Available online at www.elixirpublishers.com (Elixir International Journal)

Biosciences

Elixir Biosciences 108 (2017) 47568-47569

ISSN: 2229-712X

Experimental Study of Valine Molecule

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ARTICLE INFO

Article history:
Received: 26 April 2017;
Received in revised form:
28 June 2017;
Accepted: 7 July 2017;

Keywords:
IR,
Raman Spectra.

ABSTRACT

Valin is a type of amino acid which is essential for growth of the living organism. We have monitored the IR ,Raman & electronic absorption spectra of the valine molecule in solid form.The IR spectra has been observed in the range 4000-400 cm^{-1} in the solid as well as liquid form. Similarly Raman spectra of the same molecule has also been monitored under the same range . The electronic absorption spectra have been monitored in the range 400-200 nm. In this paper we have made the several assignments of observed peaks. There are some new peaks has been found, which were not reported by earlier workers.

Introduction

Valine molecule is a type of amino acids. It contains 19 atoms and has S_1 modes of vibrations which are infrared as well as Raman active. Stepanion et al[1]studied the conformational behavior of non ionized α-valine. The structure and relative energies of the nine lowest energy valine conformers were calculated at the DFT/ B3LYP/6-31+G and MP2/6-31 + +G** andMP2/6-31++G** levels of theory. These authors [1] also recorded and analyzed the matrix isolation IR spectrum of valine which allowed a definite identification of bands corresponding to three lowest energy valine confirmers I, II and III. By comparing the calculated and the observed intensity of bands for different conformers, they estimated the conformational conformation of valine in Ar matrix. They concluded that almost 94% valine is in confirmer I while 5% of these are in confirmer II and the remaining portion is in III conformation a number of spectroscopic studies on valine and their C-deutrated analogues [2],L-valine nitrate [3],tri L-valine selenate [4], have been reported in the literature. Raman optical activity of L-valine has been reported by Gargo et al[5]. Stepnain et al[1] have assigned a high frequency band at 3561 cm^{-1} due to OH starching vibration for conformer I and at 3183 cm^{-1} due to the same OH stretch for conformer II. They also observe a band at 3422 cm^{-1} and assigned to asymmetric NH_2 stretching vibration. Another region which provides information on the valine conformational composition is the C=O stretching vibration (1800-1700) cm^{-1}. An intense band in this region is seen at 1761 cm^{-1} and is attributed to the lower energy confirmer I in the region below 1500 cm^{-1} most of the experimental bands are assigned to the lowest energy confirmer I with some characteristic bands of confirmer II. The structural and electronic properties of L valine have also been studied by tulip et al[6] . They have also shown that amino and carboxy functional groups are the dominant factors in determining band structure. In the present paper we have reported spectra of valine molecule.

Large number of bands are observed in the structure some of the peaks observed here are new and not reported by earlier workers. The IR, Raman, and electronic absorption spectrum of the valine molecule are shown in Fig 1, 2&3 respectively.

Result and discussion

A broad band appears in the IR spectrum of valine at 2927 cm^{-1} and is due to C-H stretch in CH_2 group. There is no corresponding peak is seen in Raman spectrum .Similarly in the Raman spectrum four peaks are seen at 2880,2865,2835,2810 cm^{-1} and are attributed to CH_2 stretch. The peaks at 2835 and 2880 cm^{-1} are new a peak is observed in Raman spectrum at 2585 cm^{-1}. This is perhaps due to combination (1152+1448) cm^{-1}. A broad band is seen at 2104 cm^{-1} in IR spectrum. This is perhaps due to a combination of CH_3 bend and rocking vibration of NH_2 group (1065+1032) cm^{-1}. In Raman spectrum a broad band is seen at 1640 cm^{-1}. This is due to the asymmetric stretch of CO_2 group. The corresponding peak is absent in IR spectrum. A very intense band in the Raman spectrum appears at 1480 cm^{-1} due to HCH bending. A band in IR spectrum at 1423 cm^{-1} and its corresponding band at 1448 cm^{-1} in Raman spectrum is due to HCH bending. A medium intense band in Raman spectrum appears at 1400 cm^{-1} and in IR at 1394 cm^{-1}. This is attributed to a combination of OH bend and CH bend vibrations. A weak band at 1352 cm^{-1} in IR spectrum and at 1360 cm^{-1} in the Raman spectrum appears due to CH_3 bending. A medium intense band appears at 1271 cm^{-1} in IR and at 1288 cm^{-1} in Raman and due to twisting of the CH_2 group. The CH bending vibration causes peaks in IR and Raman spectrum at 1177 cm^{-1} and at 1200 cm^{-1} respectively. A medium intense band appears in both the spectra at 1140 cm^{-1} (IR) and 1152 cm^{-1} (Raman) due to CN stretch. Similarly the peaks observed at 1065 cm^{-1} in IR and at 1080 cm^{-1} in Raman spectrum is due to CH_3 bending vibration. A peak at 1032 cm^{-1} in IR and at 1048 cm^{-1} in the Raman spectrum peaks are seen due to CH_3 bending.

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At 968 cm^{-1} an intense band is seen in the Raman spectrum due to NH_2 wagging. The corresponding band in the IR appears at 949 cm^{-1}. At 928 cm^{-1} there is a band in Raman spectrum due to CN stretch .a medium intense band at 872 cm^{-1} appears in Raman spectrum due to NH_2 bend and corresponding IR band is at 900 $cm^{-1.}$ Due to OH torsion a peak appears at 840 cm^{-1} in Raman spectrum and at 823 cm^{-1} in IR spectrum. An intense band is seen at 760 cm^{-1} in the Raman spectrum with the corresponding band in IR at 775 cm^{-1} and is assigned to CC stretch. An intense band is observed in IR spectrum at 665 cm^{-1} and in Raman at 633 cm^{-1}. These bands are due to C=O bending. A much intense bend is observed in IR spectrum at 543 cm^{-1} and it may be due to CC bending. The corresponding band is not seen in Raman spectrum. In Raman spectrum as well as in the IR spectrum intense band at 435 cm^{-1} and at 428 cm^{-1} respectively is seen and is assigned as CC torsion.

Table 1. A comparison Of IR And Raman Frequencies Of Valine Molecule.

S.NO.	I.R. frequency (cm^{-1})	Raman frequency ($cm^{-1)}$	Assignment
1	2927	2880	Asym CH_2 Stretch
2	------	2865	Asym CH_2 stretch
3	------	2835	Sym CH_2 Stretch
4	-------	2810	Sym CH_2 Stretch
5	--------	2710	CH Stretch
6	--------	2585	Combi (1152+1448)
7	2104	-------	Combi (1065+1032)
8	-------	1640	CO2 Asym Stretch
9	------	1480	HCH Bend
10	1423	1448	HCH Bend
11	1394	1400	OH Bend + CH Bend
12	1352	-------	CH_3 Bend
13	1329	1360	CC Stretch, OH Bend
14	1271	1288	CH Bend
15	1177	1200	CH Bend
16	1140	1152	CN Stretch, CC Stretch
17	1065	1080	CH_3 Bend
18	1032	1048	CH_3 Bend
19	-----	968	CC Stretch, CH Bend
20	949	928	CN Stretch
21	900	872	NH_2 Bend
22	823	840	OH Torsion, NH_2 Bend
23	775	-----	CC Stretch, C=O Bend
24	715	710	CC Stretch, C=O Bend
25	665	633	C=O Bend, CC Bend
26	543	----	CC Bend
27	472	-----	CO Bend
28	428	435	NCC Bend, CC Torsion

Asy=asymmetric, sym=symmetric, combi=combination, bend=banding

Electronic absorption spectrum of valine

Electronic absorption spectrum of valine has been recorded in region of 200-400 nm. .01 gm of valine molecule was dissolved in 2 ml of triply distilled water. In the spectrum of this solution a peak appears at 212 nm. On further dilution (same amount of valine dissolved in 4 ml of water) a new peak appears at 204 nm. The pH of this solution is 7. On changing the pH of solution from 7 to 2 the peak remains unchanged (i e 204 nm). However at 10 pH a peak appears at 220 nm.

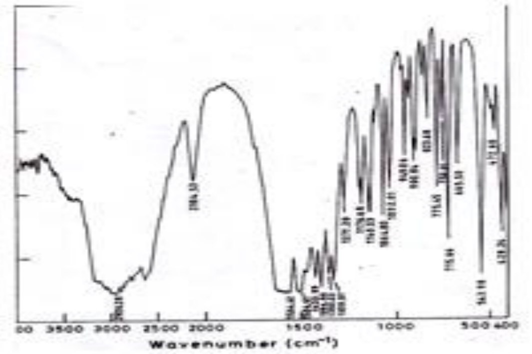

Figure 1. IR Spectra Of Valine Molecule.

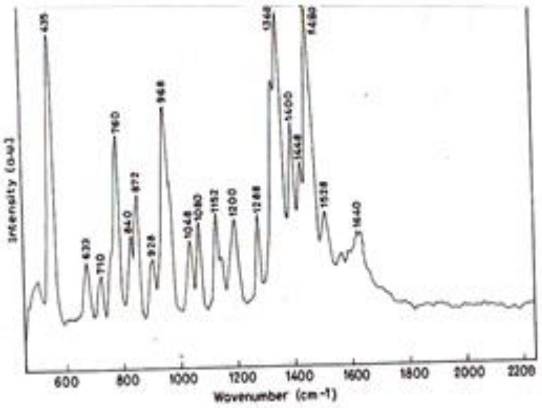

Figure 2. Raman Spectra Of Valine Molecule.

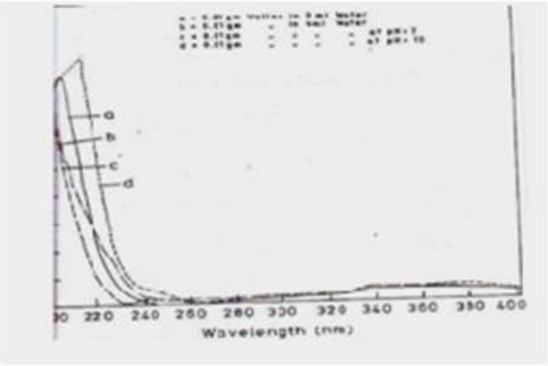

Figure 3. Electronic Absorption Spectra Of Valine Molecule.

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