Asian Journal of Chemistry; Vol. 23, No. 12 (2011), 5584-5586

ASIAN JOURNAL OF CHEMISTRY

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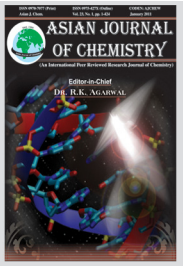

FTIR Investigation of Structural Change Due to Radiation Damage in Biomolecule†

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AJC-10337

The objective of this paper is the development of an over dynamical characterization of bio-molecules under the purview of this work. The developed sucrose specimen was supposed to exhibit change in molecular structure over that in pure sucrose due to rapture of some bonds. FTIR analysis on pure sucrose was carried out to examine its molecular structure and dynamical information. Infrared absorption spectrum of sucrose was analyzed from measured data of FTIR spectra. The change in characteristics bond stretching due to radiation damage is detected clearly. Some characteristics frequencies are absent due to radiation damage by irradiation of laser beam having energy greater than the bond strength of sucrose. The FTIR analysis successfully confirms the effect of radiation damage of sucrose molecule due to irradiation laser on it. The laser irradiation on pure Sucrose molecule caused damage, in its molecular structure and its finger print is detectable from FTIR study.

Key Words: Infrared spectroscopy, Bio polymer, Sucrose, Vibrational levels, Radiation damage.

INTRODUCTION

In an n-atom non linear molecule there are (3n-6) possible vibrational modes[1]. The vibration includes bond bending and bond stretching. The energy difference between vibrational states corresponds to the energy level of IR radiation. Normally two major region in the IR spectrum of a molecule are the functional group region (7000 to 1500 cm^{-1}) which includes the X-H stretching region and finger print region (1500 to 350 cm^{-1}). The later region is very important in bio-molecular dynamics[2] and it may provide much relevant information about the internal motion of the molecule and is related bio-molecular function in living systems.

Biological molecules share a structural complexity that is also reflected in their complex dynamical behaviour. The internal motions in most of the bio-molecules are partly vibrational and partly rotational. The complex motion involves groups of atom undergoing a plethora of continuous or jump-like diffusion. The strategy developed in this proposed research is to combine the results from quantum theory with that of spectroscopy and to compare them with that of the available result. The proposed combined study will provide geometry of motion and distribution of relaxation times of various parts (within a range of time scales permissible by this study) of bio-molecules along with effect of hydration. This technique can investigate on very small (1 mg) or less amount of specimen in its native/environmental condition. In fact it is superior in the said context over that other technique like inelastic Neutron scattering or XRD and NMR (in some cases) studies. An over all database to be prepared to develop a characterization technique of bio-molecule from this out come of the proposed project. The outcome may serve as a new addition to Physics of complex system and related technological applications. Bio-molecules have very low excitation energy *ca.* 10 meV and often very small amount of specimens are available. Neutron scattering technique are often found to be in adequate to study the dynamics of bio-molecules. In an earlier study[3] infrared absorption spectrum of biomolecule of gum acacia was analyzed from measured data of FTIR spectra. The change in characteristics bond vibration detected clearly. The obtained shift of the characteristics frequency caused due to change of molecular structure introduced by polymerization effect.

Sucrose is an organic compound, disaccharide in nature and may be derived from glucose and fructose. The glycosidic bond in sucrose is formed between the reducing ends of both glucose and fructose and not between the reducing end of one and the nonreducing end of the other. In this present work vibrational and rotational characteristic of sucrose molecule along with its characteristics change due to irradiation Laser on it are studied. Both functional group and finger print region

†Presented to the National Conference on Recent Advances in Condensed Matter Physics, Aligarh Muslim University, Aligarh, India (2011).

are taken into consideration for analyzing the obtained shift in FTIR absorption spectrum of pure sucrose and Laser irradiated sucrose. The objective of this paper is to study the effect of radiation damage on sucrose.

EXPERIMENTAL

The sucrose specimen (S1) was collected in crystal form from Merck (India). Some of these crystals specimen were pressed to get the powder form for suitable analysis. A small portion of the sucrose specimen was taken and irradiated by He-Ne laser beam for *ca.* 45 min. Now the new specimen (S2) was supposed to be damaged by laser radiation.

General procedure: The developed irradiated sucrose specimen (S2) is supposed to exhibit change in molecular structure over that in S1 due to radiation damage by He-Ne laser beam. FTIR analysis on pure sucrose specimen was carried out to examine its molecular structure and dynamical information of it. FTIR analysis on specimen S2 was also carried out. Comparing the vibrational and rotational spectrum of the two specimens effect of radiation damage caused by the irradiation on bio-molecule may be analyzed.

The analysis was carried out using FTIR model, IR affinity 1, Shimadzu, Japan, at high resolution (resolution was 0.5 cm^{-1} with 100 scans) using KBr window.

RESULTS AND DISCUSSION

Fig. 1 shows the comparison of the FTIR spectra between the developed sucrose specimens within wave number range 380 to 349 cm^{-1}.

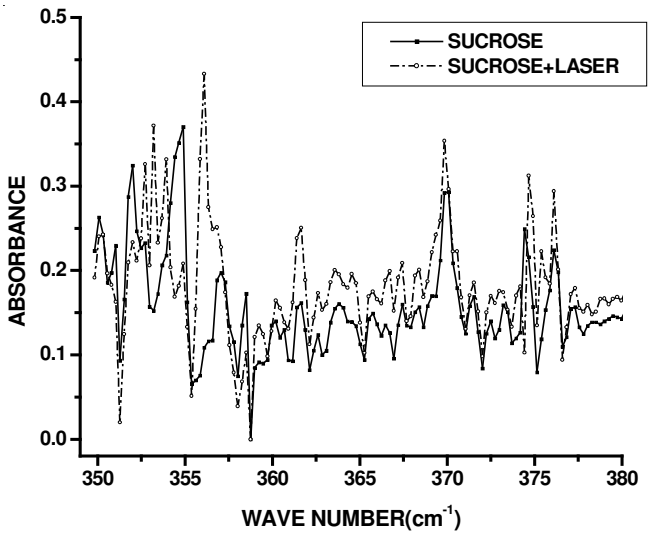

Fig. 1. FTIR absorption spectrum of specimen S1 and S2 in finger print region at 27 ºC

Fig. 2 shows comparison the FTIR spectra of S1 and S2 specimens between wave number 3405 to 3365 cm^{-1}.

After analyzing Figs. 1 and 2, and entire FTIR spectrum between wave number 4000 to 350 cm^{-1} of both the specimens S1 and S2 (Tables 1 and 2). The comparison of peak position and the corresponding absorption intensity between the specimens S1 and S2 were made clearly. Table-1 shows that the positions of most of the peaks remain same and only the positions of the peaks at wavenumber (cm^{-1}) 419.74, 417.58,

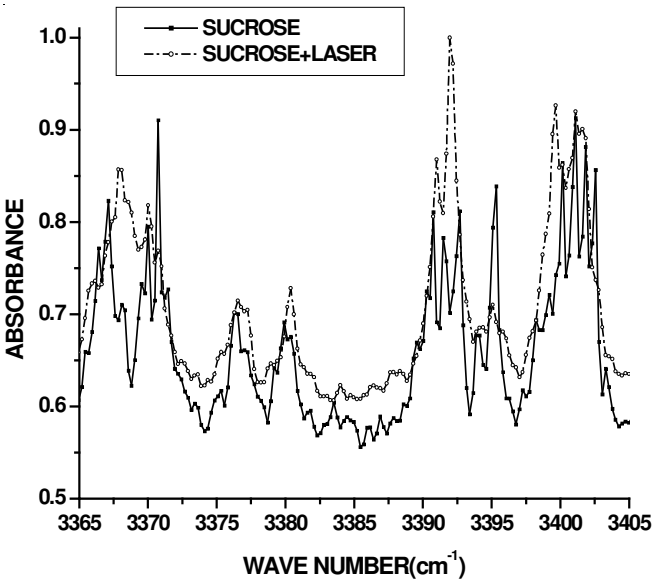

Fig. 2. FTIR absorption spectrum of specimen S1 and S2 in functional group region at 27 ºC

402.39, 400.46, 393.71, 380.45, 373.21, 370.08, 367.43, 360.68, 357.06, 351.03, 350.07, were changed. Whereas from Table-2 it was found that only the position of the peaks at wave number (cm^{-1})3469.83, 3466.45, 3441.86, 3420.40, 3359.41, 3296.72, remain same and the position of most of the peaks changed. This suggests that irradiation affect vibrational mode more than that of the rotational mode.

The comparison of the FTIR spectra of S1 and S2 specimens between wave number 1080 to 1045 cm^{-1} is shown in Fig. 3.

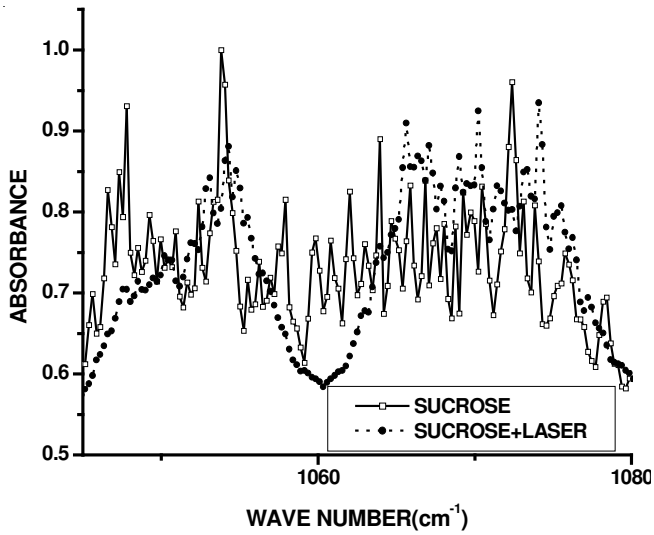

Fig. 3. Comparison of FTIR absorption spectrum of specimen S1 and S2 at 27 ºC

Temperature dependent vibrational modes of the glycosidic bond[4] in sucrose are found 1200 to 1000 cm^{-1}. Peaks found at wave number (cm^{-1}) 1072.39, 1065.88, 1063.95, 1062.02, 1060.81, 1059.05, 1057.92, 1053.82, 1047.79 for pure sucrose molecule from Fig. 3 represent the glycosidic bond in sucrose molecule which are absent in the FTIR spectra of irradiated sample. This indicate that during the irradiation

TABLE-1
POSITION OF SIGNIFICANT PEAKS AND CORRESPONDING INTENSITY OF DIFFERENT SPECIMENS (S1 AND S2) BETWEEN 420 TO 350 cm^{-1}

Pure Sucrose		Radiation damaged Sucrose	
Peak position	Intensity	Peak position	Intensity
350.07	0.2630	350.31	0.2428
351.03	0.2292	–	–
352.00	0.3244	352.00	0.2336
352.72	0.2328	352.72	0.3263
354.89	0.3702	354.89	0.2083
357.06	0.1974	356.10	0.4331
358.51	0.1726	358.51	0.1026
360.19	0.1398	360.19	0.1642
360.68	0.1295	–	–
361.64	0.1619	361.64	0.2507
362.61	0.1238	362.61	0.1735
365.74	0.1492	365.74	0.1752
366.46	0.1354	366.43	0.2090
367.43	0.1596	366.70	0.1992
370.08	0.2933	369.84	0.3536
371.53	0.1688	371.53	0.1856
372.49	0.1399	372.49	0.1699
373.21	0.1593	372.97	0.1756
376.11	0.2243	376.11	0.2941
377.31	0.1566	377.31	0.1790
380.45	0.1603	378.04	0.1591
381.89	0.1536	381.89	0.1743
382.86	0.1506	382.86	0.1813
393.71	0.1791	394.43	0.2231
396.84	0.1944	396.84	0.2065
400.46	0.2346	400.22	0.2472
402.39	0.2066	–	–
417.58	0.1841	417.82	0.2010
418.54	0.2114	418.54	0.2290
419.74	0.1877	419.99	0.1990

most of the glycosidic bond were damaged which can not be reproduced. But the peaks arise due to -OH bonds are present at wavenumbers[5] ranging from 3600 to 3200 cm^{-1}. These peaks are not absent in the FTIR absorption spectrum of irradiated sucrose but their positions are shifted from that of the pure sucrose specimen.

Conclusion

The analysis shows that there is a definite change in molecular vibration spectra over its corresponding pure bio-molecule.

TABLE-2
POSITION OF SIGNIFICANT PEAKS AND CORRESPONDING INTENSITY OF DIFFERENT SPECIMENS (S1 AND S2) BETWEEN 3600 TO 3140 cm^{-1}

Sucrose		Sucrose + Laser	
Peak position	Intensity	Peak position	Intensity
3140.49	0.5080	3222.71	0.5038
3290.94	0.8712	3294.31	0.6814
3296.72	0.7960	3296.72	0.7102
3302.03	0.7487	3302.23	0.7166
3350.73	0.8146	3357.72	0.6463
3359.41	0.7297	3359.41	0.7106
3363.99	0.6428	3366.16	0.7362
3411.97	0.7113	3418.23	0.6203
3420.40	0.6304	3420.40	0.6632
3427.40	0.6309	3425.47	0.6135
3437.04	0.7439	3437.28	0.7069
3441.86	0.5615	3441.86	0.5867
3443.79	0.5690	3445.72	0.5992
3465.01	0.6060	3463.80	0.5563
3466.45	0.7238	3466.45	0.5696
3469.83	0.7748	3469.83	0.5600
3475.62	0.5819	3473.20	0.5319
3592.30	0.5014	3562.41	0.5073

The laser irradiation on pure sucrose molecule caused damage, in its molecular structure and its finger print is detectable from FTIR analysis. The glycoside bond of sucrose is affected due to radiation damage.

ACKNOWLEDGEMENTS

The authors are thankful to UGC, New Delhi for financial support [MRP No F35-7/2008(SR)].

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