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Synthesis and characterization of L-amino acid doped 2-aminopyridine co-crystals using Powder XRD, FTIR and UV-Vis spectrum.

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ABSTRACT

The FTIR spectrum shows that the carbonyl group of L-Leucine, L-Glutamic acid and L-Tyrosine interact with 2-aminopydine through N—H···O hydrogen bonding. 2-aminopyridine protonated and L-amino acids deprotonated during the reaction, resulting in the formation of 2-aminopyridiniumleucinate, bis2-aminopyridinium glutamate and 2-aminopyridiniumtyrosinate co-crystals. The UV-Vis spectrum shows that the molecules are closely packed, undergoes $n \rightarrow \pi^*$ transition in all these three co-crystal and the cut off wavelength value indicate that bis2-aminopyridinium glutamate and 2-aminopyridiniumtyrosinate co-crystals have Non-linear optical property compared to 2-aminopyridiniumleucinate crystals. The cell parameter calculated from powder XRD pattern.

1. Introduction

Several co-crystal structures have been reported that are based upon 2-aminopyrimidine whether or not a salt or co-crystal forms seems to be related to the ancillary groups that are bonded to the 2-aminopyriddine moiety. For example all 2-aminopyridines that interact with carboxylic acids appear to be in the form of salts whereas 2-aminopyrimidines form either neutral or ionic Supra molecular hetero synthase and melamine tend to exist as mono-protonated salts. An analysis of the Cambridge structural info reveals that seventy seven of compounds that contain each 2-aminopyridine and acid moieties generate 2-aminopyridine– acid Supra molecular hetero synthase instead of carboxylic acid or 2-amino pyridine-supramolecular-homosynthons[1].

The 2-amino pyridine–carboxylic acid system has been the subject of theoretical and spectroscopic. 2-aminopyridine can be protonated in acidic solution. The bonding of the H atom to the ring N atom of 2-aminopyridine rather than the amine N atom gives an ion for which an additional resonance structure can be written. As this has a lot of resonance energy (additional ionic resonance) than 2-aminopyridine itself. 2-aminopyridine is a strong base, like amides. The positive charge in the 2-aminopyridinium ions of 2-amino pyridininum–fumarate–fumaric acid is on the amine-group[2]. The Supra molecular Synthase present are analysed and their effect upon the crystal packing is presented in the context of crystal engineering salt $C_5H_7N_2^+$. $C_6H_7O_7^-$ is formed by the protonation of the pyridine N atom and de protonation of the central carboxylic group of citric acid. Systematic structural and statistical analysis focusing on the identification of robust Supra molecular synthase or patterns are essential for crystal engineering and the design of new solid-state structures with desired properties. Organic crystals, especially salts are now considered as potential materials for optical applications because of their flexibility in molecular design, thermal stability and delocalized clouds of pi electrons.

In all the reported structures, the charge–assisted 2-aminopyridinium–carboxylate or neutral 2-acetamino pyridine-carboxylic hetero synthase is observed as suggested by statistical analysis. The crystal structure of 2-amino 5-chloropyridinium–L-tartrate shows that depicts of the presence of the other competing functionalities on the carboxylic acid the most frequent 2-aminopyridinium–carboxylate hetero synthase is still observed[3]. Hydrogen bonding plays a key role in molecular recognition and crystal engineering research. The design of highly specific solid state compounds is of considerable significance in organic chemistry due to the important applications of these compounds in the development of new optical, magnetic and electronic system[4-6]. Amino acids also play pivotal role in the physical properties of peptides and proteins. Because their side chain rings can be stacked one with another. Amino acids alone or together with insulin were able to regulate expression of several genes involved in the metabolism of carbohydrates and lipids. The properties of α-amino acids area unit advanced, yet simplistic in that every molecule of an amino acid involves two functional groups: carboxyl (-COOH) and amino ($-NH_2$). Side chains having pure organic compound alkyl group or aromatic teams area unit thought of non-polar, and these amino acids are comprised of Phenylalanine, Glycine, Alanine, Isoleucine, Methionine, and Tryptophan. Meanwhile, if the aspect chain contains totally different polar teams like amides, acids, and alcohols, they are classified as polar. Their list includes, Serine, Asparagine, Threonine, Glutamine, and Cysteine. If the aspect chain contains acid, the amino acids in the acidic-polar classification are Aspartic Acid and Glutamic Acid. The side chain consists of a carboxylic acid in amino acids like Lysine, and Arginine. Glutamate is involved in neuro-inflammation in autism and Glutamate is a major excitatory

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Neuro-transmitter in the brain[7]. Glutamic acid performs a vital role in brain disorders like Parkinson illness, dementia praecox, and brain disorder and conjointly helps in correcting behavioural disorders of childhood. Aspartic acid, an excitatory neurotransmitter, is a metabolite in the urea cycle and helps in the removal of ammonia[8]. Leucine, an essential amino acid, helps in the formation of sterols in adipose and muscle tissue[9]. It stimulates the synthesis of muscle protein. Tyrosine is one of the building blocks of protein and is especially important for its role as a precursor to dopamine. It becomes an essential amino acid and should be provided to the organism[10]. In this work an investigation is done and reported that the 2-aminopyridine interact with L-Glutamic acid, L-Leucine and L-Tyrosine amino acids and forms salts.

2. Material Preparation

During the preparation suitable pH is maintained. Colourless 2-aminopyridinium-leucinate co-crystals prepared by mixing the 2-aminopyridine and L-Leucine in 2: 1 ratio through slow evaporation method. Colourless bis-2-aminopyridinium glutamate co-crystals prepared by mixing the 2-aminopyridine and L-glutamic acid in 2: 1 ratio through slow evaporation method. Light brownish colour 2-aminopyridinium tyrosinate co-crystal prepared by mixing the 2-aminopyridine and L-tyrosine in 2: 1 ratio through slow evaporation method

3. Result and Discussion

3.1. Powder XRD

Powder x-ray diffraction pattern collected from diffracto-meter XPERT-PRO, with starting position 2θ = 10.0231°, end position 2θ = 80.9231°, step size 2θ = 0.0500°, specimen length = 10.00 mm, measurement temperature = 25°C, Cu as anode material and K-Alpha = 1.54060 Å. The powder XRD pattern shown in figure 1.

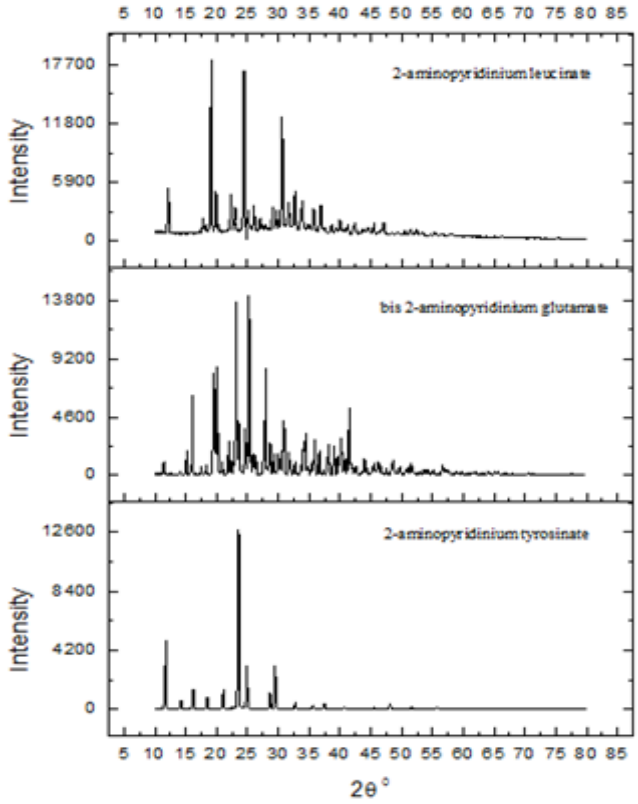

Figure 1. XRD pattern of L-amino acid based 2-aminopyridine co-crystals.

2-aminopyridinium-leucinate co-crystals crystallized in tetragonal structure with

$a = b = 3.99\text{Å}, c = 7.41\text{Å}, \alpha = \beta = \gamma = 90°$,

bis-2-aminopyridinium glutamate co-crystals crystallized in tetragonal structure with

$a = b = 13.57\text{Å}, c = 21.92\text{Å}, \alpha = \beta = \gamma = 90°$ and

2-aminopyridinium-tyrosinate co-crystals crystallized in triclinic structure with $a = 6.49\text{Å}, b = 7.92\text{Å}, c = 4.82\text{Å}, \alpha = 91.20°, \beta = 95.46°, \gamma = 107.18°$

3.2 FTIR spectrum

FTIR spectrum for powdered solid samples collected from JASCO IR spectrometer, between the ranges 399 cm^{-1} – 4000 cm^{-1} with Scanning Speed - 2 mm/sec. Hydrogen bonding plays a key role in molecular recognition[5] and crystal engineering research[4]. The design of high specific solid state compounds is of considerable significance in organic chemistry due to the important applications of these compounds in the development of new optical, magnetic and electronic system[6]. 2-aminopyridine can be protonated in acidic solution. The bonding of the H atom to the ring N atom of 2-aminopyridine rather than the amine N atom gives an ion for which an additional resonance structure can be written[2]. Based on these our investigation also show that the 2-aminopyridine was protonated and carbonyl group of L-leucine, L-glutamic acid and L-Tyrosine were deprotonated resulted as co-crystals. This was confirmed from the solid FTIR spectrum of these co-crystals and is shown in figure 2. The absorption peaks at 3559 cm^{-1}, 3518 cm^{-1}, 3569 cm^{-1} are due to the presence of $O_{(carbonyl)}\cdots H_{(pyridine\ N)}$ Hydrogen bond between 2-aminopyridine and L-leucine, L-Glutamic acid and L-tyrosine respectively.

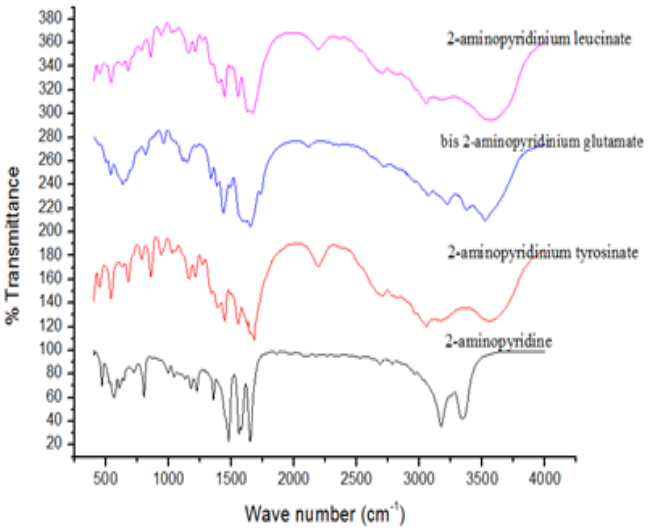

Figure 2. FTIR spectrum of L-amino acid based 2-aminopyridine co-crystals.

And this indicates the amine stretching present in these co-crystals. The peak at 3000 cm^{-1} disappears in all the co-crystals and new peak at 1686 cm^{-1}, 1734 cm^{-1}, 1665 cm^{-1} appears in the co-crystals of 2-aminopyridine with L-leucine, L-Glutamic acid and L-tyrosine respectively. This indicates the condensation / interaction of 2-aminopyridine with L-leucine, L-Glutamic acid and L-tyrosine. The structure of these three co-crystals shown in figure 3.

The absorption at 782 cm^{-1} & 859 cm^{-1} for L-leucine, 817 cm^{-1} for L-Glutamic acid and at 855 cm^{-1} for L-tyrosine is due to the N-H wagging in primary and secondary amine present in these co-crystals. The stretching vibration of the C = O of carbonyl compound observed at 1681 cm^{-1}, 1958cm^{-1}, 1664 cm^{-1} for the co-crystals formed due to L-Leucine, L- Glutamic acid and L- tyrosine respectively.

And also C-O stretch found at 1211 cm^{-1} for L-Leucine, 1337 cm^{-1} for L-glutamic acid and at 1212 for L-tyrosine co-crystal. The absorption at 1158 cm^{-1} , 1334 cm^{-1}, 1156 cm^{-1} is due to the primary and secondary amine C-N stretch present in co-crystal formed due to L-leucine, L- Glutamic acid and L- tyrosine respectively. The absorption at 1445 cm^{-1} in L-Leucine co-crystal is due to CH_3 bending. From these peaks it is concluded that 2-aminopyridinium-leucinate, bis 2-aminopyridinium glutamate and 2-aminopyridinium-tyrosinate co- crystals formed using slow evaporation method.

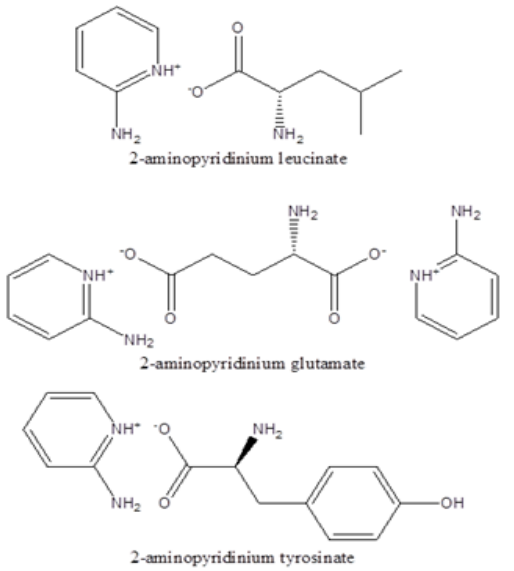

Figure 3. Structure of L-amino acid based 2-aminopyridine co-crystals.

3.3. UV-Vis spectrum

The UV- Vis spectrum collected from JASCO UV Vis between the ranges 200 nm to 900 nm with the Scan speed 10 nm/min.

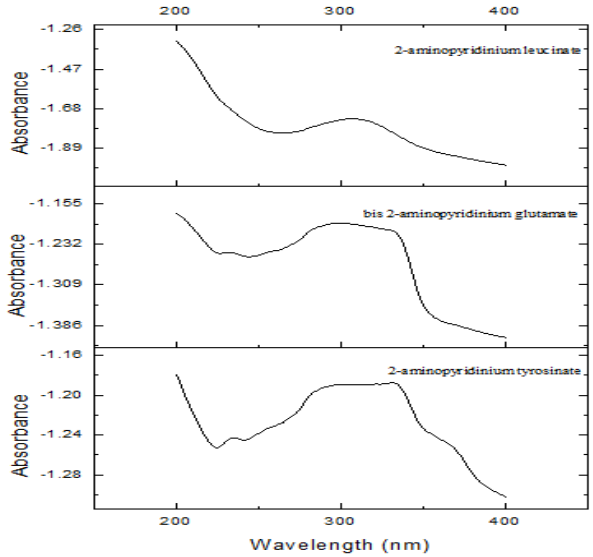

Figure 4. UV Vis spectrum of L-amino acid based 2-aminopyridine co-crystals.

The optical behaviour of powdered 2-aminopyridinium-leucinate co-crystal, bis-2-aminopyridinium glutamate co-crystal and 2-aminopyridiniumtyrosinate co-crystal specimen analysed using UV-Vis spectrometer and shown in figure 4 and the cut off wavelength of powdered crystal observed at 240 nm for 2-aminopyridiniumleucinate co-crystals, at 285 nm for bis2-aminopyridinium glutamate co-crystals and at 275 nm for 2-aminopyridiniumtyrosinate co-crystals. Peak broadening in the range between 295 nm to 330nm in 2-aminopyridinium glutamate co-crystals and between 286 nm to 334nm in 2-aminopyridiniumtyrosinate co-crystals specimen is due to the electron level transition is accompanied by simultaneous change between more vibrational level indicating that the molecules are closely packed together and they exert influences on each other. This is due to the conjugation of the carbonyl group with double bond shift in these two crystals. In all the three co-crystals, the heteroatom withdraws electron from carbonyl carbon and makes carbonyl oxygen lone pairs of electrons more stabilized due to its involvement in increasing C=O bond order and undergo $n \rightarrow \pi^*$ transition.

4. Conclusion

By slow evaporation method the L-amino acid based 2-aminopyride co-crystals were grown and they characterized by Powder XRD, FTIR and UV-Vis spectrum. The interaction between the L-amino acid and 2-aminopyridine were confirmed by the hydrogen bonding interactions.

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