

Vibrational Study of Aspartic Acids

Dr. Santosh Kumar

Department of Applied Sciences, IEC Group of Institutions, 4, Knowledge Park-I, Greater Noida 201306 UP India
bhu.santosh71@gmail.com

Abstract — Aspartic acid is a type of amino acid which is essential for growth of body. Author studied the IR and Raman Spectroscopy of the molecule in the range of 4000-400 cm^{-1} and recorded the UV visible spectra of Aspartic acid in the range 400-200 nm at different concentrations and pH values. Several peaks were assigned.

Keywords: *Vibrational study, Aspartic acid, Raman spectrum.*

I. INTRODUCTION

MOST of the amino acids exist in biological systems in the L-form [1-3]. Aspartic acid recemises from the L- to the D-form in living as well as non living systems at a rate of about 0.12-0.14% per year [4-10]. This fact can be used to determine age and due to which aspartic acid has a place of special interest amongst the amino acids [4-10].

Aspartic acid is a non-essential amino acid and found in abundance in plant proteins. Both aspartic acid and glutamic acid and almost all proteins are linked to other amino acids only through their side carbonyl groups. Some of the amino acids that are synthesized from aspartic acid are arginine, asparagines, lysine, methionine, threonine, isoleucine and different nucleotides. It is important from this point of view also Aspartic acid is needed for stamina, brain and neutral health and assists the liver by removing excess ammonia and other toxins from the blood stream. Its role is important in function of RNA, DNA, as the production of immunoglobulin and antibody synthesis. [11]. Aspartic acid forms a dianion at high pH and a monocation at low pH, thus existing in species of different stoichiometry. There are two tautomeric zwitterionic structures for Aspartic acid, and each may have different rotamers.

Nagy and Noszal [12] reported theoretical calculations with available experimental results for the conformational/tautomeric equilibrium of aspartic acid zwitterionic aqueous solution. Navarrete *et al.* [13] studied the Infrared and Raman spectra of aspartic acid dipeptide and glutamic acid dipeptide solid samples. Wang and Ando [14] have reported a study of structure and dynamics of poly aspartic acids sodium blends by CCP/MAS NMR method. Mary and Ramkrishnan[11] made IR and Laser Raman spectral studies of D, L- aspartic

acid [15-17]. In this paper the infrared, Raman spectra of aspartic acid in the 400-4000 cm^{-1} region were studied. Also, the electronic spectra of this molecule at different concentrations as well as at different pH values were studied.

II. RESULTS AND DISCUSSION

The infrared and Raman spectra of aspartic acid are shown in Figures 1 and Figure 2 respectively. A band is observed in the infrared spectrum at 3134 cm^{-1} due to symmetric stretching of NH_3^+ , but corresponding band is absent in Raman spectrum. In this region of spectrum Navarrete *et al.* [13] reported an intense peak at 3115 cm^{-1} in IR spectrum. A peak is observed at 3042 cm^{-1} in IR spectrum. This is assigned to CH_2 stretching (asym). This peak does not appear in Raman spectrum. Navarrete *et al.* [13] also observed this peak at 3021 cm^{-1} and similar assignment has been made by these workers. Similarly a band has been observed at 2924 cm^{-1} due to asymmetric stretching of CH_2 group in I.R. spectrum but not seen in the Raman spectrum. There are two bands at 2879, 2843 cm^{-1} in Raman spectrum due to symmetric stretch of CH_2 group but these bands are not seen in IR spectrum.

There is a band at 1685 cm^{-1} due to asymmetric stretching of COO^- observed in both IR and Raman spectrum. Similarly a band appears at 1618 cm^{-1} in IR and at 1620 cm^{-1} in Raman spectrum due to asymmetric stretch of COO^- . In IR spectrum there is a band at 1504 cm^{-1} and its corresponding band is seen in Raman spectrum at 1540 cm^{-1} . These peaks are considered due to symmetric bending of NH_3^+ . There are three bands in Raman spectrum within the region of 1400-1487 cm^{-1} at 1487, 1418, 1400 cm^{-1} . These peaks are assigned as bending of CH_2 group, symmetric stretch of COO^- group and combined effect of stretching of $\text{C=O} + \text{OH}$ Bending respectively. Due to bending of CH group, there are two bands observed at 1333 cm^{-1} and at 1361 cm^{-1} in Raman spectrum but only a single band appears in IR spectrum at 1346 cm^{-1} .

This is considered to be due to the combined effect of bending of OH group and stretching of CC bond. There is a peak at 1311 cm^{-1} in IR spectrum and at 1287 cm^{-1} in Raman spectrum. There are two bands due to torsional motion of CH_2 group at 1251 cm^{-1} and at 1210 cm^{-1} in Raman spectrum but only one band is seen

at 1213 cm^{-1} in IR spectrum. The rocking of NH_3^+ group leads to two bands in Raman spectrum at 1113 cm^{-1} and 1139 cm^{-1} . Due to stretching of CN group as well as stretching of CC bond, there are bands observed in IR spectrum at 1070 cm^{-1} and in Raman spectrum at 1072 cm^{-1} . A band is observed at 1033 cm^{-1} in IR spectrum and is assigned as due to stretch of CN group. Its corresponding band does not appear in Raman spectrum.

A band is seen at 980 cm^{-1} in Raman spectrum due to stretching of CN as well as CC bond but not observed in IR spectrum. Similarly an intense band is observed at 934 cm^{-1} in Raman spectrum due to out of plane bending of OH group which are not seen in IR spectrum. Due to rocking of CH_2 group there is a band at 893 cm^{-1} in IR spectrum. A band is seen in Raman spectrum also at the same frequency. A similar band is seen at 852 and 857 cm^{-1} respectively again due to rocking of CH_2

group. There are two bands in Raman spectrum at 733 cm^{-1} and 778 cm^{-1} due to bending of COO^- group but corresponding bands do not appear in IR spectrum.

A band at 695 cm^{-1} due to COOH group observed in Raman spectrum which does not appear in IR spectrum. There is a band at 640 cm^{-1} in IR and at 643 cm^{-1} in Raman spectrum. This is due to bending of COO^- group. There also appears a band in Raman spectrum at 586 cm^{-1} due to bending of COO^- group but not seen in infrared spectrum of this molecule. A band is seen at 500 cm^{-1} in IR and at 510 cm^{-1} in Raman due to bending of HOCC bond. Due to bending of NCC as well as of bending of OCC a band appears in IR at 476 cm^{-1} and in Raman at 487 cm^{-1} respectively. The deformation motion of NH_2 group leads a band at 418 cm^{-1} in IR spectrum but not seen in Raman spectrum. These bands are tabulated in Table 1.

TABLE 1-- A COMPARISON OF IR AND RAMAN FREQUENCIES OF ASPARTIC ACID

S. NO.	IR Frequencies (cm^{-1})	Raman Frequencies (cm^{-1})	Assignment
1.	3234	----	Symmetric stretch NH_3^+
2.	3042	----	Asy Stretch of CH_2
3.	2132	----	Asy Stretch of CH_2
4.	----	2879	Symmetric stretch CH_2
5.	----	2843	Symmetric stretch CH_2
6.	1685	1685	Asymmetric Stretch of COO^-
7.	1618	1620	Asymmetric Stretch of COO^-
8.	1504	1540	Symmetric Bending NH_3^+
9.	----	1487	Bending CH_2
10.	----	1418	Symmetric Stretch COO^-
11.	----	1400	Stretch CO , Bending OH
12.	----	1361	Bending CH
13.	1346	1333	Bending CH
14.	1311	1287	Bending OH, Stretch CO
15.	----	1251	Torsion CH_2
16.	1213	1210	Torsion CH_2
17.	----	1139	Rocking NH_3^+
18.	----	1113	Rocking NH_3^+
19.	1070	1072	Stretch CN, Stretch CC
20.	1033	----	Stretch CN
21.	----	980	Stretch CN, Stretch CC
22.	----	934	Out plane Bending OH
23.	893	893	Rocking CH_2
24.	852	857	Rocking CH_2
25.	----	778	Out plane Bending COO^-
26.	----	733	Bending COO^-
27.	----	695	Bending COOH
28.	640	643	Bending COO^-
29.	----	586	Bending COO^-
30.	500	530	Out plane Bending HOCC
31.	476	487	Bending NCC, Bending OCC
32.	418	----	Deformation NH_2

Electronic absorption spectrum:

Electronic absorption spectrum: The electronic absorption spectrum of the same molecule was recorded (Figure 3) by taking 0.01 gm in 4 ml distilled water in region 200-400 nm at pH = 7. In this case peaks appear at 206 nm. On changing the pH of this solution peaks are seen at 204 nm and at 224 nm at pH = 2 and pH = 10 respectively.

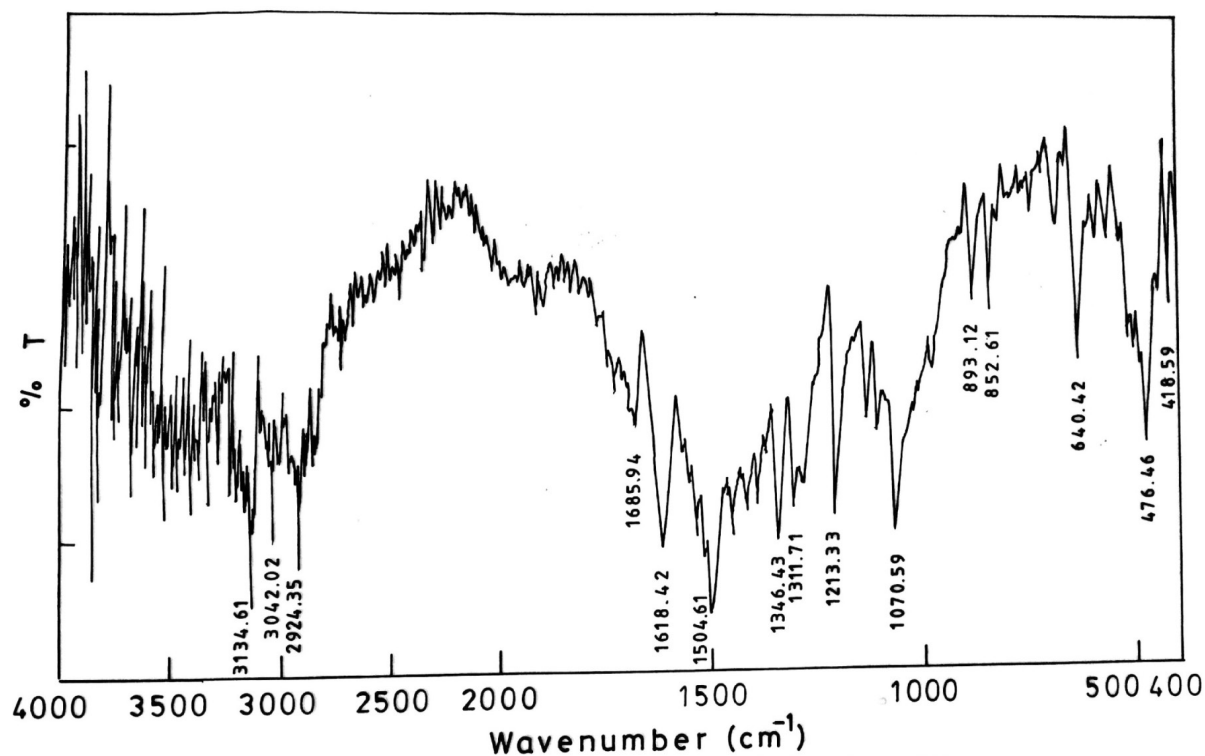


Figure 1. Infrared spectrum of aspartic acid in solid form.

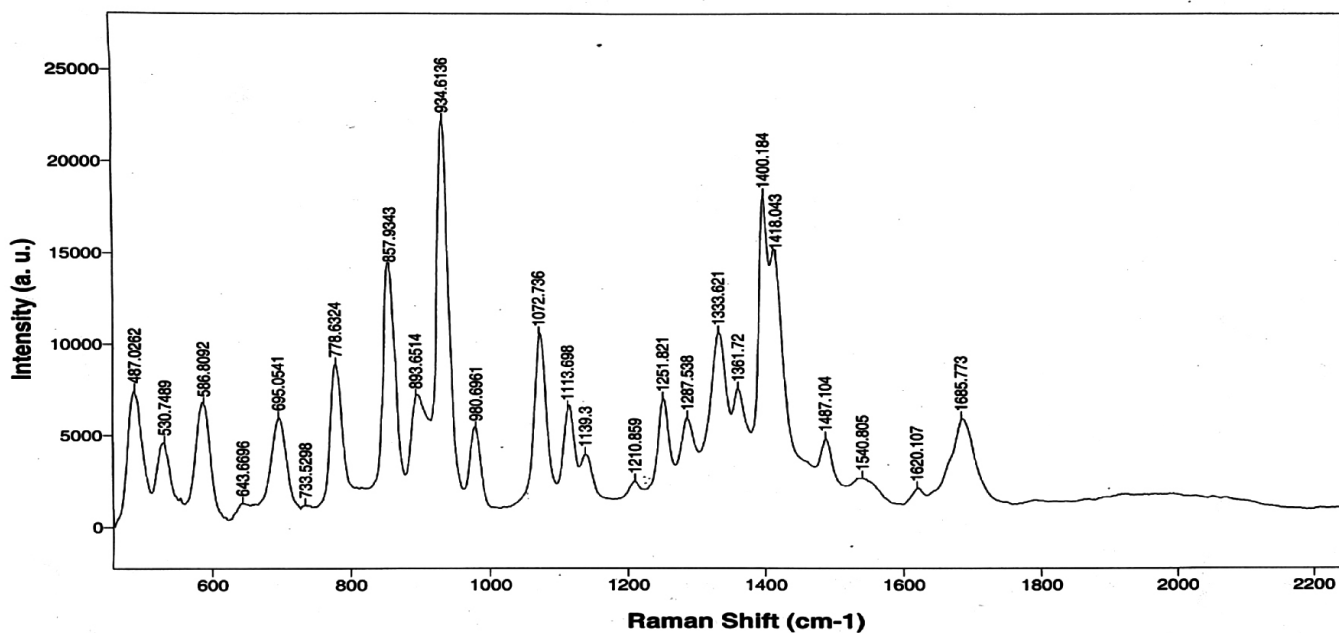


Figure 2a. Raman spectrum of aspartic acid

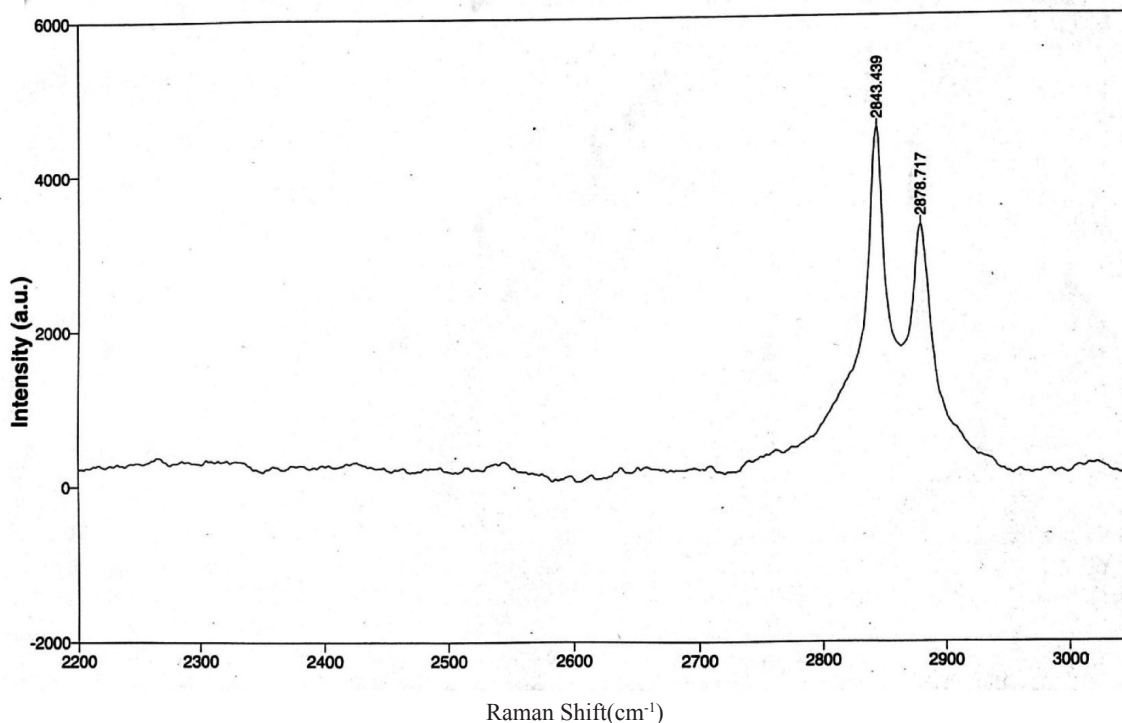


Figure 2b. Infrared spectrum of aspartic acid in solid form.

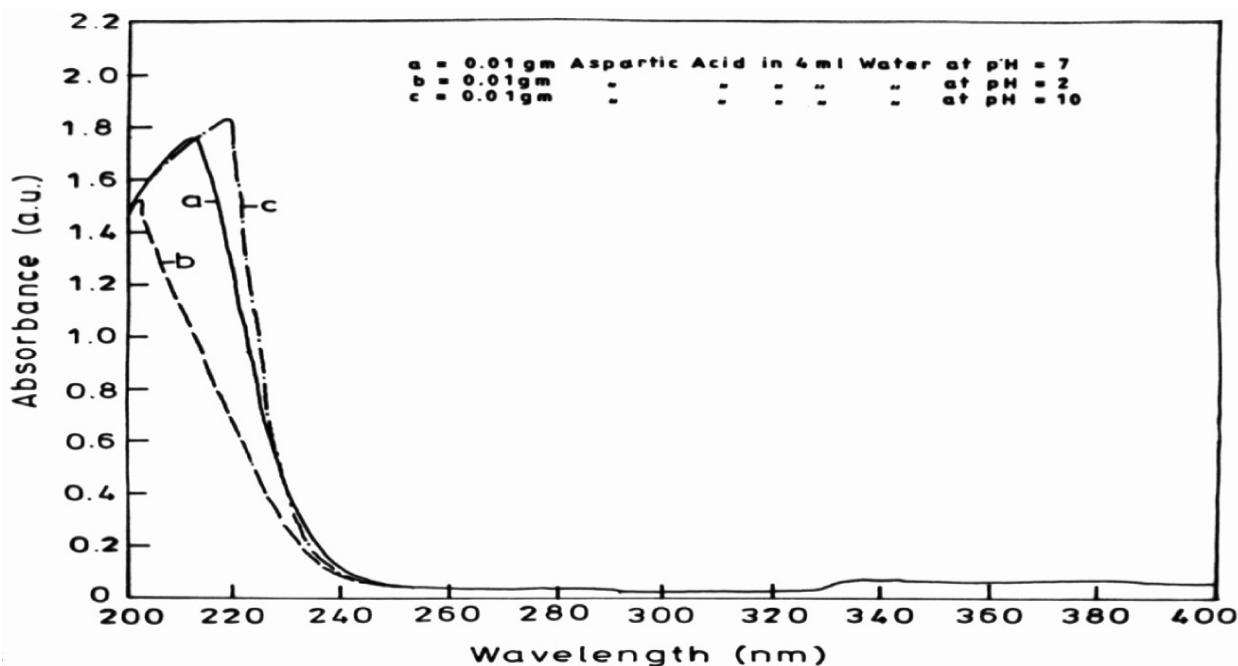


Figure 3. Electronic absorption spectrum of aspartic acid at different pH values.

III. CONCLUSION

The observed IR and Raman peaks are in good agreement mutually. The observed peaks have also been supported by others. Some unobserved peaks have also been monitored.

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Dr. Santosh Kumar is currently working as Associate Professor in the Department of applied sciences, IEC College of Engineering and Technology Gr. Noida. Obtained MSc from VBSPU University, Jaunpur in 1994 and PhD from BHU in 2006. Published over dozen papers in international and national journals. He is also an author of a book with title "*Vibrational Spectroscopy of Some Biomolecules*", VDM Publishers, Germany. Presently he is working in the area of laser spectroscopy and its applications.