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Research Article

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Growth and Characterisation of Purine derivative Adenine Nucleobase.

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Abstract

Adenine is an important class of purine derivative nucleobase. Adenine found wide applications in electronic and optical fields. In the present work, Pure Adenine are grown from slow evaporation technique, Grown crystals are subjected to FT-IR, UV-Vis, and Fluorescence spectral studies. Crystal structure of grown crystals is obtained from powder XRD pattern. Band gap determination is also carried out from the UV-Vis data. The surface morphology of the crystals are analyzed by SEM studies. Elemental analysis is also carried out by EDAX analysis.

Keywords: Band gap, EDAX, FT-IR, UV-Vis

1. Introduction

Organic non-linear materials are attracting a great deal of attention, as they have large optical susceptibilities, inherent ultra fast response times and high optical thresholds for laser powder as compared with organic materials[1]. A number of such materials have been reported in literature for their potential application [2-4]. In this study, the growth of the purine derivative material, adenine and its morphology, spectroscopic properties are discussed. Adenine is one of the two purine nucleobases used in forming nucleotides of the nucleic acids. In DNA, adenine binds to thymine via two hydrogen bonds to assist in stabilizing the nucleic acid structures. In RNA, which is used for protein sunthesis, adenine binds to uracil.[5,6].

2. Experimental Method

2.1. Crystal Growth Method

The selection of the solvent is an important step in the growth of crystals from solution by slow evaporation method. Here, water was selected as the solvent for the crystal growth experiments. Commercially available Adenine was used for the growth. Exactly 0.2M solution of Adenine of 1g was taken and heated in a magnetic stirrer for about 1 hour. Then the solution was filtered using micro filter paper and the solution was closed with the filter paper and several holes were made in the paper. Good quality crystals were harvested within a week.

3. Crystal Characterization

3.1 FTIR Spectral Analysis

The formation of the characteristic bands corresponding to functional groups were tested by FT-IR spectral analysis recorded in 4000-400cm^{-1} region using infrared spectrometer by using KBR peller technique. The wavenumbers corresponding to 3125.58cm^{-1}, 3296.41cm^{-1}, 3360.08cm^{-1}, 3656.5cm^{-1} are assigned to N-H stretching vibration, then the bands at 2979.57cm^{-1}, 2803.28cm^{-1} are assigned to C-H stretching vibrations. Also, the peak at 1683.8cm^{-1} signifies the C=C stretching, the bands at 1454.78cm^{-1}, 1507.23cm^{-1}, 1612.13cm^{-1} correspnds to NH_2 bending. The peak at 1418.16cm^{-1} is attributed to C-N stretching. The peak at 872.60cm^{-1} and 661.49cm^{-1} signifies C-C out-of-plane bending and N-H deformation respectievely. The FTIR spectrum of adenine crystals is shown in the Figure.(1) and the vibrational frequencies are tabulated in Table.(1).[7-9]

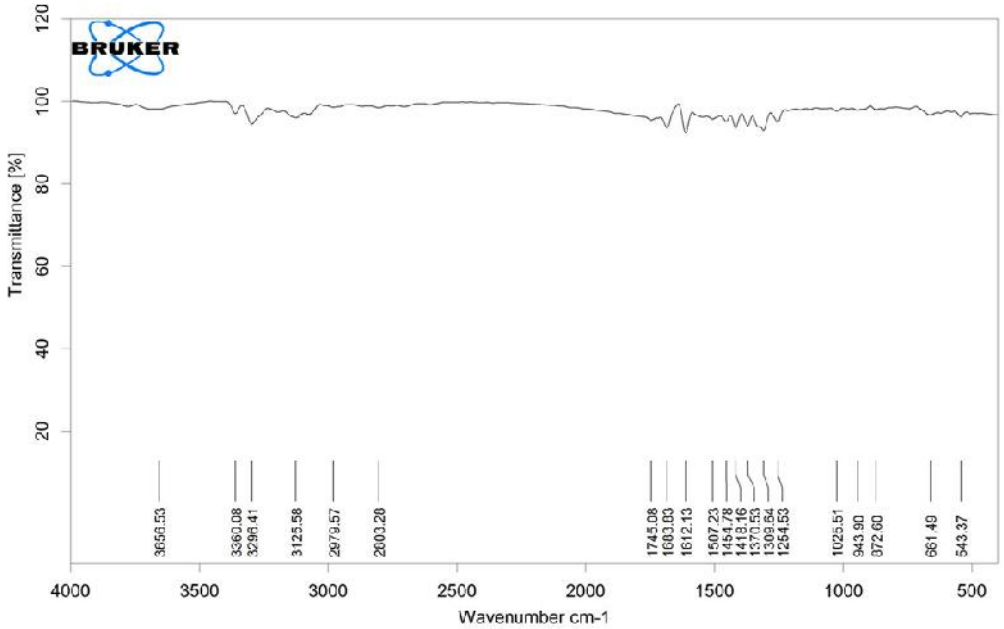

Figure.1 FTIR Spectrum of Pure Adenine

Table1. Vibrational Frequencies of Pure Adenine

Adenine Wave Number in cm^{-1}	Assigned Frequencies
3656.53 3360.08 3296.41 3125.58	N-H Stretching
2979.57 2803.28	C-H Stretching
1683.83	C=C Stretching
1612.13 1507.23 1454.78	NH_2 bending
1418.16	C-N Stretching
872.60	C-C Out-of-plane bending
661.49	N-H Deformation

3.2 UV-Vis Spectral Analysis

The UV-Vis spectrum of the grown crystal was carried out using lambda 35 UV-Vis spectrometer in the wavelength range of 200nm & 1100nm. The UV-Vis spectral data is used to measure the concentration and the transparency of the crystal. The UV-Vis spectrum of the grown adenine crystals is shown in the Figure(2). Regarding the electronic adsorption, it has the transition in the range of 205.1nm and 260.1 nm. The absorbance becomes almost constant for the entire visible region.

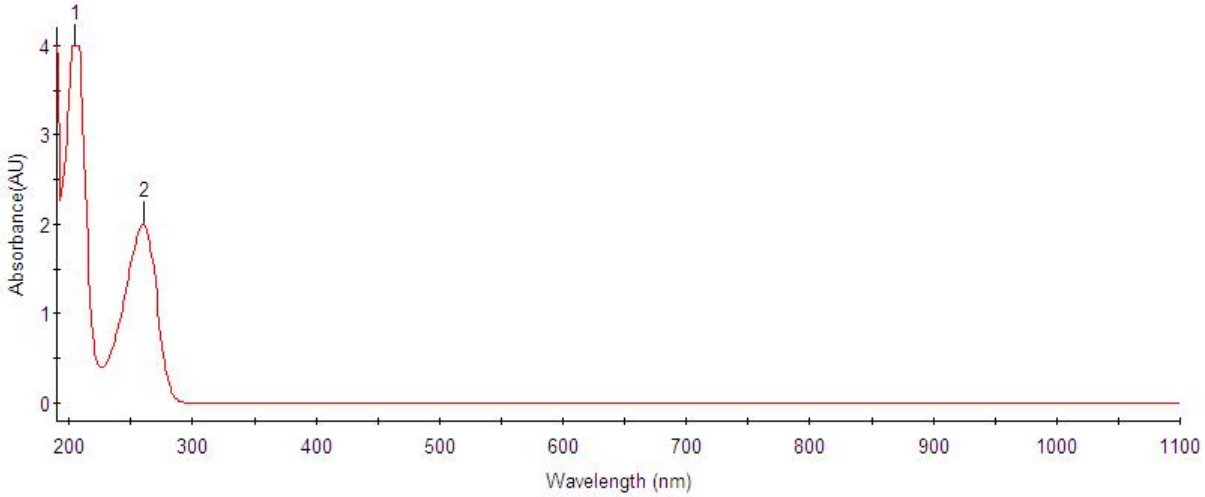

Figure.2 UV-Vis Spectrum of Pure Adenine

3.3 Band Gap Energy determination

The band gap energy measurement was also carried out for adenine crystals. The plot of $(\alpha\beta\gamma)^2$ against hν is shown in the figure(3), a trend line was added to extrapolate and it cut the X-axis of 5.81eV in adenine crystals. The band gap measurement suggested that the adenine crystals have wider applications in various optical field and have electronic properties.

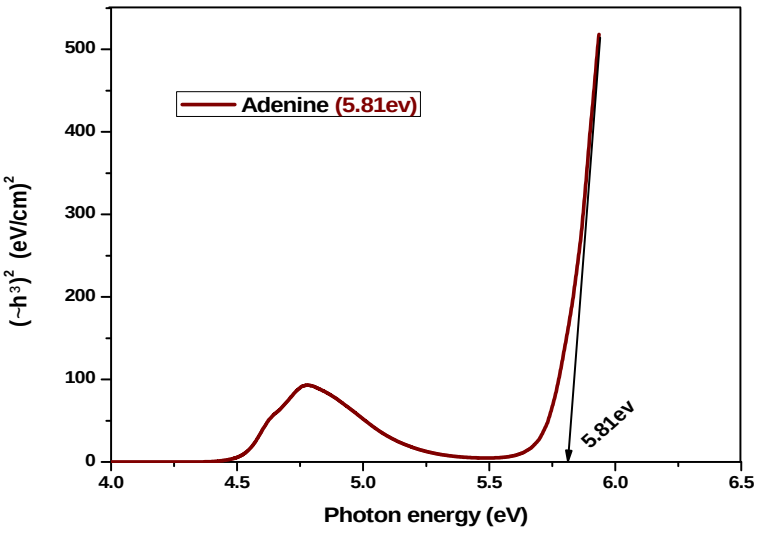

Figure.3 Band gap energy of pure Adenine

3.4 Fluoresence Spectra

The fluorescence spectrum of adenine crystals are measured in the range of 320.00nm to 750 nm are shown in the Figure(4). It has been observed that the fluorescence spectra has broad excitation spectra in the range of 417.56nm^{-1} and a sharp emission spectra in the range of 605.61nm^{-1}, The observed results suggested that the Adenine crystals have fluorescence property which emits light.

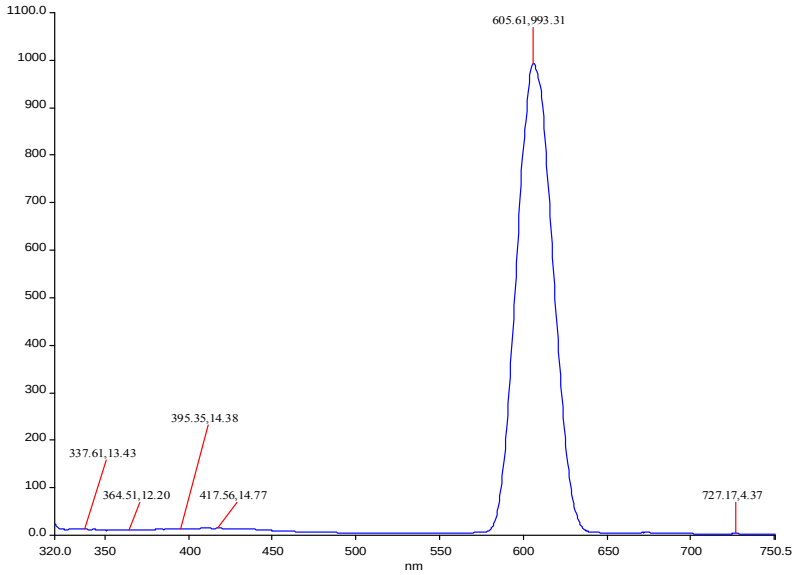

Figure.4 Fluorescence Spectra of Pure Adenine

3.5 Powder X-ray Diffraction Analysis

The crystallinity nature of the obtained sample was identified by powder X-ray difractometer. The sharp intensity peaks shows the measure of crystalline nature of the compound. The XRD patterns of Adenine crystals are shown in the Figure.(5)

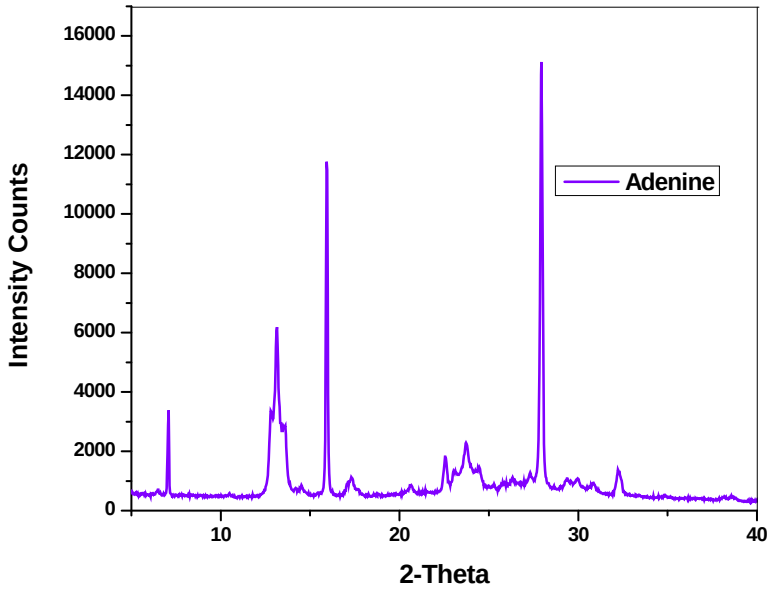

Figure.5 Powder XRD Spectra of Pure Adenine

3.6 SEM Analysis

The image in SEM is produced by scanning the sample with a focused electron beam and detecting the secondary back scattered electrons from the conventional SEM image. The SEM images of Adenine is shown in the Figure(6). It is observed that the surface of the grown crystal is smooth. It is also seen that there are particles, agglomerating into uniformly grown clusters.

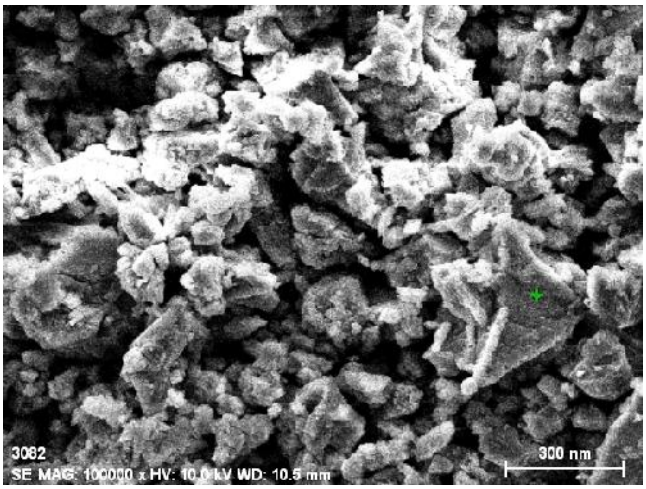

Figure. 6 SEM image of Pure Adenine

3.7 Energy Dispersive X-ray Analysis

Figure(7) shows EDAX spectrum of Adenine crystals. The peaks shows the presence of Carbon and Nitrogen. It was observed that the atomic % of C and N are 48.63% and 51.15% respectively. The above results suggested that the pure nature of the grown crystals.

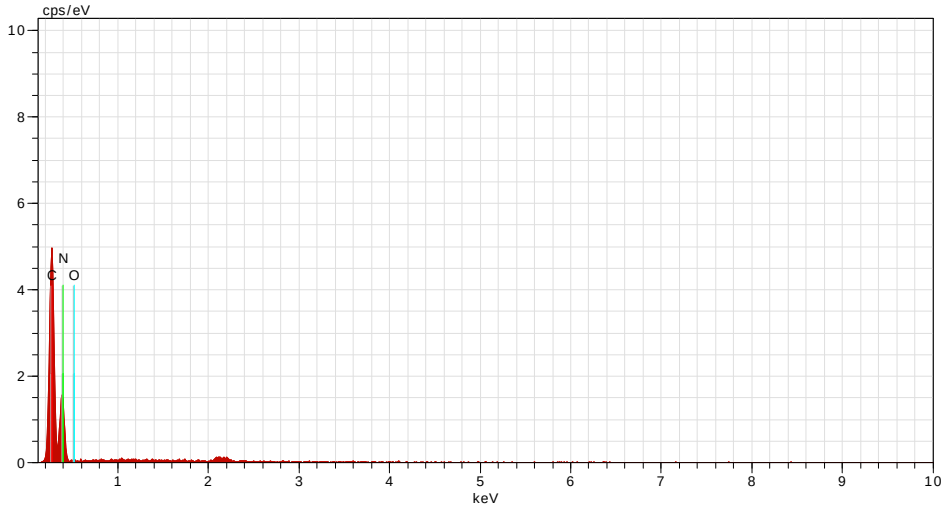

Figure.7 EDAX Spectrum of pure Adenine

4. Conclusion

Purine deravative nucleobase of Adenine crystal is grown by slow evaporation method. The fundamental vibration and the functional groups present in the grown crystals have been confirmed by FTIR spectral analysis. UV-Vis spectra show that the adenine crystal have constant absorption in the entire visible region. Fluorescence spectral analysis confirmed that the grown crystal fluoresces. Band gap measurement revealed the electronic properties. Powder XRD confimed the crystalline nature of the sample. SEM analysis confirmed the morphology of the crystal and EDAX analysis revealed the elemental nature of the sample.

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