

Crystal structure, vibrational and spectroscopic study of single crystal $(C_6H_{15}N_4O_2)H_2PO_4 \cdot H_2O$

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Abstract

A single crystal was selected from the reaction product of a stoichiometric mixture of phosphoric acid (H_3PO_4) to which was added the L-arginine ($C_6H_{14}N_4O_2$) and its crystal structure was determined from three dimensional X-ray diffraction data. The structure is monoclinic, space group $P2_1$, $a = 7.3450(14) \text{ \AA}$, $b = 7.9176(15) \text{ \AA}$, $c = 10.8796(22) \text{ \AA}$, $\beta = 97.98(2)^\circ$, $V = 626.57(186) \text{ \AA}^3$ and $Z = 2$, least squares refinement was converged to $R_1=0.0456$, $wR_2=0.1433$ for 3278 unique reflections. The structure consists of chains formed by edge sharing of PO_4 tetrahedra, water and arginine. The stacking along b axis consists of these chains bridged by layers formed by PO_4 water and arginine by hydrogen bonds. The Raman and infrared spectra of single crystal LAP were recorded to determine the symmetries of the vibrations of the various molecular groups such as NH_3^+ , NH_2 , CH_2 , CH , COO^- , H_2O and H_2PO_4 present in the crystal.

Key words: Crystal structure, Vibrational study, Infrared, Raman, X-ray diffraction.

1. Introduction

A large number of inorganic phosphates are presently known and a systematic survey of their main crystallographic data has been reported. Recently, the research of organic-inorganic polar crystals is very interesting for quadratic non-linear; studies of charged species (cations and anions) have become an active research area in organic chemistry and biology [1], optical phenomena. Their role as structural agents is important in molecular association processes and in mediating the tertiary structures of proteins and nucleic acids [2]. The present work continues a series of investigations into the factors influencing the dimensions of phosphate anion–organic cation interaction. We report here on the chemical preparation, crystallographic data, vibrational and spectroscopic study by IR and Raman of a organic phosphate $(\text{C}_6\text{H}_{15}\text{N}_4\text{O}_2)\text{H}_2\text{PO}_4\cdot\text{H}_2\text{O}$. Materials with optical non linearities have been studied extensively for their possible applications in optical communication, optical computation, optical processing of information, optical data storage. L-Arginine phosphate monohydrate (LAP) is one of the best non linear optical crystals [3].

2. Experimental

2.1. Chemical preparation

The Arginine ($\text{C}_6\text{H}_{14}\text{N}_4\text{O}_2$) was carefully added drop wise to phosphoric acid solution to reach the stoichiometric ratio 1:1. Schematically the synthesis reaction is:



After some days of evaporation, colorless prism-shaped prismatic monocrystals appear deep down the vessels. The crystals obtained in this way are pure and stable under normal conditions of temperature and humidity.

2.2. X-ray structure determination

X-ray structure determination single crystal study was performed by using an Enraf-Nonius CAD4 diffractometer. The main crystal data, the parameters used for intensity data collection and the reliability factor are summarized in Table 1. The crystal structure was carried out with a direct method by using the SHELXS-97 program [4] which permitted to locate all atoms. The hydrogen of carbon atoms were geometrically fixed with isotropic thermal parameters in idealized positions using HFIX option. Organic groups were located after subsequent cycles of refinement and difference-Fourier syntheses by using SHELXL-97[5]. Hydrogen atoms of the H_2PO_4^- anion water and NH_2 groups of organic cations located after subsequent cycles of refinement and difference-Fourier syntheses by using SHELXL-97[5]. The final atomic coordinates are given in Table 2. Main geometrical features, bond distances and angles are reported in Tables 3 and 4.

2.3. L-Arginine phosphate monohydrate Structure description

L-Arginine phosphate monohydrate is a single crystal which is formed by the reaction of the amino acid L-arginine with phosphoric acid. The L-arginine molecule is bound to the phosphate group by OH - O hydrogen bonds of the phosphate to carboxyl oxygen atoms and to the NH ... O hydrogen bonds of the amino and guanidyl nitrogen N (1), N (3) atoms and N (4) to the oxygen atoms of the phosphate. As shown in Figures. 1 and 2, these hydrogen bonds bind the molecules on one side of the phosphate layer. The other side is attached to another molecule of L-arginine.

The L-arginine layer between the two phosphate layers is therefore composed of double layers of L-arginine molecules and chains of water molecules. The water molecules and the carboxyl oxygen atoms O (5) are arranged around the double screw axis $(1/2, y, 0)$ to form a hydrogen bonded chain.

Table 1: Crystal structure data for (C₆H₁₅N₄O₂)H₂PO₄·H₂O

I. Crystal data	
Formula/formula weight	(C ₆ H ₁₅ N ₄ O ₂)H ₂ PO ₄ ·H ₂ O/292g.mol ⁻¹
Crystal system	Monoclinic
Space group / Z	<i>P</i> 2 ₁ / 2
parameters	<i>a</i> =7.3450(14) Å <i>b</i> =7.9176(15) Å <i>c</i> =10.8796(22) Å, β=97.98(2)°
Volume	<i>V</i> =626.57(186) Å ³
Calculated density (g/cm ³)	1.846
Absorption coefficient μ (mm ⁻¹)	0.251
F(0 0 0)	362
Size/color	(0.18 mm × 0.18 mm × 0.43 mm)/colorless
II. Intensity measurement	
Diffractionmeter,	fine-focus sealed tube
Monochromator	graphite
Wavelength (Mo Kα)	λ= 0.71073 Å
Temperature	293(2)
Theta range	3.59°/31.49°
h, k, l range	-10/10, -11/11, -15/15
Number of measured reflections	3278
Number of independent reflections	2895
III. Structure determination	
Unique reflections included (<i>I</i> > 2σ _{<i>I</i>})	
Programs used	SHELXL-97
Number of refined parameters	172
Goodness-of-fit on F ²	0.903
R (anisotropic)/R _w (anisotropic)	0.0425/ 0.1366
Extinction coefficient	0.170(15)
Δρ _{min.} / Δρ _{max.} (e/ Å ³)	-0.365/ 0.501
Largest shift/error	0.000

Table 2: Final atomic coordinates and U equivalent temperature factors for (C₆H₁₅N₄O₂)H₂PO₄·H₂O

Atoms	X	Y	Z	U _{eq}
P01	0.1762(8)	-0.22925(7)	0.98806(6)	0.0225(1)
O02	0.1331(3)	-0.2831(3)	0.84626(1)	0.0372(5)
O03	0.2090(3)	-0.3965(3)	1.0641(2)	0.0367(5)
O04	0.3497(3)	-0.1288(3)	1.01197(1)	0.0311(4)
O05	0.3141(3)	0.4684(3)	0.7632(2)	0.0310(5)
O06	0.8464(3)	0.1051(4)	0.5243(3)	0.0431(6)
N07	0.3156(3)	0.2040(3)	0.9228(2)	0.0251(4)
O08	0.0071(3)	-0.1391(3)	1.0148(2)	0.0389(5)
N09	0.5060(3)	-0.2553(3)	0.6311(2)	0.0283(5)
O10	0.0792(3)	0.3556(3)	0.6381(2)	0.0453(6)
C11	0.3139(4)	0.0007(4)	0.6051(3)	0.0275(5)
N12	0.6950(4)	-0.4158(4)	0.7699(3)	0.0434(7)
C13	0.4519(4)	-0.1103(4)	0.5513(2)	0.0281(5)
C14	0.3911(4)	0.0755(4)	0.7299(3)	0.0250(5)
C15	0.2085(4)	0.3476(3)	0.7252(3)	0.0267(5)
N16	0.8123(3)	-0.1851(4)	0.6824(2)	0.0396(7)
C17	0.2478(3)	0.1774(3)	0.7886(2)	0.0235(5)
C18	0.6718(4)	-0.2835(4)	0.6936(2)	0.0286(6)

As shown in Table 4, the directions of hydrogen bonding around the oxygen atom of water are approximately tetrahedral [6]. The atomic nitrogen atom N (2) forms a hydrogen bond bifurcated at the oxygen atom of the water O

(W) and the carboxyl oxygen atom O (6) of the neighboring molecule is translated by b. The anionic arrangement can be described by chains of the inorganic entities gives a projection, along the c direction, of this anionic arrangement. Adjacent PO₄ groups are linked with O(W1) molecule so as to form an infinite chain [PO₄(H₂O)]_n³ⁿ⁻ spreading along the a direction. The organic cations are anchored onto the inorganic entities to stabilize the chains through a hydrogen bond network. The PO₄ group, its environment, established by strong hydrogen bonds, is depicted in figure 3 as an ORTEP representation [7], shown in Table 3. The detailed geometry of PO₄³⁻ anion indicates that among the P–O distances of the PO₄ tetrahedron, two different types are distinguished: the longest one, ranging from [1.562(2) – 1.589(2) Å], corresponds to the bridging oxygen atoms, the shortest [1.494(2) – 1.496(2) Å], do not deviate significantly from those observed in a regular PO₄ tetrahedron.

Table 3: Main interatomic distances (Å°) and bond angles (°) for (C₆H₁₅N₄O₂)H₂PO₄·H₂O:

PO4 tetrahedron				
P01	O02	O03	O04	O08
O02	1.589(2)	106.38(12)	111.21(13)	104.94(12)
O03	2.5235(5)	1.562(2)	107.10(11)	111.87(14)
O04	2.5450(5)	2.4589(4)	1.494(2)	115.06(13)
O08	2.4471(4)	2.5335(4)	2.5224(4)	1.496(2)

Table 4: Bond lengths (Å°) and angles (°) in the hydrogen-bonding scheme for (C₆H₁₅N₄O₂)H₂PO₄·H₂O:

	D-H	H...A	D...A	D-H...A
N16-H01h...O02	0.8600(1)	2.0127(5)	2.8580(7)	167.37(1)
N16-H01g...O06	0.8600(1)	2.0669(3)	2.9020(4)	163.58(1)
N07-H00b...O04	0.8600(1)	2.8660(5)	2.0087(4)	153.90(1)
N12-H01d...O05	0.8600(1)	2.1482(4)	2.9351(5)	151.93(1)

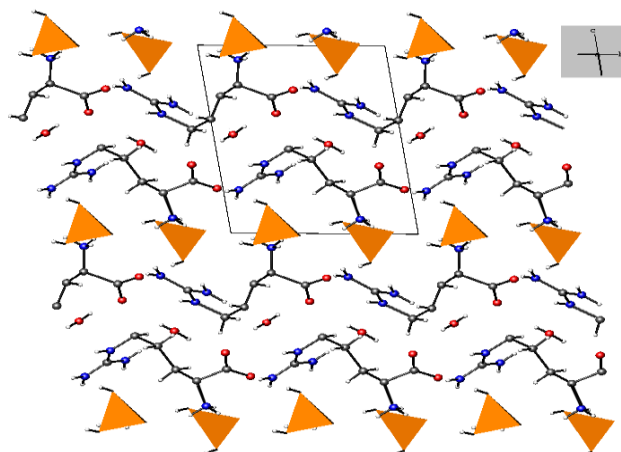


Figure 1: Projection along the c-axis of the atomic arrangement in (C₆H₁₅N₄O₂)H₂PO₄·H₂O

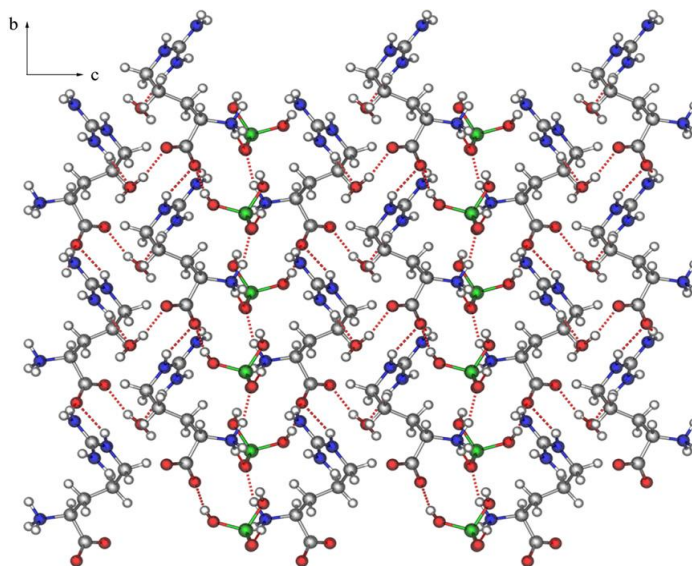


Figure 2: The crystal structure of $(\text{C}_6\text{H}_{15}\text{N}_4\text{O}_2)\text{H}_2\text{PO}_4\cdot\text{H}_2\text{O}$ viewing along (a) axis with hydrogen bonds been displayed.

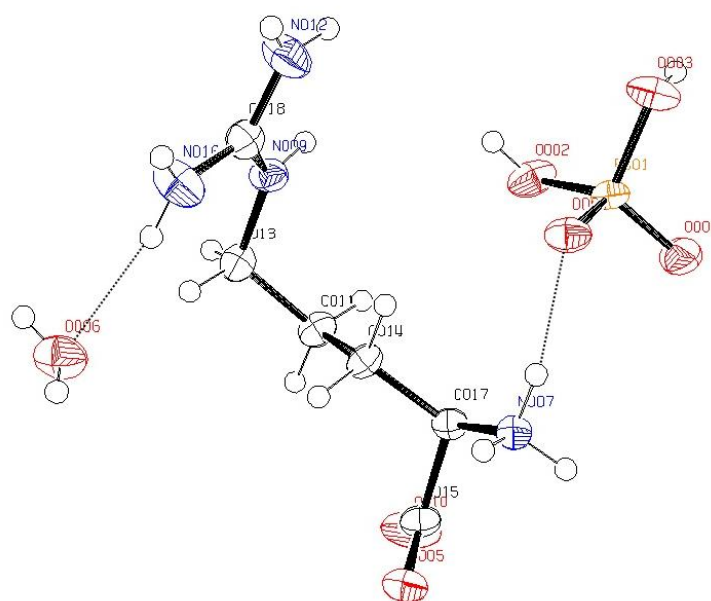


Figure 3: ORTEP representation of $(\text{C}_6\text{H}_{15}\text{N}_4\text{O}_2)\text{H}_2\text{PO}_4\cdot\text{H}_2\text{O}$ (H-bonds are represented by dashed lines). Thermal ellipsoids are scaled to enclose 50% probability.

3. Vibrational study of the single crystal $(\text{C}_6\text{H}_{15}\text{N}_4\text{O}_2)\text{H}_2\text{PO}_4\cdot\text{H}_2\text{O}$

The single crystal $(\text{C}_6\text{H}_{15}\text{N}_4\text{O}_2)\text{H}_2\text{PO}_4\cdot\text{H}_2\text{O}$ crystallizes in the monoclinic system, with P2_1 (C_2) space group, with 2 units per cell. This structure consists of a group $[\text{H}_2\text{PO}_4]^-$ and a molecule of water and an organic cation $(\text{C}_6\text{H}_{15}\text{N}_4\text{O}_2)^+$.

3.1- Internal modes of vibration of the ion $[\text{H}_2\text{PO}_4]^-$

The fixation of two hydrogen atoms on two oxygen atoms of the $[\text{PO}_4]^{3-}$ group reduces the ideal symmetry Td to C_{2v} , becoming the ideal symmetry of the group $[\text{H}_2\text{PO}_4]^-$ whereas the $[\text{H}_2\text{PO}_4]^-$ group observed in $(\text{C}_6\text{H}_{15}\text{N}_4\text{O}_2)\text{H}_2\text{PO}_4\cdot\text{H}_2\text{O}$, has the local symmetry C_1 . Based on the fact that the structure of the studied compound is composed of isolated $[\text{H}_2\text{PO}_4]^-$ groups, we have found it necessary to carry out the enumeration by the site group [8] method of the $[\text{H}_2\text{PO}_4]^-$ group. Application of the site group method requires knowledge of the symmetry of the C_{2v} molecular group

of $[\text{H}_2\text{PO}_4]^-$. The latter has 15 active internal vibrations in IR and Raman except the A_2 mode which is active only in IR.

$$\Gamma[\text{H}_2\text{PO}_4]^- : 6A_1(\text{IR, Ra}) + 4B_1(\text{IR, Ra}) + 2A_2(\text{Ra}) + 3B_2(\text{IR, Ra})$$

3.2- Normal modes of ion vibration $[\text{PO}_4]^{3-}$

The representation of the internal modes of the grouping the ion $[\text{PO}_4]^{3-}$ of symmetry T_d in the free state.

$$\Gamma[\text{PO}_4]^{3-} : A_1(\text{Ra}) + E(\text{Ra}) + 2F_2(\text{Ra, IR})$$

The F_2 modes are active in IR and Raman, A_1 and E modes are active only in Raman. The 9 normal vibrations are divided into 4 stretching vibrations and 5 mode bending vibrations, respectively $1F_2$ and $1A_1$, $\Gamma_{\text{str}} = F_2(\nu_3) + A_1(\nu_1)$, and F_2 and E , $\Gamma_{\text{ben}} = F_2(\nu_4) + E(\nu_2)$. The calculated frequencies for the degenerated triplet F_2 mode ν_3 vibrations, of asymmetric elongations and ν_1 , of mode A_1 , of symmetrical elongations are $(1139, 1139, 1139 \text{ cm}^{-1})$ of mode F_2 and 952 cm^{-1} of A_1 mode. The different modes of vibration of the anion $[\text{PO}_4]^{3-}$ are shown in the following order: $\nu_3 > \nu_1 > \nu_4 > \nu_2$ [9].

3.3- The correlation between the molecular group T_d of $[\text{PO}_4]^{3-}$ and the molecular group C_{2v} of $[\text{H}_2\text{PO}_4]^-$

The appearance of some modes under a single band and the total lifting of the degeneracy for others can be explained by the analysis of the C_{2v} group. Indeed, the correlation between the molecular group T_d of $[\text{PO}_4]^{3-}$ and the molecular group C_{2v} of $[\text{H}_2\text{PO}_4]^-$ shows the following effects (table 5):

- The vibrations ν_1 (A_1) and ν_2 (E) active in Raman in T_d by cons in their correlation modes A_1 , A_2 , B_1 and B_2 in C_{2v} is active in IR and Raman.
- The vibrations ν_3 (F_2) and ν_4 (F_2) active in IR and Raman in T_d remain active in IR and Raman in C_{2v} .

Table 5: Correlation diagram of the internal vibrations of the $[\text{PO}_4]^{3-}$ group in $[\text{H}_2\text{PO}_4]^-$

Molecular group $[\text{PO}_4]^{3-}$ T_d		Molecular group $[\text{H}_2\text{PO}_4]^-$ C_{2v}	
Vibrations	Modes	Modes	Vibrations
$\nu_{\text{as}}(\text{P-O})$	$F_2(\text{Ra, IR})$	$B_1(\text{Ra, IR})$	$\nu_{\text{as}}(\text{P-O})$
		$B_2(\text{Ra, IR})$	$\nu_{\text{as}}(\text{P-OH})$
$\nu_{\text{s}}(\text{P-O})$	$A_1(\text{IR})$	$A_1(\text{Ra, IR})$	$\nu_{\text{s}}(\text{P-O})$
		$A_1(\text{Ra, IR})$	$\nu_{\text{s}}(\text{P-OH})$
$\delta_{\text{as}}(\text{O-P-O})$	$F_2(\text{Ra, IR})$	$B_1(\text{Ra, IR})$	$\rho r(\text{PO}_2)$
		$B_2(\text{Ra, IR})$	$\rho w(\text{PO}_2)$
		$A_1(\text{Ra, IR})$	$\delta(\text{P(OH)}_2)$
$\delta_{\text{s}}(\text{O-P-O})$	$E(\text{IR})$	$A_1(\text{Ra, IR})$	$\delta(\text{OPO})$
		$A_2(\text{IR})$	$\rho t(\text{PO}_2)$

3.4- Internal vibrations of $[\text{H}_2\text{PO}_4]^-$ in single crystal $(\text{C}_6\text{H}_{15}\text{N}_4\text{O}_2) \text{H}_2\text{PO}_4 \cdot \text{H}_2\text{O}$

The distribution of the $[\text{H}_2\text{PO}_4]^-$ vibrations in the C_2 factor group is obtained by performing, on the one hand, correlations between the molecular group C_{2v} of $[\text{H}_2\text{PO}_4]^-$ and the site group C_1 that it occupies and secondly correlations between the C_1 site group and the C_2 group of the mesh. The results obtained are grouped in the (table 6).

Table 6: Correlation diagram of the $[\text{H}_2\text{PO}_4]^-$ in the single crystal $(\text{C}_6\text{H}_{15}\text{N}_4\text{O}_2) \text{H}_2\text{PO}_4 \cdot \text{H}_2\text{O}$

Activity	MG C_{2v}	SG C_1	FG C_2
	6A1 (IR, Ra) 4B1 (IR, Ra) 2A2 (IR, Ra) 3B2 (IR, Ra)	15 A (IR, Ra)	15 A (IR, Ra) 15 B (IR, Ra)
IR	15	15	30
Ra	15	15	30
Coincidence	15	15	30

From this table, we deduce the representation of the vibration of the $[\text{H}_2\text{PO}_4]^-$ ion in the single crystal L-Arginine phosphate monohydrate. The number so is 30.

$$\Gamma[\text{H}_2\text{PO}_4]^- : 15\text{A (IR, Ra)} + 15\text{B (IR, Ra)}$$

Due to the presence of this symmetry, active modes in Raman also active in IR.

3.5- Internal vibrations of H_2O in single crystal $(\text{C}_6\text{H}_{15}\text{N}_4\text{O}_2) \text{H}_2\text{PO}_4 \cdot \text{H}_2\text{O}$

In the single crystal L-Arginine phosphate monohydrate, the molecules of H_2O they all occupy the site of symmetry C_1 . The Counting of the normal modes of internal vibration of these molecules is given in the (table7).

Table 7: Correlation diagram of the H_2O in the single crystal $(\text{C}_6\text{H}_{15}\text{N}_4\text{O}_2) \text{H}_2\text{PO}_4 \cdot \text{H}_2\text{O}$

Activity	MG C_{2v}	SG C_1	FG C_2
	2A ₁ (IR, Ra) B ₂ (IR, Ra)	3 A (IR, Ra)	3 A (IR, Ra) 3 B (IR, Ra)
IR	3	3	6
Ra	3	3	6
Coincidence	3	3	6

The distribution of the 6 internal vibrations of H_2O is given by the following irreducible representation:

$\Gamma[\text{H}_2\text{O}] : 3\text{A (IR, Ra)} + 3\text{B (IR, Ra)}$ We can observe, on the Raman scattering and infrared absorption spectra, 6 Raman lines of symmetry 3A and 3B and 6 infrared bands of type 3A and 3B. Using the internal coordinates, we can deduce that the fundamental vibrations of H_2O in the C_{2v} free state of symmetry are as follows [10]:

- $\nu_s(\text{OH})$: Valence vibration of the symmetrical O-H bond (type A_1).
- $\nu_{as}(\text{OH})$: valence vibration of the asymmetric O-H bond (type B_2).

- $\delta(\text{HOH})$: Vibration of angular deformation of the H-O-H bond (type A_1).

4. Interpretation of infrared and Raman scattering spectra of single crystal $(\text{C}_6\text{H}_{15}\text{N}_4\text{O}_2)\text{H}_2\text{PO}_4\cdot\text{H}_2\text{O}$

The infrared absorption and Raman scattering spectra of $(\text{C}_6\text{H}_{15}\text{N}_4\text{O}_2)\text{H}_2\text{PO}_4\cdot\text{H}_2\text{O}$ are shown in Figures 4 and 5 respectively. The proposed allocations of the bands for the fundamental vibrations of this compound are given in Table 8. In the single crystal $(\text{C}_6\text{H}_{15}\text{N}_4\text{O}_2)\text{H}_2\text{PO}_4\cdot\text{H}_2\text{O}$, each anion $[\text{H}_2\text{PO}_4]^-$ has two types of distances: the terminal P-OH bond in $\text{P}(\text{OH})_2$, and the terminal P-O bond assigned in PO_2 . For this reason, the assignments of the bands on the two infrared and Raman spectra can be made according to the vibrations of $\text{P}(\text{OH})_2$, PO_2 and O-H.

4-1 Infrared Absorption Spectrum of the Compound $(\text{C}_6\text{H}_{15}\text{N}_4\text{O}_2)\text{H}_2\text{PO}_4\cdot\text{H}_2\text{O}$.

The infrared absorption spectrum of the single crystal $(\text{C}_6\text{H}_{15}\text{N}_4\text{O}_2)\text{H}_2\text{PO}_4\cdot\text{H}_2\text{O}$ is reported in Figure 4. The frequencies observed are interpreted as follows:

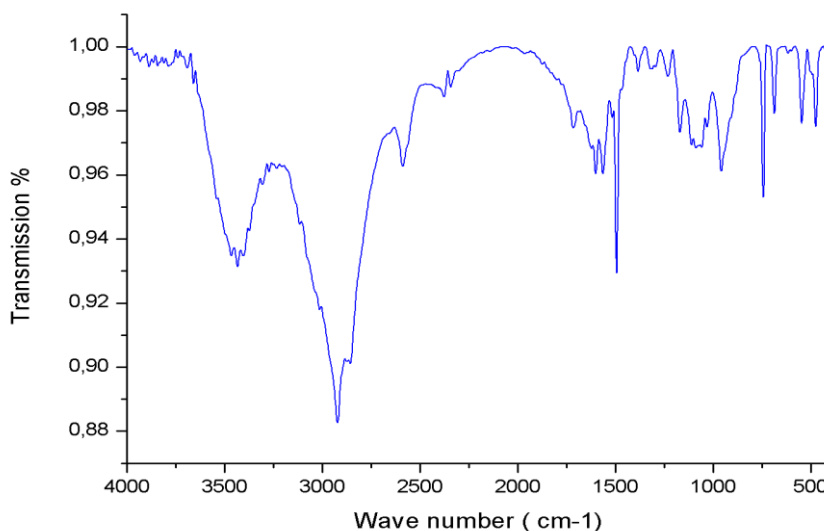


Figure 4: IR spectra of the single crystal $(\text{C}_6\text{H}_{15}\text{N}_4\text{O}_2)\text{H}_2\text{PO}_4\cdot\text{H}_2\text{O}$

Vibration of water molecules

The two broad bands between 3474 and 3098 cm^{-1} are due to the syntactic and antisymmetric valence vibrations of water molecules of type A_1 and B_2 , and the band located at 1556 cm^{-1} is attributed to the deformation vibration of H_2O of type A_1 . The band observed at 592 cm^{-1} is due to the rocking mode of the water molecule [10-11].

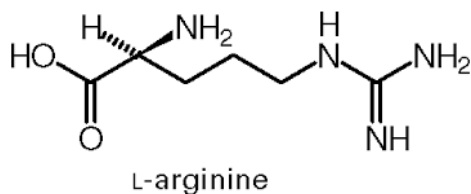
Vibrations of the group $[\text{H}_2\text{PO}_4]^-$

The two bands of weak intensities located at 1226 and 1010 cm^{-1} are assigned to $\text{P}=\text{O}$ stretching vibrations.

The band at 534 cm^{-1} is attributed to the deformation vibration in the P-OH plane, while the band seen at 480 cm^{-1} is due to the out-of-plane deformation vibration of P-OH.

Internal vibrations of the L-arginine molecule.

The L-arginine molecule has no symmetry so all modes of vibration will be active both infrared and active in Raman. The molecular structure discussed above shows that the L-arginine molecule has the molecular groups NH_3^+ , NH_2 , NH , CH_2 , CH and COO^- [12].



4-2 Raman scattering spectrum of the compound $(C_6H_{15}N_4O_2) H_2PO_4 \cdot H_2O$.

The Raman spectrum of single crystal $(C_6H_{15}N_4O_2) H_2PO_4 \cdot H_2O$ in the range of 4000-200 cm^{-1} is shown in Figure 5. This figure shows the position and relative intensity of the bands in the Raman spectrum. It is obvious that there are large parts between 2000-2700 cm^{-1} of the spectrum where no intensity is observed.

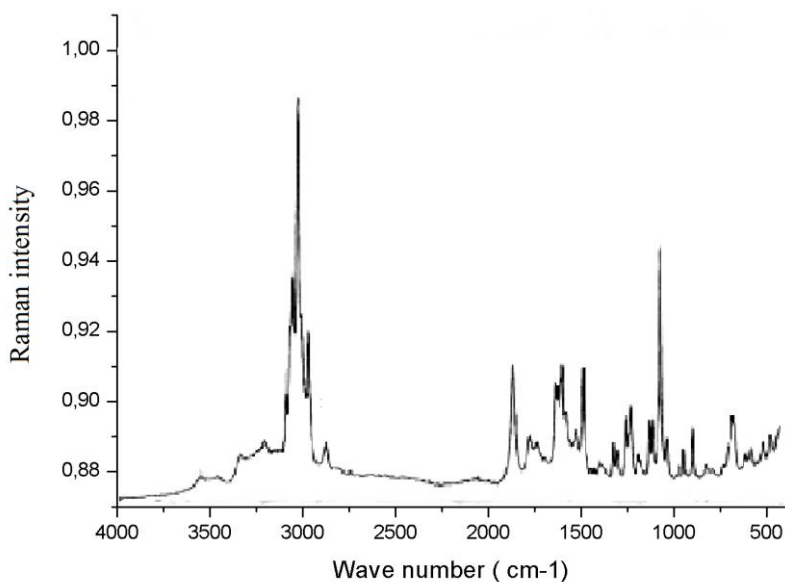


Figure 5: Raman spectra of the single crystal $(C_6H_{15}N_4O_2)H_2PO_4 \cdot H_2O$

The Raman spectrum is remarkable for a very intense group at 890 cm^{-1} that is assigned to C-C stretching. This group is given the same mission, whose implication is that not all units of hydrogen phosphate are equivalent. A low intensity Raman band is at 1054 cm^{-1} and is assigned to CH_2 Rocking vibration and P=O symmetric stretching. Other Raman bands are observed at 1231 cm^{-1} P=O stretching, 1324 cm^{-1} C-O asymmetric stretching, 1479-1624 cm^{-1} NH_3^+ symmetric deformation and NH_2 in-plane-deformation, 1721-1961 cm^{-1} C=O stretching and 2773 - 2962 cm^{-1} CH_2 asymmetric stretching and CH stretching. The frequencies of water modes are $\nu_2 = 3652$ cm^{-1} , $\nu_1 = 1595$ cm^{-1} and $\nu_3 = 3756$ cm^{-1} [13]. The symmetry of the site of the water molecule in the $(C_6H_{15}N_4O_2) H_2PO_4 \cdot H_2O$ is C_1 and, in addition, the water molecules are involved in the hydrogen bonding. Consequently, the frequencies ν_1 and ν_3 of $(C_6H_{15}N_4O_2) H_2PO_4 \cdot H_2O$ are nearly 200 cm^{-1} lower than the corresponding frequencies of the free molecule. The results of the analysis of the band components of the Raman and infrared spectra are shown in Table 8.

Table 8: Assignments of the IR and Raman frequencies of $(\text{C}_6\text{H}_{15}\text{N}_4\text{O}_2)\text{H}_2\text{PO}_4\cdot\text{H}_2\text{O}$.

IR	RAMAN	Assignments
3474	3468	N-H asymmetric stretching and vas O-H
3368	3384	
3242	3254	
3098	3120	ν_{δ} H-O-H
2924	2962	C-H stretching
	2933	
2870	2874	CH ₂ asymmetric stretching
2668	2773	
2430	-	
1882	1961	C=O stretching
1714	1721	
1620	1624	N-H bending
1556	-	NH_3^+ symmetric deformation / NH_2 in-plane deformation
1520	1479	
1470	1443	CH ₂ in-plane deformation
1352	1324	C-O asymmetric stretching
1226	1231	P=O stretching
1194	-	C-O stretching
1010	1054	CH ₂ Rocking and P=O symmetric stretching
926	890	C-C stretching
840	-	COO ⁻ Scissoring
704	708	NH ₂ out of plane deformation
592	-	O-H out of plane deformation
534	-	δ_{as} O-P-O
480	486	P-OH deformation
464	-	COO ⁻ Rocking
	340	External modes of N-H...O and O-H...O
	282	
	264	

Conclusion

The single crystal L-Arginine phosphate monohydrate $(\text{C}_6\text{H}_{15}\text{N}_4\text{O}_2)\text{H}_2\text{PO}_4\cdot\text{H}_2\text{O}$ was prepared by direct method. The $(\text{C}_6\text{H}_{14}\text{N}_4\text{O}_2)$ was carefully added drop wise to phosphoric acid solution to reach the stoichiometric ratio 1/1. Its structure was reinvestigated and solved by direct methods from the data collected by using single crystal X-ray diffraction. The infrared and Raman scattering spectra allowed us to determine the symmetries of various modes of molecular vibration in the single crystal L-Arginine phosphate monohydrate. The assignment of Raman and infrared bands to various molecular vibrations in the L-Arginine phosphate monohydrate crystal has been made taking into account the molecular structure and crystalline data. In view of the above, the vibrations of the $(\text{C}_6\text{H}_{15}\text{N}_4\text{O}_2)\text{H}_2\text{PO}_4\cdot\text{H}_2\text{O}$ crystal can be considered as being composed of the following vibrations : vibrations of the water molecule; internal vibrations of the L-arginine molecule; internal vibrations of the phosphate group with symmetry C_{2v} .

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