iJRASET
International Journal For Research in Applied Science and Engineering Technology

INTERNATIONAL JOURNAL FOR RESEARCH

IN APPLIED SCIENCE & ENGINEERING TECHNOLOGY

Volume: 3 **Issue:** IX **Month of publication:** September 2015

DOI:

www.ijraset.com

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Volume 3 Issue IX, September 2015
ISSN: 2321-9653
International Journal for Research in Applied Science & Engineering Technology (IJRASET)

Growth And Characterization of ADP With β-Alanine Single Crystals

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Abstract-In Semi Organic crystal, ADP with β-Alanine was grown by slow evaporation method at room temperature. The characterization of Powder X-ray diffraction and spectroscopic studies of FT-IR, UV-Visible Spectra and AC Impedance spectra were taken. The miller indices was determined by powder X-ray diffraction.FT-IR spectra were assigned the vibrational analysis of grown crystals. The optical transparency of crystal was shown by UV-Visible spectra. The band gap of the crystal is 5.93 eV. AC Impedance spectra were recorded by HIOKI 3532 LCR meter interfaced with computer. The conductivity of grown crystal was calculated by using AC Impedance spectra.

Key words: ADP, β-Alanine, Slow evaporation method, Powder X-ray Diffraction, FT-IR, UV-Visible spectroscopy, AC Impedance spectroscopy.

I. INTRODUCTION

In recent years the more achievements are in semi-organic single crystals. The Ammonium Dihydrogen Phosphate (ADP) is an in-organic material. This is mixed with the organic compound of amino acid groups to produce a new material. Here the β-Alanine was used. The semiorganic crystal mostly used to produce the ultrasonic waves except the quartz crystals. The ADP with β-Alanine crystals are used the piezo –electric transducers.

II. EXPERIMENTAL WORK

Equimolar ratio of ADP and β-Alanine salts are dissolved with distilled water. The dissolved solution stirred from magnetic stirrer with 15 minutes. After the stirring process the solution is filtered by filter paper and the solution is placed in the petty disc. The mouth of the petty disc tightly covered by news paper or any cover with small holes. The petty disc placed without direct sunlight and dust but air circulation is free. After 3 days nucleation will be started. Some seed crystals formed. The solutions are slowly evaporated by the holes; all the solution will be evaporated. After 30 days bulk crystals were formed by the slow evaporation process. The crystal formation is depends on the surroundings. The growth of crystal is fast or slow by their surrounding environment.

III. RESULT AND DISCUSSION

A. Fourier Transform Infrared Analysis

If the grown crystal has been taken for the FTIR spectra in the region 4000-400 cm^{-1}. The FTIR spectrum is very useful to confirm the functional groups present in the growth crystal. Pure and complex FTIR spectra were recorded and the frequencies, functional groups present are shown in the table [1].

Volume 3 Issue IX, September 2015
ISSN: 2321-9653
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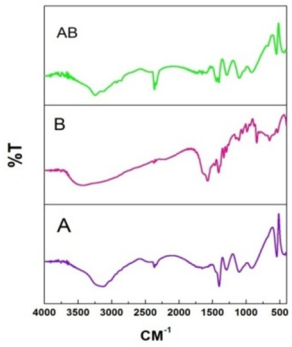

FTIR Spectrum for pure and complex.

A-ADP, B-β-ALANINE, AB-COMPLEX

FTIR frequency assignment Table

ADP (CM^{-1})	β- ALANINE (CM^{-1})	COMPLEX (AB) (CM^{-1})	ASSIGNMENTS
3128.54	---	3124.68	O-H Stretching, P-O-H Stretching, N-H Vibration of ammonium
---	2929.87	2924.09	CH_2 Vibration
2370.51	2370.51	2370.51	NH_3^+ torsion, Band due to hydrogen bond
1654.92	---	1683.86	O-H bending of water
---	1575.84	1546.91	NH_3^+ symmetric bending
---	1463.97	1442.75	CH deformation
1400.32	1408.04	1404.18	Bending vibration of Ammonium, COO^- symmetric stretching
1294.24	1294.24	1288.45	Combination of the asymmetric stretching vibration of PO_4 with lattice, COO^- symmetric stretching
1103.28	1107.14	1101.35	P-O-H vibration, COO^- symmetric stretching
---	1055.06	1024.20	C-N stretching

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920.05	---	920.05	P-O-H vibration
---	651.94	675.09	COO^- scissoring
543.93	534.28	547.78	PO_4 vibration, COO^- rocking
443.63	---	432.05	PO_4 vibration

The functional groups of O-H stretching, P-O-H stretching and N-H vibration of ammonium are assigned at the range 3124.68 cm^{-1}. This peak were also presented in the pure ADP at the frequency 3128.54 cm^{-1}, [2], CH_2 vibrational frequency occurs at the range 2924.09 cm^{-1} and this functional group due to the β-Alanine at the range 2929.87 cm^{-1} [3].

The torsional oscillation of NH_3^+ group and the band due to the hydrogen bond are occurred at 2370.51 cm^{-1} [4]. The O-H bending vibration of water due to the band at 1683.86 cm^{-1} and this frequency shifted from pure ADP at the range 1654.92 cm^{-1}. Symmetric bending vibration of NH_3^+ assigned at the band 1546.91 cm^{-1}. This bending vibration is occurred by β-Alanine [5]. The CH deformation due to the organic compounds, at the range is 1442.75 cm^{-1}. In the pure β-Alanine, it has small amount of shifting at the range 1463.97 cm^{-1} [6]. The band 1404.18 cm^{-1} is due to the bending vibration of ammonium. The combination of asymmetric stretching vibration of PO_4 with lattice assigned at the range 1288.45 cm^{-1}. The frequencies 1404.18, 1288.45 and 1101.35 cm^{-1} are assigned the COO^- symmetric stretching. The P-O-H vibration occurs at 1101.35 cm^{-1} and 920.05 cm^{-1}. C-N stretching vibration of β-Alanine was assigned at the range 1055.06 cm^{-1}. COO^- scissoring and rocking vibrations are occurred at the bands 675.09 cm^{-1} and 547.78 cm^{-1} [3,7]. The frequency ranges 547.78 cm^{-1} and 432.05 cm^{-1} are due to the PO_4 vibrations.

B. Powder X-Ray Diffraction

The powder X-ray diffraction spectrum is shown below.

The crystalline quality of the grown crystals and their cell dimensions were studied by powder X-ray diffraction analysis using a Rigaku X-ray diffractometer with Cu Kα radiation source K_α = 1.540 Å in the 2θ range 20º–80º [8]. The hkl planes are determined by peak indexing method. The hkl plane table is given below.

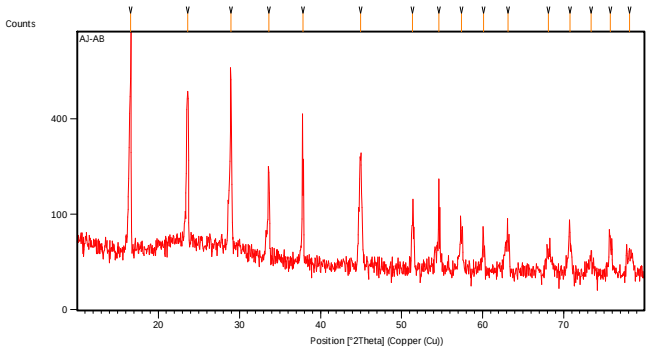

Fig: powder XRD for grown Crystal

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Table: Powder XRD

2θ	D	$1000/d^2$	$(1000/d^2)/CF$	hkl
16.5866	5.34481	35.0054	1	100
23.6189	3.76696	70.4722	2	110
28.9594	3.08330	105.1885	3	111
33.6201	2.66576	140.7206	4	200
37.8144	2.37917	176.6644	5	210
51.3723	1.77864	316.0995	9	300
54.6530	1.67938	354.5700	10	310
57.4049	1.60525	388.0740	11	311
60.1386	1.53865	422.3965	12	222
63.1405	1.47254	461.1750	13	320
70.7918	1.33098	564.4908	16	400
73.4150	1.28977	601.1397	17	410
75.7641	1.25552	634.3847	18	411
78.1509	1.22304	668.5265	19	331

C. UV-Visible Absorption Spectroscopy

Optical transparency range of single crystals plays very important role in optical technology [9]. For such non linear optical crystals principal role begin to play intrinsic defects due to intermolecular voids and phonon subsystem [10]. The UV-Visible spectra of grown crystals are taken in range 200-1100 nm.

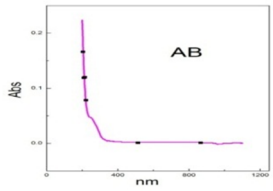

Fig: UV absorption spectrum

The absorption ranges of the crystals are 209 nm and 223 nm respectively. We used the following formula to calculate the bandgap [11,12]. The cut off wavelength is 209 nm and the band gap value is 5.93 eV. The absorption ranges are very small. It indicates that the transparency of grown crystals were high. The grown crystals are transparent in the UV region.

D. Dissipation Factor From AC Impedance Spectra

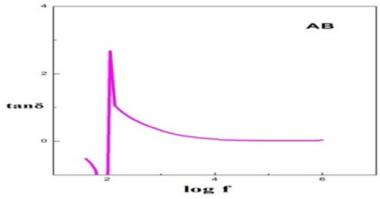

Fig: Dissipation factor

The dielectric dissipation factor of the AB crystal is shown in above [13]. In the figure sharp peaks were observed at high frequencies. The maximum loss tangent as a result of resonant condition induced by the relaxation time of polarization is equal to the period of applied field.

IV. CONCLUSION

The ADP with β-Alanine single crystal was grown by slow evaporation method at room temperature. This is an semi organic crystal. The frequency assignments are determined by FT-IR spectra. The band gap measured with UV-absorption spectra. The band gap value is 5.93 eV. The Dissipation factor graph was drawn form the AC Impedance spectra.

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SUMMARY AND CONCLUSIONS

The ADP with β-Alanine and Ammonium Thiocyanate single crystals were grown by slow evaporation method. ADP and β-Alanine is taken in the ratio 1:1. ADP with β-Alanine and Ammonium Thiocyanate are taken in the ratio 1:1:1. The grown crystals are colourless and transparent. The grown crystals were characterised using powder XRD, density measurement, FTIR studies, UV-Visible studies and AC Impedance Spectroscopy studies.

From the density measurement the density values of the complex crystals are found in between their parent values.

From the FTIR studies, grown crystal are new complexes. The vibrational modes of grown crystals are the combination of all the vibrational modes of the parent materials.

From the UV-Visible Spectroscopy, the grown crystals are transparent in the UV region.

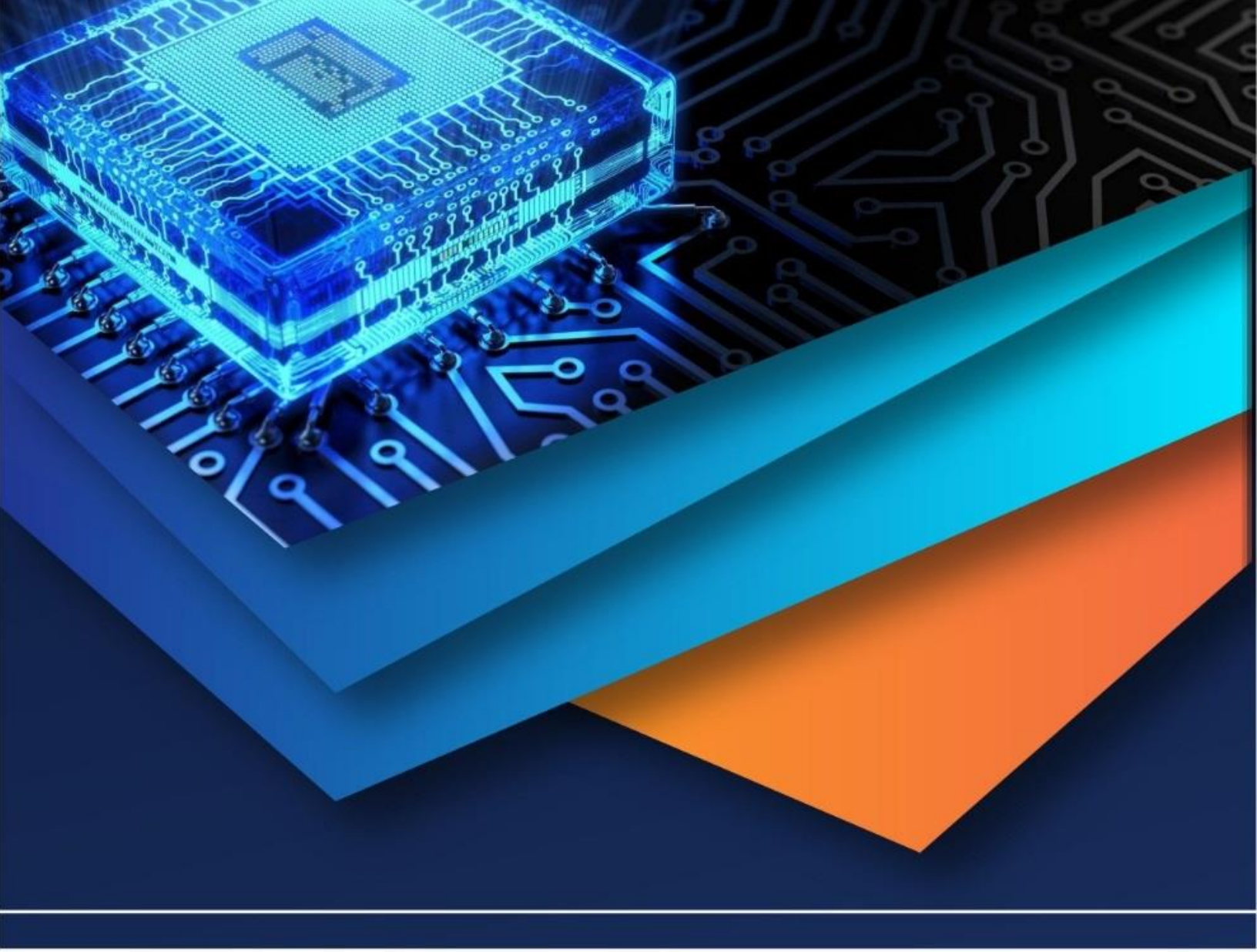
The bandgap energy for AB crystal is 5.93eV.

The bandgap energy for ABT crystal is 5.56 eV.

From the powder XRD hkl planes were determined. This hkl planes are not coincide with any prior JCPDS file values. This confirms that the grown crystals are the new ones.

From the AC Impedance Spectroscopy studies the conductivity of the one crystal is 0.5979 Scm^{-1}.

The conductivity of another crystal has the negative region.



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