

Experimental and Theoretical Vibrational Analysis of Vitamin C

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Abstract— Vitamin C (L-Ascorbic Acid) was investigated by FTIR and Raman spectroscopy. In parallel with the experimental study, density functional theory (DFT) is employed to the structure analysis and vibrational frequencies of Vitamin C. Based on the DFT calculations different observed vibrational modes are assigned. For detailed interpretation of a mode, relative participation (in percentages) is also assigned.

Keywords—Vitamin C, FTIR and Raman spectroscopy, density functional theory, structure analysis, vibrational frequency.
Section— Physical Sciences.

I. INTRODUCTION

Vitamin C, also known as ascorbic acid, is an essential component in the diet of humans and a small range of other mammals. Ascorbic acid is a water soluble vitamin found widely in raw fruits, vegetable and other food products, such as juices and sports drinks. It contains four hydroxyls and a lactone ring. It is very easy to get oxidized and changes to dehydroascorbic acid [1] and plays a very important role as an antioxidant by destroying toxic free radicals resulting from the metabolic products of oxygen. In this role, the mixture of L-ascorbic acid and its oxidative products acts as a redox buffer. In addition to the redox function in cells, other physiological actions of L ascorbic acid may be related to chelating with metals. Deficiency of vitamin C results in scurvy. It is absolutely essential for human existence, but humans are one of the animals unable to synthesize vitamin C [2-3].

However, L ascorbic acid is very unstable to exposures in air, light, moisture, heat, metal ions, oxygen, and base, since it is easily decomposed into biologically inactive compounds such as oxalic acid, L-xylonic acid, L-threonic acid, and L-lyxonic acid [4] and because of instability, applications of vitamin C in various fields are limited. So the study of the molecule structure is very important, the better understanding of the fundamental behaviour of this molecule will be helpful to improve the utility of this substance. The FTIR and Raman spectroscopy gives much information about the structure of Vitamin C.

II. EXPERIMENT

The FTIR spectrum was recorded in the KBr pellet on a Perkin Elmer PERX1FTIR spectrometer. The spectral resolution of IR spectrometer was 0.5 cm^{-1} throughout the

experiment. Raman spectrum was excited by the blue lines of 488 nm beam provided by Ar laser. Raman spectrum was recorded from 250 to 1900 cm^{-1} with the help of an iHR 550 JY Horiba spectrograph fitted with TE cooled CCD detector.

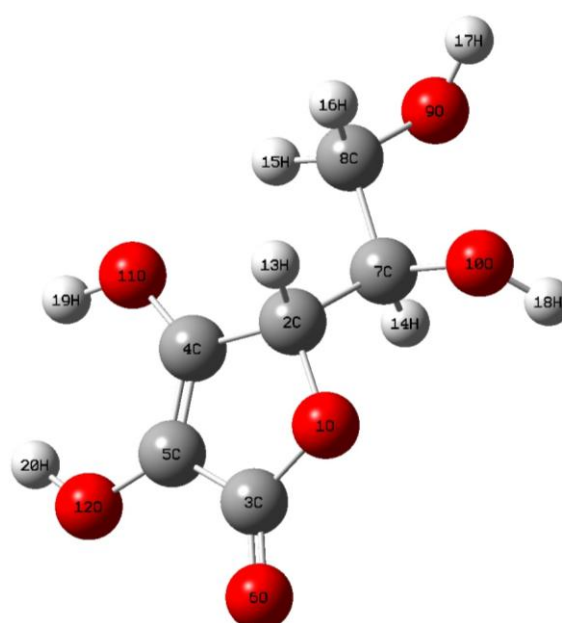


Fig. 1 Optimized structure and labelling scheme of vitamin C.

III. RESULTS AND DISCUSSION

The optimized structure of vitamin C, obtained from density functional theory calculations, is shown in Fig. 1. This geometry was optimized by minimization of potential energy calculations with B3LYP functional [6-7] and 6-31+dp basis sets using Gaussian 03 Revision D.01 program package [5]. The attainment of the local minima on the potential energy surface has been confirmed by the absence of imaginary value of vibrational wavenumber. The recorded FTIR and Raman spectra are shown in Fig.2 and 3. The observed normal modes of vibrations, for both IR and Raman active, along with theoretically calculated are listed in table 1. Scaling has been done with the help of linear fitting (scaled wavenumber = $m \cdot \text{calculated wavenumber} + c$; $m = 0.96985$ and $c = 7.00613$).

The observed IR and Raman bands of Vitamin C are assigned on the basis of DFT calculations and their comparative intensities. The relative contribution of different

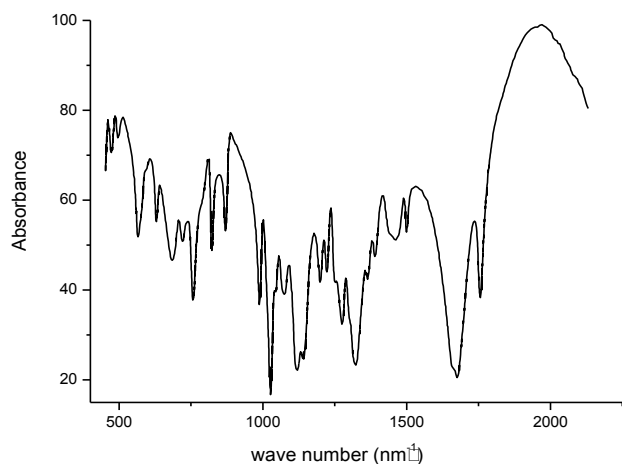


Fig.2 IR spectrum of vitamin C in 400 – 2250 cm^{-1} region.

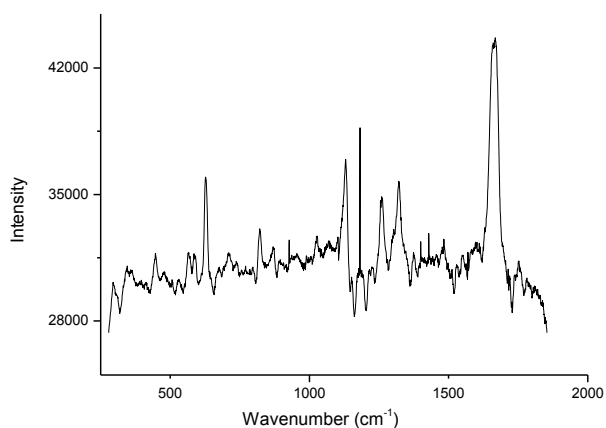


Fig. 3 Raman spectrum of Vitamin C in 100 – 1900 cm^{-1} region.

modes of vibration to a particular band are also calculated and assigned. O-H stretching is one of the most important group. O-H stretching is assigned to 3525 cm^{-1} of observed IR spectrum. The assignment to the other most important groups for the present molecule is presented as bellow.

A. CH Modes :-

The bands in the region 3050 to 2900 cm^{-1} of IR spectrum are assigned to the C-H stretching modes. These are assigned to the 3042 and 2916 cm^{-1} of the IR spectrum. These assignments are also in agreement with the previously studies [8].

B. CH₂ Modes

The calculations predicted the CH₂ bending modes at 1467 cm^{-1} which is assigned to the 1458 and 1456 cm^{-1} in IR and Raman observed modes respectively.

C. Skeletal Modes

The strong intensity peaks are observed at 1675 and 1668 cm^{-1} in IR and Raman respectively which are assigned C=C stretching mode, calculated at 1731 cm^{-1} . C=C stretching is also calculated at 1789 and 1079 cm^{-1} are assigned to 1781 cm^{-1} of the Raman band 1075 cm^{-1} of the IR band respectively. Comparing with the calculated values the C-C stretching modes are assigned to $676, 798, 870, 989, 1028, 1070$ and 1131 cm^{-1} bands in Raman and $684, 869, 1026$ and 1020 cm^{-1} in IR. The C-O stretching mode is observed at 1103 and 1070 cm^{-1} . The torsion mode (O=C-O-C) associated with the lactone ring is assigned to 720 and 710 cm^{-1} of IR and Raman bands respectively. The C-C-O bending is assigned to $295, 531$ and 642 in the Raman bands. In the spectra, we observe a larger number of bands than possible fundamentals for the molecules. It may be due the fact that in solid crystalline state sample is present in aggregated form due to which splitting of bands takes place. Further calculations are in progress.

TABLE I

POSITIONS OF OBSERVED IR AND RAMAN BAND AND THEIR ASSIGNMENTS

Observed Bands (cm^{-1})			Assignments
Experimental		Calculated	
IR	Raman		
	295	287	δ (C-C-O) 54%
		313	δ (H-O-C) 23% + τ (O-C=C-C) 42%
		326	ν (C-C) 10% + δ (C-C-C) 46%
	345		
	358	368	τ (H-O-C=C) 52%
		379	τ (H-O-C=C) 15% + τ (H-O-C=C) 37%
	396	404	τ (H-O-C-C) 60% ?
	413	427	τ (H-O-C=C) 61% + τ (O-C-C-C) 11%
		430	τ (H-O-C-C) 67% + τ (O-C-C-C) 14%
	447	448	τ (H-O-C-C) 16% + τ (H-O-C-C) 19% + τ (O-C-C-C) 22%
471			
	479		
494			
	507		
	531	529	δ (C-C-O) 10% + δ (C-C-O) 27% + τ (C-C=C-O) 30%
565	566	552	ν (O-C) 15% + δ (C=C-O) 46%
	585		
	590		
628	627	609	δ (C=C-O) 31% + τ (C=C-C=O) 33%
	642	668	δ (C-C-O) 52%
684	676	676	ν (C-C) 12% + ν (C-C) 18% + δ (O-C=O) 36% + δ (C-C-C) 10%
720	710	719	ν (C-C) 79% + τ (O-C=C-C) 11%

	738		
757	758		
	771		
	786		
	798	791	ν (C-C) 44% + δ (O-C=O) 12%
821	821		
869	870	869	ν (C-C)17% + ν (C-C) 13% + ν (CC) 18% + τ (CCOH) 30%
988			
	895		
	917		
	952		
	989	980	ν (O-C) 10% + ν (C-C) 51%
	998		
	1006	1003	δ (C-O-C) 29% + δ (O-C=O) 12%
1026	1028	1026	ν (C-C) 39% + δ (H-O-C) 12% + τ (CCOH) 15%
		1049	ν (O-C) 51%
	1070	1065	ν (O-C) 11% + ν (C-C) 38%
1075		1079	ν (C=C) 59%
	1103	1100	ν (O-C) 52%
1120	1131	1143	ν (C-C) 19% + δ (H-O-C) 40%
	1152	1162	δ (H-O-C) 37% + δ (H-C-C) 35%
1198			
	1183		
	1217		
1221			
	1225	1239	δ (C-C-O-H) 70%
	1261	1253	δ (H-O-C) 18% + δ (H-C-C) 45% + τ (C-C-O-H) 15%
1274		1269	δ (H-O-C) 17% + δ (H-C-O) 45%
	1280	1289	ν (O-C) 28% + δ (H-O-C) 44%
	1303		
1322	1322	1328	δ (H-O-C) 17% + τ (H-C-C-C) 34%
		1341	ν (C-C) 23% + δ (H-O-C) 12% + δ (H-C-O) 11% + OUT (C-C-C-H) 15%
		1350	δ (H-O-C) 10% + δ (H-C-C) 15% + δ (C-C-C-H) 28%
1363	1374	1369	δ (H-O-C) 24% + δ (H-C-C) 16% + δ (CCCH) 33%
1388			
	1401	1406	δ (H-O-C) 14% + δ (H-C-C) 29% + τ (HCCC) 21%
	1432	1413	ν (O-C) 16% + δ (H-O-C) 22% + δ (C-CO) 18% + δ (O-C=O) 13%
1458	1456	1467	δ (H-C-H) 81% + τ (HCCC) 13%
1498	1484		
	1499		
	1513		
	1530		
	1550		
	1601		

	1611		
	1661		
1675	1668	1731	ν (C=C) 73%
1754	1752		
	1781	1789	ν (C=C) 85%
	1810		
	1838		
2916		2917	ν (C-H) 88%
		2939	ν (C-H) 88%
		2980	ν (C-H) 96%
3042		3050	ν (C-H) 95%
3525		3680	ν (O-H) 99%

* ν , δ and τ represent stretching, bending and torsion vibrations, respectively

CONCLUSIONS

Observed bands are assigned by using DFT calculations. The low wavenumber bands are mainly arise from torsion modes of lactone ring. All the observed bands are almost matches well with the calculated values except some extra bands. These extra bands may be because of the reason that we have observed the spectra in crystalline form and the calculations are done only for a single molecule. These bands may be obtained for dimer and trimer structure calculations.

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