0406(3)
O(4)	0.0330(1)	-0.0463(1)	0.28801(9)	0.0354(3)
O(5)	-0.4554(1)	0.5773(1)	0.15711(9)	0.0415(3)
O(6)	-0.55800(9)	0.7465(1)	0.18163(8)	0.0322(3)
O(7)	-0.5962(1)	0.5581(1)	0.2366(1)	0.0513(4)
O(8)	-0.6421(1)	0.5998(1)	0.0751(1)	0.0513(4)
O(W1)	0.1413(2)	-0.1036(2)	0.5387(1)	0.0546(5)
O(W2)	-0.6408(2)	0.4110(2)	0.0209(1)	0.0602(5)
O(W3)	-0.4848(4)	0.8976(3)	0.0923(2)	0.129(2)
O(W4)	-0.6036(2)	0.8944(2)	-0.0308(2)	0.0863(8)
N(1)	-0.1452(1)	-0.6949(1)	-0.2745(1)	0.0264(3)
N(2)	-0.3507(1)	-0.6036(1)	0.2297(1)	0.0363(4)
N(3)	-0.8494(1)	0.3488(1)	0.2422(1)	0.0267(3)
N(4)	-0.6310(1)	0.3419(1)	0.2600(1)	0.0374(4)
C(1)	-0.1885(1)	-0.6437(2)	0.3439(1)	0.0307(4)
C(2)	-0.2673(2)	-0.5547(2)	0.3017(1)	0.0344(4)
C(3)	-0.3076(2)	-0.6557(2)	0.1610(1)	0.0362(4)
C(4)	-0.2269(1)	-0.7446(1)	0.2001(1)	0.0298(4)
C(5)	-0.1019(2)	-0.5962(2)	0.4165(2)	0.0478(5)
C(6)	-0.1765(2)	-0.7910(2)	0.1319(2)	0.0421(5)
C(7)	-0.7760(2)	0.4018(2)	0.3199(1)	0.0315(4)
C(8)	-0.6724(2)	0.3417(2)	0.3381(1)	0.0389(4)
C(9)	-0.7047(2)	0.2884(2)	0.1836(1)	0.0376(4)
C(10)	-0.8101(1)	0.3464(2)	0.1621(1)	0.0323(4)
C(11)	-0.8198(2)	0.3968(2)	0.3983(2)	0.0490(5)
C(12)	-0.8889(2)	0.2878(2)	0.0885(2)	0.0500(5)

Note. Esds are given in parentheses. $U_{eq} = (1/3) \sum_i \sum_j U_{ij} a_i^* a_j^* a_i a_j$.

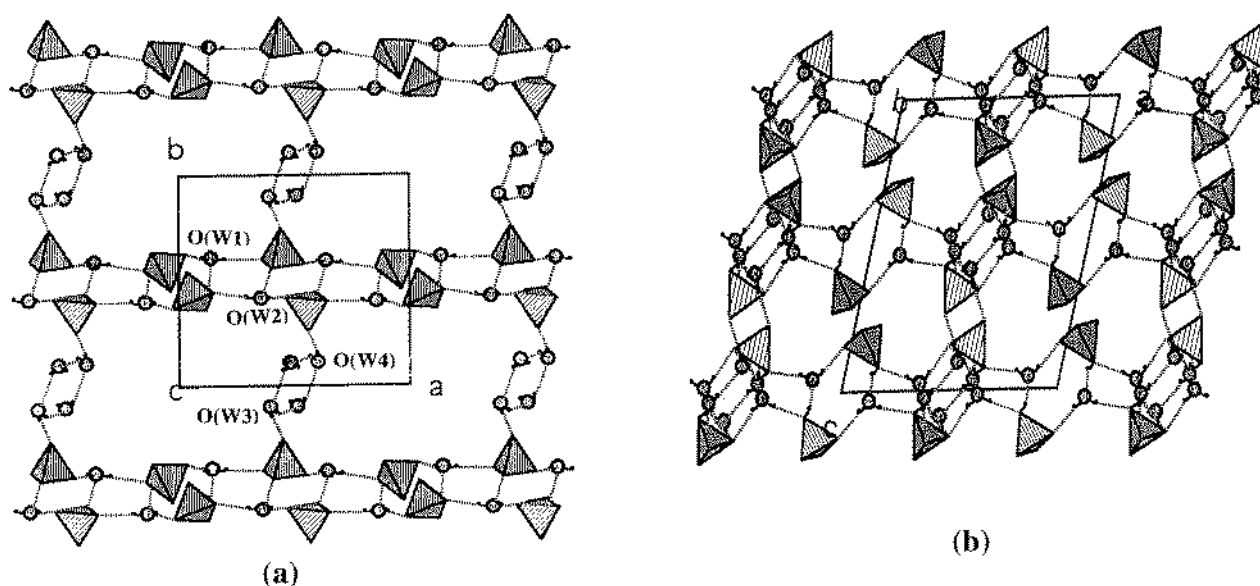


Figure 2: (a) Projection along the c direction of anionic layer located at the plane $z=0$. (b) projection along the b direction of the anionic arrangement. The PO4 groups are represented by polyhedra. Large circles represent water O atoms and small black ones water H atoms. Hydrogen bonds are denoted by full and dotted lines.

The detailed geometry of HPO_4^{2-} (table III) indicates that the P—O bonds are significantly shorter [1.500(1)-1.520(1) Å] than the P—OH bonds [1.590(2) and 1.598(2)Å]. The H···O bonds which maintain the cohesion of the ribbons, are characterized by relatively short distances, from 1.90(3) to 2.19(3) Å. Concerning the organic groups, the main characteristics are reported in table III; each cation is anchored into the anionic arrangement by N—H···O hydrogen bonds. This interaction contributes to the cohesion of the structure. All the D(donor)—H···A (acceptor) hydrogen bonds are listed in table IV with an upper limit of 2.31(3)Å for the H···A distances and a lower limit of 123(4)° for the D—H···O angles [12-15]. It is to be noted that distances including the located but not refined H(2W1) and H(2W2), are given, in table IV, without standard deviations.

TABLE III: Main inter atomic distances(Å) and bonds angles(°) in the 2.6DMPHP.

<i>The Phosphoric Group</i>				
		P(1)O ₄ tetrahedron		
P(1)	O(1)	O(2)	O(3)	O(4)
O(1)	1.598(2)	107.0(1)	104.7(1)	106.3(1)
O(2)	2.497(2)	1.508(1)	114.9(1)	111.1(1)
O(3)	2.453(2)	2.536(2)	1.500(1)	112.0(1)
O(4)	2.493(2)	2.495(2)	2.501(2)	1.517(1)
		P(2)O ₄ tetrahedron		
P(2)	O(5)	O(6)	O(7)	O(8)
O(5)	1.509(1)	112.0(1)	113.2(1)	106.9(1)
O(6)	2.511(2)	1.520(1)	111.1(1)	105.2(1)
O(7)	2.517(2)	2.495(2)	1.506(1)	108.0(1)
O(8)	2.489(2)	2.471(2)	2.504(2)	1.590(2)
P—P = 6.372(2)		P—O(1)—H(O1) = 110 (4)		P—O(8)—H(O8) = 96(3)
<i>The 2.6-dimethylpiperazinium groups</i>				
N(1)—H(1N1)	0.97(2)	H(1N1)—N(1)—H(2N1)		106(2)
N(1)—H(2N1)	0.87(2)			
N(2)—H(1N2)	0.88(2)	H(1N2)—N(2)—H(2N2)		106(2)
N(2)—H(2N2)	0.87(2)			
N(1)—C(1)	1.491(2)	N(1)—C(1)—C(5)		110.2(2)
C(1)—C(5)	1.502(3)	N(1)—C(1)—C(2)		108.5(2)
C(1)—C(2)	1.510(3)	C(5)—C(1)—C(2)		112.1(2)
C(2)—N(2)	1.479(3)	C(1)—C(2)—N(2)		110.8(2)
N(2)—C(3)	1.484(3)	C(2)—N(2)—C(3)		111.6(2)
C(3)—C(4)	1.514(3)	N(2)—C(3)—C(4)		111.1(2)
C(4)—N(1)	1.492(2)	C(3)—C(4)—C(6)		111.2(2)
C(4)—C(6)	1.511(3)	C(3)—C(4)—N(1)		109.6(2)
		C(4)—N(1)—C(1)		113.3(1)
		N(1)—C(4)—C(6)		109.6(2)

TABLE III (continued)

N(3)—H(1N3)	0.88(2)	H(1N3)—N(3)—H(2N3)	108(2)
N(3)—H(2N3)	0.82(2)		
N(4)—H(1N4)	0.88(2)	H(1N4)—N(4)—H(2N4)	109(2)
N(4)—H(2N4)	0.94(3)		
N(3)—C(7)	1.487(2)	N(3)—C(7)—C(8)	109.1(2)
C(7)—C(8)	1.506(3)	N(3)—C(7)—C(11)	110.5(2)
C(7)—C(11)	1.498(3)	C(11)—C(7)—C(8)	111.0(2)
C(8)—N(4)	1.473(3)	C(7)—C(8)—N(4)	111.3(2)
N(4)—C(9)	1.479(3)	C(8)—N(4)—C(9)	111.5(2)
C(9)—C(10)	1.515(3)	N(4)—C(9)—C(10)	111.2(2)
C(10)—N(3)	1.486(2)	C(9)—C(10)—N(3)	109.2(2)
C(10)—C(12)	1.511(3)	C(9)—C(10)—C(12)	112.1(2)
		C(12)—C(10)—N(3)	109.5(2)
		C(10)—N(3)—C(7)	114.0(1)

TABLE IV: Bond lengths(Å) and angles(°) in the hydrogen-bonding scheme in 2,6DMPHP.

	N(O)—H	H...O	N(O)...O	N(O)—H...O
N(1)—H(1N1)...O(4) ^{a)}	0.97(2)	1.69(2)	2.657(2)	174(2)
N(1)—H(2N1)...O(2) ^{b)}	0.87(2)	1.80(2)	2.642(2)	163(2)
N(2)—H(1N2)...O(6) ^{c)}	0.88(2)	1.86(2)	2.732(2)	169(2)
N(2)—H(2N2)...O(5) ^{b)}	0.87(2)	1.79(3)	2.646(2)	166(2)
N(3)—H(1N3)...O(4) ^{d)}	0.88(2)	1.79(2)	2.665(2)	175(2)
N(3)—H(2N3)...O(3) ^{e)}	0.82(2)	1.79(3)	2.605(2)	170(2)
N(4)—H(1N4)...O(7)	0.88(2)	1.78(3)	2.647(2)	167(2)
N(4)—H(2N4)...O(6) ^{f)}	0.94(3)	1.75(3)	2.684(2)	174(2)
O(1)—H(O1)...O(W1)	0.57(3)	2.19(3)	2.673(3)	143(5)
O(8)—H(O8)...O(W2)	0.87(4)	2.13(5)	2.703(2)	123(4)
O(W1)—H(1W1)...O(2) ^{g)}	0.79(2)	1.90(3)	2.670(2)	166(2)
O(W1)—H(2W1)...O(8) ^{h)}	0.759*	2.044*	2.780(3)	163.52*
O(W2)—H(1W2)...O(5) ⁱ⁾	0.82(3)	1.96(3)	2.773(2)	172(3)
O(W2)—H(2W2)...O(1) ^{j)}	0.840*	1.929*	2.764(3)	172.45*
O(W3)—H(1W3)...O(7) ^{k)}	0.97(5)	1.80(5)	2.763(4)	172(5)
O(W3)—H(2W3)...O(W4) ^{l)}	0.60(2)	2.31(3)	2.792(5)	138(4)
O(W4)—H(1W4)...O(W3)	0.75(2)	2.18(2)	2.801(5)	141(2)
O(W4)—H(2W4)...O(6)	0.76(3)	2.14(4)	2.885(3)	167(4)

Note. a)-x, y-0.5, -z+0.5 e)x-1, y, z i)-x-1, -y+1, -z
 b)x, y-1, z f)-x-1, y-0.5, -z+0.5 j)x-1, -y+0.5, z-0.5
 c)-x-1, y-1.5, -z+0.5 g)-x, -y, -z+1 k)x, -y+1.5, z-0.5
 d)-x-1, y+0.5, -z+0.5 h)x+1, -y+0.5, z+0.5 l)-x-1, -y+2, -z

* Fixed values.

IV- THERMAL BEHAVIOR

Figure 3 shows both TG and DTA thermograms of 2,6DMPHP. Thermal decomposition occurs in three stage between 92 and 300°C. The first process starts at a low temperature of 92°C and is complete at 141°C. It corresponds to the loss of the first water molecule of the formulae (weight loss, calculated 7.25%, observed 6.98%). Indeed this water departure must be related to the large temperature factors of O(W3) and (OW4) water molecules, since their U equivalent are respectively 29 to 54% higher than those of O(W1) and O(W2). The second stage from 141 to 170°C is attributed to the elimination of the last water molecule from the formulae. The experimental weight loss (7.48%) is closed to the calculated value (7.25%). Thus the first two endotherms are considered to result from the evolution of the water molecules from the structure. The third stage representing a set of endotherms from 170 to 300°C is assigned to the degradation of the organic cations. The TG curve shows a rather vigorous and continuous weight loss corresponding probably to the evolution of ammonia from the structure [16]. When the temperature of pyrolysis is reached, a black residue is obtained. Figure 4 showing the DSC thermogram, registered from RT to 300°C reveals the same thermal behavior as 2,6DMPHP in accordance with what is observed in the TG-DTA curves. Indeed the two large endothermic effects at 123 and 145°C correspond to the dehydration with an overall $\Delta H=82.61$ kJ/mol.

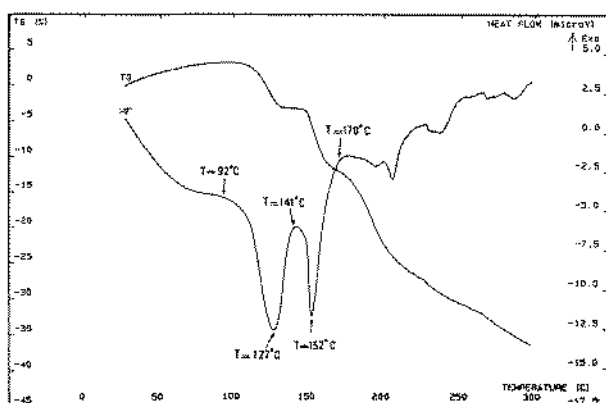


Figure 3: TG-DTA analysis of 2,6DMPHP.

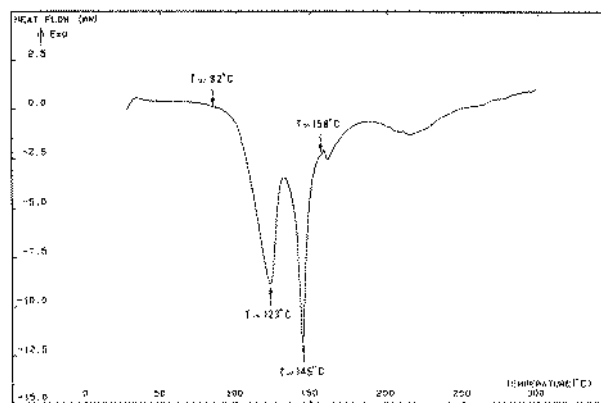


Figure 4: DSC curve of 2,6DMPHP.

V- IR SPECTROSCOPIC INVESTIGATION

The normal modes of vibration in an isolated PO_4 tetrahedron with an ideal T_d symmetry have been widely studied [17]. The ν_1 and ν_2 symmetric and asymmetric stretching modes are observed in $1200\text{-}900\text{cm}^{-1}$ region, whereas the ν_2 and ν_4 symmetric and asymmetric bending modes are distinguished in the $600\text{-}400\text{cm}^{-1}$ domain [18], [19]. The group-theoretical analysis shows that the number of normal modes of the PO_4 tetrahedron is given by the representation $\Gamma_{\text{int}} = A_1 + E + 2F_2$. The localization of a proton on one of the oxygen atoms reduces the ideal symmetry from T_d to C_{3v} . The correlation of group to sub-group shows that these modes can be divided into $2A_1 + E$ stretching and

A_1+2E bending vibrations in the C_{3v} symmetry of HPO_4 group. Meanwhile the HPO_4 , observed in the 2,6DMPHP has the lower local symmetry C_1 . This symmetry lowering gives rise to the splitting of the degenerate IR modes and activates the inactive ones. Indeed the C_1 local symmetry leads to 4 stretching and 5 bending vibrations (table V). The interpreting of the IR spectrum (figure 5) is made in terms of internal modes of two atomic groups, PO_3 and POH, included in HPO_4^{2-} anion. With regard to the compounds including HPO_4 tetrahedron the two stretching vibrations, asymmetric and symmetric of PO_4 group, are observed respectively at 1080 and 990 cm^{-1} [17]; while that related to POH group occurs at 860 cm^{-1} [20]. Then, we attribute the three intense bands at 1064, 980 and 855 cm^{-1} to these three vibrations in the 2,6DMPHP compound. The splitting of F_2 stretching mode of PO_4 into two intense components at 1064 cm^{-1} (E) and 980 cm^{-1} (A_1) corroborates the symmetry lowering of HPO_4 in the solid state. The intense bands at 532 and 503 cm^{-1} are respectively assigned to the two bending vibrations $\delta_{as}(PO_3)$ and $\delta_s(PO_3)$. Moreover the remaining observed bands in the spectrum can be assigned to CH_3 , CH_2 , NH_2 and H_2O symmetric and asymmetric stretching and deformation modes.

TABLE V: Tentative assignment of the observed IR frequencies outside the stretching domain of PO_4 .

$\nu(cm^{-1})$	assignment	$\nu(cm^{-1})$	assignment
3486 vs	① $\nu OH_2 + \nu_{as} NH_2^+$ + $\nu CH_2 + \nu CH_3 + \nu CH$	1667 sh	③ $\delta OH_2 + \delta NH_2^+$ + $\delta CH_2 + \delta CH_3$
3438 vs		1619 w	
3375 sh		1523 w	
3376 vs		1478 sh	
3070 s		1463 w	
2989 s		1384 w	
2952 sh		1361 w	
2896 sh		1315 vw	
2762 s			
2642 sh	② Bands of combination and harmonics	1225 w	④ νCH + $\delta POH + \delta CH$
2468 s		1226 w	
2339 s		1138 m	
2151 sh		1033 s	
2070 sh		937 w	⑤ $\gamma POH + \gamma CH$
1982 sh		876 w	
		843 sh	
		755 vw	
		664 sh	
		646 sh	
		604 s	

Note. vs, very strong; s, strong; sh, shoulder; m, medium; w, weak; vw, veryweak.

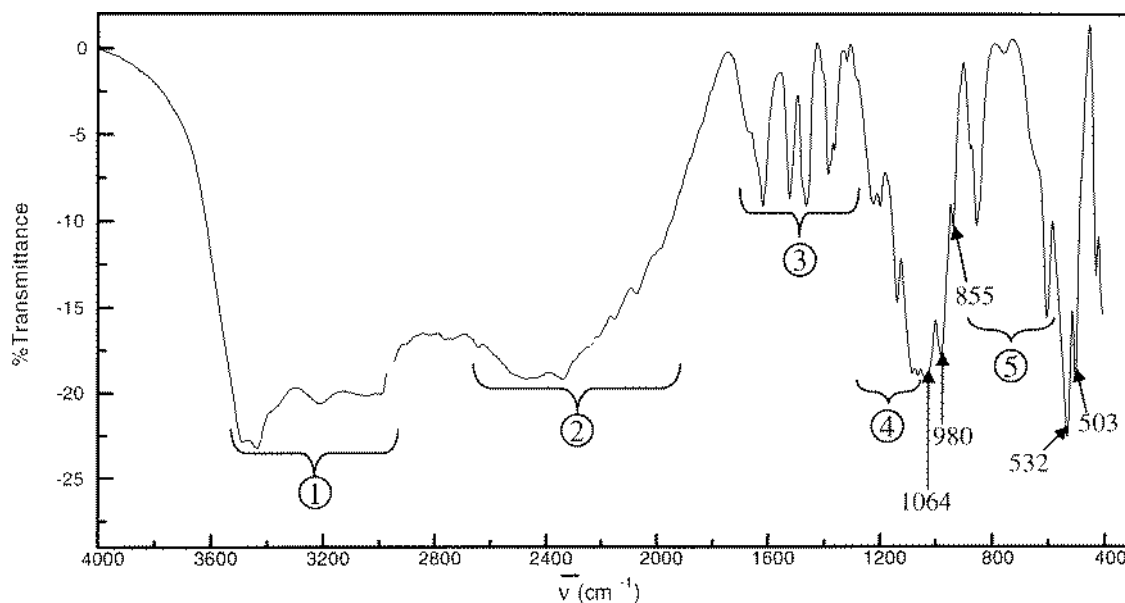


Figure 5: IR spectrum of 2,6DMPHP in polycrystalline form.

This attribution must be made by comparison with frequencies of other compounds including similar entities. Nevertheless, the attribution will not be very easy because of the lack of deuterated compounds and the Fermi resonance of the overtone of the corresponding asymmetric bending vibrations.

VI- CONCLUSION

Crystals of 2,6DMPHP have been prepared by slow evaporation, at room temperature, of aqueous solution of H_3PO_4 and 2,6-dimethylpiperazin. The structural cohesion is established by a three dimensional network of $O(W)-H\cdots O$, $O(P)-H\cdots O$ and $N-H\cdots O$ hydrogen bonds. Organic cations are anchored to the anionic arrangement, by the third type of hydrogen bonds, namely, $N-H\cdots O$ originating from the $N-H$ donors. The thermal behavior study, summarized by elimination of the water molecules in two steps and the pyrolysis, specify the stability of 2,6DMPHP. Indeed this hydrate compound has low thermal stability owing to the ionic and covalent nature of its interatomic bonding and to the existence of unreliable water molecules in the structure. IR spectrometric investigation, supported by group theoretical analysis allows the attribution of bands to the different atomic motions.

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