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Qualitative and Quantitative Analysis of Antipsychotic Drugs-A Spectroscopic Study

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Sertraline hydrochloride and olanzapine are basic compounds of pharmaceutical application for antidepressant and antipsychotic treatment, respectively. Sertraline comes under the category of aryl and aryloxyalkylamines antidepressant drugs. Olanzapine is a relatively new benzodiazepine which has been found useful in the treatment of schizophrenia. In the present work the FTIR and Raman spectra of these two drugs were recorded in the solid state. The fundamental modes of vibration were assigned based on the position, shape and relative intensity of the recorded spectra and in correlation with the vibrational bands of structurally related molecules. By employing FTIR spectral technique the quality of the drugs under various storage conditions have been studied. The assay of the tablets of these drugs were done using UV-visible spectroscopy and compared with the labeled amount.

Key Words: FTIR Spectroscopy, Raman spectroscopy, Antidepressant, Antipsychotic, Vibrational frequency, Drug assay.

INTRODUCTION

Sertraline hydrochloride (1) (4-(3,4-dichlorophenyl)-1,2,3,4-tetrahydro-Nmethyl-1-naphthalenamine hydrochloride) selectively blocks serotonin reuptake and is used for the treatment of depression, as well as dependency- and other anxietyrelated disorders. Sertraline belongs to those medicinal agents having one or more asymmetric centers in which the isomers show significant differences in their biological activity and therefore, it is necessary to produce the biologically active 1S,4S-enatiomer, sertraline with high optical purity¹. Typical antipsychotics are classified by their chemical structure and the potency with which they bind to dopamine type 2 (D2) receptors². Olanzapine (2-methyl-4-(4-methyl-1-piperazinyl)-10*H*thieno-[2,3-b][1,5]benzodiazepine) is a relatively new benzodiazepine which belongs to the class of the thienobenzodiazepines and has proven efficacy against the positive and negative symptoms of schizophrenia, bipolar disorder and other psychosis³. Olanzapine is the most widely studied of all first-line typical agents for the treatment of bipolar disorder and significant evidence of its mood-stabilizing properties exists⁴. The structure of sertraline hydrochloride and olanzapine is shown in Fig. 1(a-b).

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Fig. 1. (a) Sertraline hydrochloride (b) Olanzapine

It is essential to design pharmaceutical products that consistently deliver the intended performance, which demands monitoring of their quality incessantly. Quality of drug plays a vital role indicating the suitability of drug product for its intended use. In this work, a quality analysis of antipsychotic drugs sertraline and olanzapine has been carried out by employing FTIR and FT-Raman spectroscopic techniques. The change in quality of these drugs when stored under various conditions has been studied. Based on the structure of these drug molecules and other similar molecules, vibrational band assignment has been made from the FTIR and FT-Raman vibrational spectra.

EXPERIMENTAL

Sertraline hydrochloride and olanzapine of the pharmaceutical grade were procured for Orchid Chemicals, Mumbai, India and were used as received.

FTIR, FT-Raman and UV-visible spectroscopy: The FTIR spectra of the drugs sertraline and olanzapine were recorded with ABB Bomem series spectro-photometer over the region of 4000-400 cm⁻¹ by adopting KBr pellet technique at Dr. CEEAL Analytical Lab, Chennai, India. The FT-Raman spectra were recorded over the region 3700-100 cm⁻¹ by Raman spectrophotometer Nexus 670 at CECRI, Karaikudi, India. The UV-visible spectral measurements were carried out using Shimadzu-1601 spectrophotometer at Ceeal Analytical Lab, Chennai. All the spectra were recorded at the room temperature.

RESULTS AND DISCUSSION

Vibrational spectral analysis: The IR spectrum of a compound is the superposition of the absorption bands of specific functional groups. By observing the position, shape and relative intensities of the vibrational bands in FTIR and FT Raman spectra of the drug molecules sertraline and olanzapine a satisfactory vibrational band assignment has been made. They are summarized in Tables 1 and 2 for sertraline and olanzapine, respectively.

Sertraline has two planar phenyl rings that are approximately perpendicular to each other and unsaturated ring in a half-chair conformation. Sertraline hydrochloride molecule has three groups namely methyl ammonium chloride, a hydrophobic phenyl Vol. 22, No. 8 (2010)

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TABLE-1

VIBRATIONAL BAND ASSIGNMENTS FOR SERTRALINE HYDROCHLORIDE

Frequency (cm ⁻¹)		- Vibrational hand assignment			
FTIR	FT Raman	v ibrational band assignment			
3361 s	_	NH ₂ symmetric stretching			
3076 w	3060 s	C-H stretching			
3037 w	3028 w	C-H stretching			
3008 w	2989 s	C-H stretching			
2940 mw	2960 mw	C-H stretching of N bonded CH ₂ group			
2920 s	_	$N^{+}H_{2}$ asymmetric stretching			
2817 mw	_	C-H stretching of N bonded CH ₃ group			
2751 mw	_	$N^{+}H_{2}$ symmetric stretching			
2620 m	_	NH…Cl stretching			
1620 s	-	Methyl bonded N^+H_2 deformation (scissors)			
1616 s	_	N-H bending			
1585 w	1592 m	Aromatic ring stretching			
1582 mw	_	$N^{+}H_{2}$ symmetric deformation			
1564 vw	1561 vw	Aromatic ring stretching			
1468 vs	1471 vw	CH_3/CH_2 asymmetrical scissoring			
1465 w	1471 vw	CH ₂ scissoring vibration			
1460 w	1452 w	CH ₃ asymmetric deformation			
1428 mw	1428 vw	CH_2/NH_2 symmetric deformation			
1408 m	-	Symmetric scissoring methyl group attached to N_2 atom			
1401 s	1391 w	C-H deformation			
1348 w	1348 w	C-NH ₂ stretching			
1270 w	1290 m	CH ₃ /CH deformation			
1212 mw	1216 mw	CH ₃ twisting			
1138 s	1133 m	Aromatic ring stretching			
1058 vw	1058 w	CH ₃ deformation			
1044 m	1042 m	C-N stretching			
1025 m	1002 vw	Aromatic ring stretching			
955 m	963 w	C-H twisting			
922 mv	917 w	NH_2 wagging			
891 w	888 mv	C-H stretching			
824 m	829 m	C-H twisting			
803 w	811 w	NH ₂ twisting			
787 s	785 m	NH ₂ rocking			
780 s	781m	NH_2 wagging			
704 mw	705 mw	C-H twisting			
672 mw	673 m	N-H twisting			
621 w	622 w	C-H twisting			
590 mw	590 w	Aromatic ring twisting			
565 w	564 mw	Aromatic ring twisting			
512 vw	513 mw	Aromatic ring twisting			

ring and an aromatic ring with electronegative two Cl atoms⁵. Olanzapine crystallizes in atleast 25 solid forms, including polymorphs, solvates and hydrates⁶. The many different structure in which the compound crystallizes probably differ only slightly in their packing arrangement, irrespective of the solvate content. This hypothesis

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TABLE-2 VIBRATIONAL BAND ASSIGNMENTS FOR OLANZAPINE

]	Frequency (cm ⁻¹)	
FTIR	FT Raman	
3291 mw	_	N-H stretching
2933 ms	3008 m	C-H stretching
2837 m	_	CH ₂ symmetric stretching
1585 s	_	C-N stretching
1558 m	1558 mw	C-N stretching
1516 w	1517 w	N-H deformation
1471 w	1472 w	CH_2 deformation
1447 vw	1445 w	CH_2 deformation
1412 s	1411 m	CH ₃ deformation
1379 vw	1377 w	CH_2 wagging
1369 m	1370 m	C-C stretching
1357 vw	1353 w	CH_2 wagging
1331 vw	1331 vw	CH_2 wagging
1289 m	1290 m	CH ₂ twisting
1271 m	_	C-N stretching
1259 w	1259 vw	CH ₂ twisting
1223 s	1224 m	C-N stretching
1201 m	1202 m	CH ₂ twisting
1179 m	1179 m	C-H deformation
1155 m	1154 m	Aromatic ring stretching
1142 s	1142 mw	Aromatic ring stretching
1120 w	_	C-H deformation
1102 vw	1103 w	C-N stretching
1073 m	_	CH ₂ twisting
1042 w	1043 w	Aromatic ring deformation
1009 m	_	Aromatic ring deformation
964 m	965 m	C-S stretching
927 mw	_	Aromatic ring deformation
887 mw	886 m	Aromatic ring deformation
853 m	852 w	C-H out of plane bending
846 w	845 w	C-H out of plane bending
817 w	819 w	C-N stretching
783 m	784 w	Aromatic ring deformation
767 w	769 w	Aromatic ring deformation
745 s	748 w	C-H out of plane deformation
670 w	669 w	Aromatic ring stretching
610 vw	606 w	Aromatic ring deformation
566 m	_	C-C in-plane deformation

was verified by Polla *et al.*⁷ showing that all of the crystalline forms of olanzapine are built through the piling of (olanzapine)₂ centrosymmetric racemic pairs, stacked into columns parallel to the crystallographic (100) direction and connected with each other through N-H…N hydrogen bonds or solvate mediated interactions.

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Considering the CH₃NH₂ group^{8,9} of sertraline the vibrational modes are the C-H stretching modes, the NH₂ scissors, N-H stretching modes, NH₂ bond. NH₂ symmetric stretching vibrations occur at 3361 cm⁻¹. The band at 780 cm⁻¹ corresponds to the NH₂ wagging and the band at 1616 cm⁻¹ corresponds to the N-H bending motions. The C-N stretching is located at 1044 cm⁻¹. The absorption of the N⁺H₂ group are lower by about 200 cm⁻¹. In this region also occurs stretching modes of CH₃. The asymmetric stretching of N⁺H₂ has been assigned to the ranges 2920-2915 cm⁻¹. A very weak band has been observed at 2918 cm⁻¹. The band observed at 2751 cm⁻¹ is assigned to the symmetric stretching of N^+H_2 . The calculated band at 2620 cm⁻¹ is assigned to the v(NH…Cl). The deformation vibration (scissors) of methyl bonded N^+H_2 group is found in the region¹⁰ 1620-1560 cm⁻¹. The bands at 1582, 1428 and 803 cm⁻¹ are assigned to the $v_s(N^+H_2)$, wagging and rocking modes of sertraline hydrochloride, respectively. The band at 891 cm⁻¹ is assigned to v(C-N) stretching mode. This mode showed also coupling between the other modes. Table-4 indicates that most of the vibrational wave numbers arise on account of mixing of different normal modes. The weak bands observed at 3076, 3037 and 3008 cm⁻¹ are assigned to C-H stretching frequencies. The bands observed at 2817 and 2940 cm⁻¹ are assigned to C-H stretching of N bonded CH₃ group and CH₂, respectively. The CH₂ group (for ring) gives rise to a band near 1465 cm⁻¹ due to the scissoring vibration. The asymmetrical CH₃ deformation is also found around 1460 cm⁻¹. A methyl group attached to a nitrogen atom gives rise to a band at 1408 cm⁻¹ as a symmetric scissors. The observed IR band at 1468 cm⁻¹ is assigned to the asymmetrical CH₃ and CH₂ scissoring vibration modes, corresponding to the computed spectra¹¹. Vucis *et al.*¹ reported that the frequencies at 1130 and 1077 cm⁻¹ were observed Ph-Cl bands in N-[4-(3,4-dichlorophenyl)-3,4-dihydro-1(2H)-naphthalenylidene]-methanamine N-oxide. In the IR spectrum of sertraline-HCl, the corresponding bands are observed at 1138 and 1025 cm⁻¹. The other vibrational modes¹² of molecule studied are given in Table-2.

In the case of olanzapine starting from high wave numbers, the first feature observed in the vibrational spectra is the stretching vibration of the only N-H bond present in the molecule. This band is intense in the infrared spectra but shows only low intensity in the Raman spectra. The broad band shape and the shift toward lower wave numbers, pointed out the involvement of this band in hydrogen bonds in agreement with the reported crystalline structure¹³. At lower wave numbers, the bands associated with the C-H stretching are observed. The first group corresponds to the C-H stretching of the thiophene and benzene rings¹⁴, whereas the remaining bands are the symmetric and antisymmetric modes of the two methyl groups and the methylene functionalities of the piperazine ring¹⁵. It is interesting to notice that more bands are observed in this region than expected by considering the molecular structure. However some extra bands may be associated with overtones and combinations of lower energy modes. Proceeding to lower energy, the region between 1600 and1500 cm⁻¹ is dominated by the bands associated with the double bonds,

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which are partially coupled to C-H and N-H bending deformations. These bonds may be classified in three groups: the C-C ones belonging to the benzene and thiophene rings and the C-N bond of the azepine ring. C=C bonds¹⁶ are expected to be weak in infrared but strong in Raman, as it is verified in the case of the 1516 cm⁻¹ band, whereas the C-N should exhibit the opposite behaviour. The fact that the C-N band is observed below 1600 cm⁻¹ evidences the participation of this bond in the hydrogen bond pattern of olanzapine, as it was proposed by the X-ray diffraction structure refinement¹⁷. The next spectral region (1500-1300 cm⁻¹) is mainly dominated by the deformations of the methyl, methylene and C-H groups. In the case of coupling, it is usually between neighboring groups (e.g., methylene deformation of the piperazinyl group coupled to the methyl at 1470 cm⁻¹). Between 1300 and 1100 cm⁻¹, the contribution of the C-C and C-N stretching is dominant and the vibrational modes are spread over the complete molecule having contributions of different moieties, as may be observed in Table-2. Below 1100 cm⁻¹, vibrational modes recover some localization and the corresponding bands are less overlapped. In this region, some relevant features are identified, such as the Raman band at 1043 cm⁻¹, characteristic of the in plane bending deformation of the benzene¹⁸ and the infrared band at 745 cm⁻¹, associated with the out of plane deformation of the C-H bonds of the same group¹⁹. The deformations of the piperazinyl group, coupled to methyl group (1009 cm⁻¹) or to the azepine and thiophene moieties (965 cm⁻¹), are well identified in the infrared spectra. At lower wave numbers, the main components of the vibrational modes are the deformation and torsions of the rings giving rise to highly coupled movements²⁰. Finally, the low energy vibrational modes originate from the deformations of the skeleton of the molecule and the lattice vibrations.

Qualitative analysis using FTIR spectroscopy: The Indian Pharmacopoeia recommends that sertraline and olanzapine should be stored in tightly closed, light-resistant containers²¹. The behaviour of these drugs that were stored under the prescribed storage with those stored at altered conditions has been compared. The FTIR spectra of the samples have been recorded for the pure drugs stored in (i) well-sealed light resistant container (ii) exposed to sunlight and (iii) at ice point. Fig. 2 gives a comparison of the FTIR spectra of olanzapine at different storage conditions. Tables 3 and 4 compares the absorbance values of some selected specific modes of vibration for both the molecules. These tables indicate change in the absorbance values with change in storage condition.

The internal standard ratio is calculated among the various absorption bands of these two drugs and the results are given in Tables 5 and 6. The internal standard ratios evaluated clearly states the change in the quality of drugs due to the alteration in the storage condition.

Assay of tablets-UV-visible spectroscopy: Tablets are the popular form of dosage because of their cost effective preparation, stability and convenience in packaging, transporting and dispensing. It is popular among patients for accuracy

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TABLE-3 ABSORBANCE FOR CERTAIN MODES OF VIBRATION UNDER DIFFERENT CONDITIONS OF STORAGE FOR SERTRALINE

Frequency		Absorbance		_			
(cm^{-1})	Labeled	Labeled Exposed		Assignments			
()	condition	to sunlight	point				
3008 w	0.3414	0.3262	0.3715	C-H stretching			
2940 mw	0.5200	0.5191	0.5142	C-H stretching of N bonded CH ₂ group			
2751 mw	0.6216	0.5737	0.6261	N ⁺ H ₂ symmetric stretching			
1468 vs	0.8545	0.7928	0.9012	CH ₃ /CH ₂ asymmetrical scissoring			
1138 s	0.4532	0.4241	0.4809	Aromatic ring stretching			
955 m	0.3241	0.3115	0.3334	C-H twisting			
824 m	0.4497	0.4415	0.4684	C-H twisting			
787 s	0.5416	0.4835	0.6481	NH ₂ rocking			

TABLE-4 ABSORBANCE FOR CERTAIN MODES OF VIBRATION UNDER DIFFERENT CONDITIONS OF STORAGE FOR OLANZAPINE

Fraguanay		Absorbance		_
(cm ⁻¹)	Labeled condition	Exposed to sunlight	At ice point	Assignments
2933 ms	0.5346	0.2879	0.5937	C-H stretching
1585 s	0.8837	0.6093	1.1232	C-N stretching
1412 s	0.7459	05382	0.8742	CH ₂ deformation
1223 s	0.6092	0.4227	0.7203	C-N stretching
1142 s	0.6363	0.4667	0.7349	Aromatic ring stretching
964 m	0.5368	0.3883	0.5482	C-S stretching
846 w	0.3636	0.2346	0.4179	C-H out of plane bending
745 s	0.6591	0.4909	0.6875	Aromatic ring deformation

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Condition of	Internal standard of specific modes of vibration at 3008 cm ⁻¹						l ⁻¹	
exposure	A3008/3008	A _{2940/3008}	A _{2751/3008}	A _{1468/3008}	A _{1138/3008}	A _{955/3008}	A _{824/3008}	A _{787/3008}
Labeled condition	1.0000	1.5231	1.8207	2.5029	1.3275	0.9493	1.3172	1.5864
Exposed to sunlight	1.0000	1.5914	1.7587	2.4304	1.3001	0.9549	1.3535	1.4822
At ice point	1.0000	1.3841	1.7122	2.4258	1.2406	0.8974	1.2608	1.7445
-	Ir	nternal sta	indard of	specific m	odes of vi	ibration a	t 2940 cm	-1
	A3008/2940	A _{2940/2940}	A _{2751/2940}	A _{1468/2940}	A _{1138/2940}	A _{955/2940}	A _{824/2940}	A _{787/2940}
Labeled condition	0.6565	1.0000	1.1954	1.6433	0.8715	0.6233	0.8648	1.0415
Exposed to sunlight	0.6284	1.0000	1.1052	1.5273	0.8170	0.6001	0.8505	0.9314
At ice point	0.7225	1.0000	1.2371	1.7526	0.8963	0.6484	0.9109	1.2604
•	Ir	nternal sta	indard of	specific m	odes of vi	ibration a	t 2751 cm	-1
	A3008/2751	A _{2940/2751}	A _{2751/2751}	A _{1468/2751}	A _{1138/2751}	A _{955/2751}	A _{824/2751}	A _{787/2751}
Labeled condition	0.5492	0.8366	1.0000	1.3747	0.7291	0.5214	0.7235	0.8713
Exposed to sunlight	0.5686	0.9048	1.0000	1.3819	0.7392	0.5430	0.7696	0.8428
At ice point	0.5840	0.8084	1.0000	1.4168	0.7246	0.5241	0.7363	1.0189
	II	nternal sta	undard of	specific m	odes of vi	ibration a	t 1468 cm	l ⁻¹
	A3008/1468	A _{2940/1468}	A _{2751/1468}	A _{1468/1468}	A _{1138/1468}	A _{955/1468}	A _{824/1468}	A _{787/1468}
Labeled condition	0.3995	0.6085	0.7274	1.0000	0.5304	0.3793	0.5263	0.6338
Exposed to sunlight	0.4115	0.6548	0.7236	1.0000	0.5349	0.3929	0.5569	0.6099
At ice point	0.4122	0.5706	0.7058	1.0000	0.5114	0.3699	0.5798	0.7192
	Internal standard of specific modes of vibration at 1138 cm ⁻¹							
	II	nternal sta	indard of	specific m	odes of vi	ibration a	t 1138 cm	i ⁻¹
	In A _{3008/1138}	$\frac{\text{hternal sta}}{A_{2940/1138}}$	$\frac{\text{ndard of s}}{A_{2751/1138}}$	$\frac{\text{specific m}}{A_{1468/1138}}$	$\frac{\text{odes of vi}}{A_{1138/1138}}$	$\frac{1}{A_{955/1138}}$	$\frac{t\ 1138\ cm}{A_{824/1138}}$	$\frac{1}{A_{787/1138}}$
Labeled condition	In A _{3008/1138} 0.7533	$\frac{\text{A}_{2940/1138}}{1.1474}$	$\frac{\text{A}_{2751/1138}}{1.3716}$	specific m A _{1468/1138} 1.8855	$\frac{A_{1138/1138}}{1.0000}$	ibration a A _{955/1138} 0.7151	$\frac{t\ 1138\ cm}{A_{824/1138}}$ 0.9923	A _{787/1138} 1.1951
Labeled condition Exposed to sunlight	It A _{3008/1138} 0.7533 0.7691	$\frac{A_{2940/1138}}{1.1474}$ 1.2240	$\frac{A_{2751/1138}}{1.3716}$ 1.3527	specific m A _{1468/1138} 1.8855 1.8694	$\frac{A_{1138/1138}}{1.0000}$	ibration a A _{955/1138} 0.7151 0.7345	$\frac{t\ 1138\ cm}{A_{824/1138}}$ 0.9923 1.0410	A _{787/1138} 1.1951 1.1401
Labeled condition Exposed to sunlight At ice point	In A _{3008/1138} 0.7533 0.7691 0.8060	nternal sta A _{2940/1138} 1.1474 1.2240 1.1156	ndard of s A _{2751/1138} 1.3716 1.3527 1.3801	specific m A _{1468/1138} 1.8855 1.8694 1.9553	addes of vi A _{1138/1138} 1.0000 1.0000 1.0000	ibration a A _{955/1138} 0.7151 0.7345 0.7234	t 1138 cm A _{824/1138} 0.9923 1.0410 1.0163	A _{787/1138} 1.1951 1.1401 1.4062
Labeled condition Exposed to sunlight At ice point	In A _{3008/1138} 0.7533 0.7691 0.8060 I	$\frac{1}{A_{2940/1138}}$ 1.1474 1.2240 1.1156 nternal st	$\frac{\text{Indard of s}}{A_{2751/1138}}$ 1.3716 1.3527 1.3801 andard of	specific m A _{1468/1138} 1.8855 1.8694 1.9553 specific n	A A 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000	ibration a A _{955/1138} 0.7151 0.7345 0.7234 vibration a	t 1138 cm A824/1138 0.9923 1.0410 1.0163 at 955 cm-1	A _{787/1138} 1.1951 1.1401 1.4062 1
Labeled condition Exposed to sunlight At ice point	In A _{3008/1138} 0.7533 0.7691 0.8060 I A _{3008/955}	$\frac{A_{2940/1138}}{1.1474}$ 1.2240 1.1156 Internal st $A_{2940/955}$	ndard of s A _{2751/1138} 1.3716 1.3527 1.3801 andard of A _{2751/955}	specific m A _{1468/1138} 1.8855 1.8694 1.9553 specific n A _{1468/955}	addes of vi A _{1138/1138} 1.0000 1.0000 1.0000 nodes of v A _{1138/955}	ibration a <u>A_{955/1138}</u> 0.7151 0.7345 0.7234 vibration a A _{955/955}	$\begin{array}{c} t \ 1138 \ cm \\ \hline A_{824/1138} \\ \hline 0.9923 \\ 1.0410 \\ 1.0163 \\ \hline at \ 955 \ cm^{-} \\ \hline A_{824/955} \end{array}$	⁻¹ A _{787/1138} 1.1951 1.1401 1.4062 ¹ A _{787/955}
Labeled condition Exposed to sunlight At ice point Labeled condition	In A _{3008/1138} 0.7533 0.7691 0.8060 I A _{3008/955} 1.0534	$\begin{array}{c} \text{A}_{2940/1138} \\ \hline A_{2940/1138} \\ \hline 1.1474 \\ \hline 1.2240 \\ \hline 1.1156 \\ \hline \text{nternal str} \\ \hline A_{2940/955} \\ \hline 1.6044 \end{array}$	$\frac{A_{2751/1138}}{1.3716}$ 1.3716 1.3527 1.3801 andard of $\frac{A_{2751/955}}{1.9179}$	A 468/1138 1.8855 1.8694 1.9553 specific n A 468/955 2.6365 1.6365	A A 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 nodes of v A 1.38/955 1.3983	$\frac{A_{955/1138}}{0.7151}$ 0.7151 0.7345 0.7234 /ibration a A_{955/955} 1.0000	$\begin{array}{c} t \ 1138 \ cm\\ \hline A_{824/1138}\\ \hline 0.9923\\ 1.0410\\ 1.0163\\ \hline at \ 955 \ cm^{-}\\ \hline A_{824/955}\\ 1.3875 \end{array}$	A _{787/1138} 1.1951 1.1401 1.4062 ¹ A _{787/955} 1.6711
Labeled condition Exposed to sunlight At ice point Labeled condition Exposed to sunlight	In A _{3008/1138} 0.7533 0.7691 0.8060 I A _{3008/955} 1.0534 1.0472	$\begin{array}{c} \begin{array}{c} \text{A}_{2940/1138} \\ \hline A_{2940/1138} \\ \hline 1.1474 \\ 1.2240 \\ \hline 1.1156 \\ \hline \text{internal st} \\ \hline A_{2940/955} \\ \hline 1.6044 \\ 1.6665 \end{array}$	$\frac{A_{2751/1138}}{1.3716}$ 1.3716 1.3527 1.3801 andard of A_{2751/955} 1.9179 1.8417	A A 1.8855 1.8694 1.9553 specific n A A 2.6365 2.5451	$\frac{A_{1138/1138}}{1.0000}$ 1.0000 1.	ibration a A _{955/1138} 0.7151 0.7345 0.7234 vibration a A _{955/955} 1.0000 1.0000	$\begin{array}{r} t \ 1138 \ cm \\ \hline A_{824/1138} \\ \hline 0.9923 \\ 1.0410 \\ 1.0163 \\ \hline at \ 955 \ cm \\ \hline A_{824/955} \\ 1.3875 \\ 1.4173 \end{array}$	$\begin{array}{c} \underline{A_{787/1138}} \\ 1.1951 \\ 1.1401 \\ 1.4062 \\ \underline{A_{787/955}} \\ 1.6711 \\ 1.5522 \end{array}$
Labeled condition Exposed to sunlight At ice point Labeled condition Exposed to sunlight At ice point	In A _{3008/1138} 0.7533 0.7691 0.8060 I A _{3008/955} 1.0534 1.0472 1.1143	$\begin{array}{c} \underline{A}_{2940/1138} \\ \hline A_{2940/1138} \\ \hline 1.1474 \\ \hline 1.2240 \\ \hline 1.1156 \\ \hline nternal st \\ \hline A_{2940/955} \\ \hline 1.6044 \\ \hline 1.6665 \\ \hline 1.5423 \end{array}$	$\frac{A_{2751/1138}}{1.3716}$ 1.3716 1.3527 1.3801 andard of $\frac{A_{2751/955}}{1.9179}$ 1.8417 1.9079	$\frac{A_{1468/1138}}{1.8855}$ 1.8694 1.9553 specific n $\frac{A_{1468/955}}{2.6365}$ 2.5451 2.7031	$\frac{A_{1138/1138}}{1.0000}$ 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.3983 1.3983 1.3615 1.3874	A A	$\begin{array}{c} {\rm A}_{\rm 824/1138} \ {\rm cm}\\ {\rm A}_{\rm 824/1138}\\ {\rm 0.9923}\\ {\rm 1.0410}\\ {\rm 1.0163}\\ {\rm at}\ 955\ {\rm cm}\\ {\rm \overline{A}_{\rm 824/955}}\\ {\rm 1.3875}\\ {\rm 1.4173}\\ {\rm 1.4049} \end{array}$	$\begin{array}{c} \underline{A_{787/1138}} \\ 1.1951 \\ 1.1401 \\ 1.4062 \\ 1 \\ \hline \\ A_{787/955} \\ 1.6711 \\ 1.5522 \\ 1.9439 \\ \end{array}$
Labeled condition Exposed to sunlight At ice point Labeled condition Exposed to sunlight At ice point	In A _{3008/1138} 0.7533 0.7691 0.8060 I A _{3008/955} 1.0534 1.0472 1.1143 I I	$\begin{array}{c} \text{A}_{2940/1138} \\ \hline 1.1474 \\ 1.2240 \\ \hline 1.1156 \\ \text{nternal str} \\ \hline A_{2940/955} \\ \hline 1.6044 \\ 1.6665 \\ \hline 1.5423 \\ \text{nternal str} \end{array}$	$\frac{A_{2751/1138}}{1.3716}$ 1.3527 1.3801 andard of $\frac{A_{2751/955}}{1.9179}$ 1.8417 1.9079 andard of	$\frac{A_{1468/1138}}{1.8855}$ 1.8694 1.9553 specific n $\frac{A_{1468/955}}{2.6365}$ 2.5451 2.7031 specific n	$\frac{A_{1138/1138}}{1.0000}$ 1.0000 1.0000 1.0000 1.0000 nodes of v $\frac{A_{1138/955}}{1.3983}$ 1.3615 1.3874 nodes of v	ibration a A _{955/1138} 0.7151 0.7345 0.7234 /ibration a A _{955/955} 1.0000 1.0000 1.0000 /ibration a	$\begin{array}{c} {\rm A}_{824/1138} \ {\rm cm}\\ {\rm A}_{824/1138} \ {\rm 0.9923}\\ {\rm 1.0410}\\ {\rm 1.0163}\\ {\rm at} \ 955 \ {\rm cm}^{-}\\ {\rm A}_{824/955}\\ {\rm 1.3875}\\ {\rm 1.4173}\\ {\rm 1.4049}\\ {\rm at} \ 824 \ {\rm cm}^{-}\\ \end{array}$	$\begin{array}{c} \underline{A_{787/1138}} \\ 1.1951 \\ 1.1401 \\ 1.4062 \\ 1 \\ \hline A_{787/955} \\ 1.6711 \\ 1.5522 \\ 1.9439 \\ 1 \\ \end{array}$
Labeled condition Exposed to sunlight At ice point Labeled condition Exposed to sunlight At ice point	In A _{3008/1138} 0.7533 0.7691 0.8060 I A _{3008/955} 1.0534 1.0472 1.1143 I A _{3008/824}	$\begin{array}{c} \text{A}_{2940/1138} \\ \hline A_{2940/1138} \\ \hline 1.1474 \\ 1.2240 \\ \hline 1.1156 \\ \hline \text{nternal str} \\ \hline A_{2940/955} \\ \hline 1.6044 \\ 1.6665 \\ \hline 1.5423 \\ \hline \text{nternal str} \\ \hline A_{2940/824} \\ \end{array}$	$\begin{array}{c} \text{ndard of s} \\ \hline A_{2751/1138} \\ \hline 1.3716 \\ \hline 1.3527 \\ \hline 1.3801 \\ \hline \text{andard of} \\ \hline A_{2751/955} \\ \hline 1.9179 \\ \hline 1.8417 \\ \hline 1.9079 \\ \hline \text{andard of} \\ \hline A_{2751/824} \\ \end{array}$	$\frac{A_{1468/1138}}{1.8855}$ 1.8694 1.9553 specific m $\frac{A_{1468/955}}{2.6365}$ 2.5451 2.7031 specific n $A_{1468/924}$	$\frac{A_{1138/1138}}{1.0000}$ 1.0000 1.000 1.	ibration a A _{955/1138} 0.7151 0.7345 0.7234 /ibration a A _{955/955} 1.0000 1.0000 1.0000 /ibration a A _{955/824}	$\begin{array}{c} \begin{array}{c} A_{824/1138} \\ \hline A_{824/1138} \\ \hline 0.9923 \\ \hline 1.0410 \\ \hline 1.0163 \\ \hline at 955 \ cm^{-} \\ \hline A_{824/955} \\ \hline 1.3875 \\ \hline 1.4173 \\ \hline 1.4049 \\ \hline at 824 \ cm^{-} \\ \hline A_{824/824} \end{array}$	$\begin{array}{c} \overset{-1}{\mathbf{A}_{787/1138}}\\ 1.1951\\ 1.1401\\ 1.4062\\ \overset{1}{\mathbf{A}_{787/955}}\\ 1.6711\\ 1.5522\\ 1.9439\\ \overset{1}{\mathbf{A}_{787/824}} \end{array}$
Labeled condition Exposed to sunlight At ice point Labeled condition Exposed to sunlight At ice point Labeled condition	In A _{3008/1138} 0.7533 0.7691 0.8060 I A _{3008/955} 1.0534 1.0472 1.1143 I A _{3008/824} 0.7592	$\begin{array}{c} \text{A}_{2940/1138} \\ \hline 1.1474 \\ 1.2240 \\ 1.1156 \\ \hline \text{nternal str} \\ \hline A_{2940/955} \\ \hline 1.6044 \\ 1.6665 \\ 1.5423 \\ \hline \text{nternal str} \\ \hline A_{2940/824} \\ \hline 1.1563 \\ \end{array}$	$\begin{array}{c} \mbox{mdard of s} \\ \hline A_{2751/1138} \\ \hline 1.3716 \\ \hline 1.3527 \\ \hline 1.3801 \\ \hline andard of \\ \hline A_{2751/955} \\ \hline 1.9179 \\ \hline 1.8417 \\ \hline 1.9079 \\ \hline andard of \\ \hline A_{2751/824} \\ \hline 1.3823 \\ \end{array}$	$\frac{A_{1468/1138}}{1.8855}$ 1.8694 1.9553 specific m $\frac{A_{1468/955}}{2.6365}$ 2.6365 2.5451 2.7031 specific m $\frac{A_{1468/824}}{1.9002}$	A A 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 nodes of v V A 1.38953 1.3874 1.3874 nodes of v A A 1.3874 1.0078 1.0078	ibration a A _{955/1138} 0.7151 0.7345 0.7234 /ibration a A _{955/955} 1.0000 1.0000 1.0000 /ibration a A _{955/824} 0.7207	$\begin{array}{c} \begin{array}{c} A_{824/1138} \\ \hline A_{824/1138} \\ \hline 0.9923 \\ \hline 1.0410 \\ \hline 1.0163 \\ \hline at 955 \ cm^7 \\ \hline A_{824/955} \\ \hline 1.3875 \\ \hline 1.4173 \\ \hline 1.4049 \\ \hline at 824 \ cm^7 \\ \hline A_{824/824} \\ \hline 1.0000 \end{array}$	$\begin{array}{c} \underline{A_{787/1138}} \\ 1.1951 \\ 1.1401 \\ 1.4062 \\ 1 \\ \hline A_{787/955} \\ 1.6711 \\ 1.5522 \\ 1.9439 \\ 1 \\ \hline A_{787/824} \\ 1.2044 \end{array}$
Labeled condition Exposed to sunlight At ice point Labeled condition Exposed to sunlight At ice point Labeled condition Exposed to sunlight	$\begin{tabular}{ c c c c c c c } \hline II \\ \hline A_{3008/1138} \\ \hline 0.7533 \\ \hline 0.7691 \\ \hline 0.8060 \\ \hline I \\ \hline A_{3008/955} \\ \hline 1.0534 \\ \hline 1.0534 \\ \hline 1.0472 \\ \hline 1.1143 \\ \hline I \\ \hline A_{3008/824} \\ \hline 0.7592 \\ \hline 0.7388 \\ \hline \end{tabular}$	$\begin{array}{c} \text{A}_{2940/1138} \\ \hline A_{2940/1138} \\ \hline 1.1474 \\ 1.2240 \\ \hline 1.1156 \\ \hline \text{nternal st} \\ \hline A_{2940/955} \\ \hline 1.6044 \\ 1.6665 \\ \hline 1.5423 \\ \hline \text{nternal st} \\ \hline A_{2940/824} \\ \hline 1.1563 \\ \hline 1.1758 \end{array}$	$\begin{array}{c} \mbox{mdard of $$s$} \\ \hline A_{2751/1138} \\ \hline 1.3716 \\ \hline 1.3527 \\ \hline 1.3801 \\ \hline andard of \\ \hline A_{2751/955} \\ \hline 1.9179 \\ \hline 1.8417 \\ \hline 1.9079 \\ \hline andard of \\ \hline A_{2751/824} \\ \hline 1.3823 \\ \hline 1.2994 \\ \end{array}$	$\frac{A_{1468/1138}}{1.8855}$ 1.8694 1.9553 specific m $\frac{A_{1468/955}}{2.6365}$ 2.6365 2.5451 2.7031 specific m $\frac{A_{1468/8524}}{1.9002}$ 1.7957	A A 1.0000 1.0000 1.0000 1.0000 nodes of v V A 1.3983 1.3874 Nodes of v A A 1.0078 0.9606	ibration a A _{955/1138} 0.7151 0.7345 0.7234 /ibration a A _{955/955} 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 0.7207 0.7255	$\begin{array}{r} \begin{array}{r} A_{824/1138} \\ \hline A_{824/1138} \\ \hline 0.9923 \\ \hline 1.0410 \\ \hline 1.0163 \\ \hline at 955 \ cm^{-} \\ \hline A_{824/955} \\ \hline 1.3875 \\ \hline 1.4173 \\ \hline 1.4049 \\ \hline at 824 \ cm^{-} \\ \hline A_{824/824} \\ \hline 1.0000 \\ \hline 1.0000 \end{array}$	$\begin{array}{c} {}^{-1} \\ \hline A_{787/1138} \\ \hline 1.1951 \\ \hline 1.1401 \\ \hline 1.4062 \\ \hline \\ 1 \\ \hline A_{787/955} \\ \hline 1.6711 \\ \hline 1.5522 \\ \hline 1.9439 \\ \hline \\ 1 \\ \hline A_{787/824} \\ \hline 1.2044 \\ \hline 1.0951 \\ \end{array}$
Labeled condition Exposed to sunlight At ice point Labeled condition Exposed to sunlight At ice point Labeled condition Exposed to sunlight At ice point	$\begin{tabular}{ c c c c c c } \hline II \\ \hline A_{3008/1138} \\ \hline 0.7533 \\ \hline 0.7691 \\ \hline 0.8060 \\ \hline I \\ \hline A_{3008/955} \\ \hline 1.0534 \\ \hline 1.0534 \\ \hline 1.0472 \\ \hline 1.1143 \\ \hline I \\ \hline A_{3008/824} \\ \hline 0.7592 \\ \hline 0.7388 \\ \hline 0.7931 \\ \hline \end{tabular}$	$\begin{array}{c} \text{nternal sta} \\ \hline A_{2940/1138} \\ \hline 1.1474 \\ \hline 1.2240 \\ \hline 1.1156 \\ \hline \text{nternal st} \\ \hline A_{2940/955} \\ \hline 1.6044 \\ \hline 1.6665 \\ \hline 1.5423 \\ \hline \text{nternal st} \\ \hline A_{2940/824} \\ \hline 1.1563 \\ \hline 1.1758 \\ \hline 1.0978 \end{array}$	$\begin{array}{r} \mbox{ndard of $$s$} \\ \hline A_{2751/1138} \\ \hline 1.3716 \\ \hline 1.3527 \\ \hline 1.3801 \\ \hline andard of \\ \hline A_{2751/955} \\ \hline 1.9179 \\ \hline 1.8417 \\ \hline 1.9079 \\ \hline andard of \\ \hline A_{2751/824} \\ \hline 1.3823 \\ \hline 1.2994 \\ \hline 1.3580 \\ \end{array}$	$\frac{A_{1468/1138}}{1.8855}$ 1.8694 1.9553 specific n A_{1468/955} 2.6365 2.5451 2.7031 specific n A_{1468/8524} 1.9002 1.7957 1.9239	A A 1.0000 1.0000 1.0000 1.0000 nodes of v V A 1.3983 1.3615 1.3874 nodes of v V A 1.0078 0.9606 0.9840	ibration a A _{955/1138} 0.7151 0.7345 0.7234 vibration a A _{955/955} 1.0000 1.0000 1.0000 vibration a A _{955/824} 0.7207 0.7055 0.7118	$\begin{array}{r} \begin{array}{c} 1138 \text{ cm} \\ \hline A_{824/1138} \\ 0.9923 \\ 1.0410 \\ 1.0163 \\ \hline at 955 \text{ cm} \\ \hline A_{824/955} \\ 1.3875 \\ 1.4173 \\ 1.4049 \\ \hline at 824 \text{ cm} \\ \hline A_{824/824} \\ 1.0000 \\ 1.0000 \\ 1.0000 \\ \hline \end{array}$	$\begin{array}{c} {}^{-1} \\ \hline A_{787/1138} \\ 1.1951 \\ 1.1401 \\ 1.4062 \\ 1 \\ \hline A_{787/955} \\ 1.6711 \\ 1.5522 \\ 1.9439 \\ 1 \\ \hline A_{787/824} \\ 1.2044 \\ 1.0951 \\ 1.3836 \\ \end{array}$
Labeled condition Exposed to sunlight At ice point Labeled condition Exposed to sunlight At ice point Labeled condition Exposed to sunlight At ice point	In A _{3008/1138} 0.7533 0.7691 0.8060 I A _{3008/955} 1.0534 1.0472 1.1143 I A _{3008/824} 0.7592 0.7388 0.7931 I	$\begin{array}{c} \text{nternal sta} \\ \underline{A}_{2940/1138} \\ 1.1474 \\ 1.2240 \\ 1.1156 \\ \text{nternal st} \\ \underline{A}_{2940/955} \\ 1.6044 \\ 1.6665 \\ 1.5423 \\ \text{nternal st} \\ \underline{A}_{2940/824} \\ 1.1563 \\ 1.1758 \\ 1.0978 \\ \text{nternal st} \end{array}$	$\begin{array}{c} \mbox{ndard of s} \\ \hline A_{2751/1138} \\ \hline 1.3716 \\ \hline 1.3527 \\ \hline 1.3801 \\ \hline andard of \\ \hline A_{2751/955} \\ \hline 1.9179 \\ \hline 1.8417 \\ \hline 1.9079 \\ \hline andard of \\ \hline A_{2751/824} \\ \hline 1.3823 \\ \hline 1.2994 \\ \hline 1.3580 \\ \hline andard of \\ \hline andard of \\ \hline and and of \\ \hline and and and and of \\ \hline and and and and and and and and and and$	$\frac{A_{1468/1138}}{1.8855}$ 1.8694 1.9553 specific n $\frac{A_{1468/955}}{2.6365}$ 2.6365 2.5451 2.7031 specific n $\frac{A_{1468/824}}{1.9002}$ 1.7957 1.9239 specific n	$\frac{A_{1138/1138}}{1.0000}$ 1.0000 1.0000 1.0000 1.0000 nodes of v A_{1138/955} 1.3983 1.3615 1.3874 nodes of v A_{1138/824} 1.0078 0.9606 0.9840 nodes of v	ibration a $A_{955/1138}$ 0.7151 0.7345 0.7234 /ibration a $A_{955/955}$ 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000 1.000000 1.000000 1.00000000 1.0000000000	$\begin{array}{c} {\rm A}_{824/1138} \ {\rm cm}\\ {\rm A}_{824/1138} \ {\rm 0.9923} \ {\rm 1.0410} \ {\rm 1.0163} \ {\rm at} \ {\rm 955} \ {\rm cm}^{-}\\ {\rm A}_{824/955} \ {\rm 1.3875} \ {\rm 1.3875} \ {\rm 1.4173} \ {\rm 1.4049} \ {\rm at} \ {\rm 824} \ {\rm cm}^{-}\\ {\rm A}_{824/824} \ {\rm 1.0000} \ {\rm 1.0000} \ {\rm 1.0000} \ {\rm 1.0000} \ {\rm at} \ {\rm 787} \ {\rm cm}^{-} \ {\rm at} \ {\rm 787} \ {\rm cm}^{-} \end{array}$	$\begin{array}{c} \overset{-1}{\mathbf{A}_{787/1138}} \\ 1.1951 \\ 1.1401 \\ 1.4062 \\ \overset{1}{\mathbf{A}_{787/955}} \\ 1.6711 \\ 1.5522 \\ 1.9439 \\ \overset{1}{\mathbf{A}_{787/824}} \\ 1.2044 \\ 1.0951 \\ 1.3836 \\ \overset{1}{\mathbf{A}_{783}} \end{array}$
Labeled condition Exposed to sunlight At ice point Labeled condition Exposed to sunlight At ice point Labeled condition Exposed to sunlight At ice point	In A _{3008/1138} 0.7533 0.7691 0.8060 I A _{3008/955} 1.0534 1.0472 1.1143 I A _{3008/824} 0.7592 0.7388 0.7931 I A _{3008/787}	$\begin{array}{c} \text{A}_{2940/1138} \\ \hline A_{2940/1138} \\ \hline 1.1474 \\ \hline 1.2240 \\ \hline 1.1156 \\ \hline \text{nternal str} \\ \hline A_{2940/955} \\ \hline 1.6044 \\ \hline 1.6665 \\ \hline 1.5423 \\ \hline \text{nternal str} \\ \hline A_{2940/824} \\ \hline 1.1563 \\ \hline 1.1758 \\ \hline 1.0978 \\ \hline \text{nternal str} \\ \hline A_{2940/787} \\ \hline \end{array}$	$\begin{array}{c} \mbox{ndard of s} \\ \hline A_{2751/1138} \\ \hline 1.3716 \\ \hline 1.3527 \\ \hline 1.3801 \\ \hline andard of \\ \hline A_{2751/955} \\ \hline 1.9179 \\ \hline 1.8417 \\ \hline 1.9079 \\ \hline andard of \\ \hline A_{2751/824} \\ \hline 1.3823 \\ \hline 1.2994 \\ \hline 1.3580 \\ \hline andard of \\ \hline A_{2751/787} \\ \hline \end{array}$	$\frac{A_{1468/1138}}{1.8855}$ 1.8694 1.9553 specific m $\frac{A_{1468/955}}{2.6365}$ 2.5451 2.7031 specific m $\frac{A_{1468/955}}{1.9002}$ 1.7957 1.9239 specific n $\frac{A_{1468/787}}{A_{1468/787}}$	$\begin{array}{c} \begin{array}{c} \begin{array}{c} \text{A}_{1138/1138} \\ \hline A_{1138/1138} \\ \hline 1.0000 \\ \hline 1.3873 \\ \hline 1.3873 \\ \hline 1.3874 \\ \hline 1.0078 \\ \hline 0.9606 \\ \hline 0.9840 \\ \hline 1.38777 \\ \hline \end{array}$	ibration a A _{955/1138} 0.7151 0.7345 0.7234 /ibration a A _{955/955} 1.0000 1.0000 1.0000 /ibration a A _{955/824} 0.7207 0.7055 0.7118 /ibration a A _{955/787}	$\begin{array}{c} {\rm t} 1138 \ {\rm cm}\\ {\rm A}_{824/1138}\\ {\rm 0.9923}\\ {\rm 1.0410}\\ {\rm 1.0163}\\ {\rm at} \ 955 \ {\rm cm}^{-}\\ {\rm A}_{824/955}\\ {\rm 1.3875}\\ {\rm 1.4173}\\ {\rm 1.4049}\\ {\rm at} \ 824 \ {\rm cm}^{-}\\ {\rm A}_{824/824}\\ {\rm 1.0000}\\ {\rm 1.0000}\\ {\rm 1.0000}\\ {\rm at} \ 787 \ {\rm cm}^{-}\\ {\rm A}_{824/787}\end{array}$	$\begin{array}{c} \overset{-1}{\mathbf{A}_{787/1138}} \\ 1.1951 \\ 1.1401 \\ 1.4062 \\ \overset{1}{\mathbf{A}_{787/955}} \\ 1.6711 \\ 1.5522 \\ 1.9439 \\ \overset{1}{\mathbf{A}_{787/854}} \\ 1.2044 \\ 1.0951 \\ 1.3836 \\ \overset{1}{\mathbf{A}_{787/787}} \end{array}$
Labeled condition Exposed to sunlight At ice point Labeled condition Exposed to sunlight At ice point Labeled condition Exposed to sunlight At ice point Labeled condition	$\begin{tabular}{ c c c c c c } \hline II \\ \hline A_{3008/1138} \\ \hline 0.7533 \\ \hline 0.7691 \\ \hline 0.8060 \\ \hline I \\ \hline A_{3008/955} \\ \hline 1.0534 \\ \hline 1.0534 \\ \hline 1.0534 \\ \hline 1.0534 \\ \hline 1.0472 \\ \hline 1.1143 \\ \hline I \\ \hline A_{3008/824} \\ \hline 0.7592 \\ \hline 0.7388 \\ \hline 0.7931 \\ \hline I \\ \hline A_{3008/787} \\ \hline 0.6304 \\ \hline \end{tabular}$	$\begin{array}{c} \text{A}_{2940/1138} \\ \hline A_{2940/1138} \\ \hline 1.1474 \\ \hline 1.2240 \\ \hline 1.1156 \\ \hline \text{nternal str} \\ \hline A_{2940/955} \\ \hline 1.6044 \\ \hline 1.6665 \\ \hline 1.5423 \\ \hline \text{nternal str} \\ \hline A_{2940/824} \\ \hline 1.1563 \\ \hline 1.1758 \\ \hline 1.0978 \\ \hline \text{nternal str} \\ \hline A_{2940/787} \\ \hline 0.9601 \\ \end{array}$	$\begin{array}{c} \begin{array}{c} A_{2751/1138} \\ \hline A_{2751/1138} \\ \hline 1.3716 \\ \hline 1.3527 \\ \hline 1.3801 \\ \hline andard of \\ \hline A_{2751/955} \\ \hline 1.9179 \\ \hline 1.8417 \\ \hline 1.9079 \\ \hline andard of \\ \hline A_{2751/824} \\ \hline 1.3823 \\ \hline 1.2994 \\ \hline 1.3580 \\ \hline andard of \\ \hline A_{2751/787} \\ \hline 1.1477 \\ \end{array}$	$\frac{A_{1468/1138}}{1.8855}$ 1.8694 1.9553 specific m $\frac{A_{1468/955}}{2.6365}$ 2.6365 2.5451 2.7031 specific m $\frac{A_{1468/824}}{1.9002}$ 1.7957 1.9239 specific m $\frac{A_{1468/787}}{1.5777}$	$\begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c} A_{1138/1138} \\ \hline A_{1138/1138} \\ \hline 1.0000 \\ \hline 0.000 \\ \hline 0.0$	ibration a A _{955/1138} 0.7151 0.7345 0.7234 /ibration a A _{955/955} 1.0000 1.0000 1.0000 /ibration a A _{955/824} 0.7207 0.7055 0.7118 /ibration a A _{955/884}	$\begin{array}{c} {\rm t} 1138 \ {\rm cm}\\ {\rm A}_{824/1138}\\ {\rm 0.9923}\\ {\rm 1.0410}\\ {\rm 1.0163}\\ {\rm at} 955 \ {\rm cm}\\ {\rm A}_{824/955}\\ {\rm 1.3875}\\ {\rm 1.4173}\\ {\rm 1.4049}\\ {\rm at} 824 \ {\rm cm}\\ {\rm A}_{824/824}\\ {\rm 1.0000}\\ {\rm 1.0000}\\ {\rm 1.0000}\\ {\rm 1.0000}\\ {\rm at} 787 \ {\rm cm}\\ {\rm A}_{824/787}\\ {\rm 0.8303}\\ \end{array}$	$\begin{array}{r} {}^{-1} \\ \hline A_{787/1138} \\ \hline 1.1951 \\ \hline 1.1401 \\ \hline 1.4062 \\ {}^{1} \\ \hline A_{787/955} \\ \hline 1.6711 \\ \hline 1.5522 \\ \hline 1.9439 \\ {}^{1} \\ \hline A_{787/824} \\ \hline 1.2044 \\ \hline 1.0951 \\ \hline 1.3836 \\ {}^{1} \\ \hline A_{787/787} \\ \hline 1.0000 \end{array}$
Labeled condition Exposed to sunlight At ice point Labeled condition Exposed to sunlight At ice point Labeled condition Exposed to sunlight At ice point Labeled condition Exposed to sunlight	$\begin{tabular}{ c c c c c } \hline II \\ \hline A_{3008/1138} \\ \hline 0.7533 \\ \hline 0.7691 \\ \hline 0.8060 \\ \hline I \\ \hline A_{3008/955} \\ \hline 1.0534 \\ \hline 1.0534 \\ \hline 1.0534 \\ \hline 1.0534 \\ \hline 1.0472 \\ \hline 1.1143 \\ \hline I \\ \hline A_{3008/824} \\ \hline 0.7592 \\ \hline 0.7592 \\ \hline 0.7388 \\ \hline 0.7931 \\ \hline I \\ \hline A_{3008/787} \\ \hline 0.6304 \\ \hline 0.6747 \\ \hline \end{tabular}$	$\begin{array}{c} \text{A}_{2940/1138} \\ \hline A_{2940/1138} \\ \hline 1.1474 \\ \hline 1.2240 \\ \hline 1.1156 \\ \hline \text{nternal st} \\ \hline A_{2940955} \\ \hline 1.6044 \\ \hline 1.6665 \\ \hline 1.5423 \\ \hline \text{nternal st} \\ \hline A_{2940954} \\ \hline 1.1563 \\ \hline 1.1758 \\ \hline 1.0978 \\ \hline \text{nternal st} \\ \hline A_{2940/787} \\ \hline 0.9601 \\ \hline 1.0736 \\ \end{array}$	$\begin{array}{c} \mbox{ndard of s} \\ \hline A_{2751/1138} \\ \hline 1.3716 \\ \hline 1.3527 \\ \hline 1.3801 \\ \hline andard of \\ \hline A_{2751/955} \\ \hline 1.9179 \\ \hline 1.8417 \\ \hline 1.9079 \\ \hline andard of \\ \hline A_{2751/824} \\ \hline 1.3823 \\ \hline 1.2994 \\ \hline 1.3580 \\ \hline andard of \\ \hline A_{2751/787} \\ \hline 1.1477 \\ \hline 1.1866 \\ \end{array}$	$\frac{A_{1468/1138}}{1.8855}$ 1.8694 1.9553 specific m $\frac{A_{1468/955}}{2.6365}$ 2.6365 2.5451 2.7031 specific m $\frac{A_{1468/8524}}{1.9002}$ 1.7957 1.9239 specific m $\frac{A_{1468/787}}{1.5777}$ 1.6397	A A A 1.0000 1.0000 1.0000 1.0000 1.0000 nodes of v V A 1.3873 1.3615 1.3874 nodes of v A A 1.0078 0.9606 0.9840 nodes of v A 0.8368 0.8771	ibration a A _{955/1138} 0.7151 0.7345 0.7234 /ibration a A _{955/955} 1.0000 1.0000 1.0000 /ibration a A _{955/824} 0.7207 0.7055 0.7118 /ibration a A _{955/877} 0.5984 0.6443	$\begin{array}{r} {\rm t} 1138 \ {\rm cm}\\ \hline {\rm A}_{824/1138}\\ 0.9923\\ 1.0410\\ 1.0163\\ \hline {\rm at} 955 \ {\rm cm}^{-}\\ \hline {\rm A}_{824/955}\\ 1.3875\\ 1.3875\\ 1.4173\\ 1.4049\\ \hline {\rm at} 824 \ {\rm cm}^{-}\\ \hline {\rm A}_{824/824}\\ 1.0000\\ 1.0000\\ 1.0000\\ \hline {\rm at} 787 \ {\rm cm}^{-}\\ \hline {\rm A}_{824/787}\\ \hline {\rm 0.8303}\\ 0.9131\\ \end{array}$	$\begin{array}{c} {}^{-1} \\ \hline A_{787/1138} \\ \hline 1.1951 \\ \hline 1.1401 \\ \hline 1.4062 \\ \hline \\ 1 \\ \hline A_{787/955} \\ \hline 1.6711 \\ \hline 1.5522 \\ \hline 1.9439 \\ \hline \\ 1 \\ \hline A_{787/824} \\ \hline 1.2044 \\ \hline 1.0951 \\ \hline 1.3836 \\ \hline \\ 1 \\ \hline A_{787/787} \\ \hline 1.0000 \\ \hline 1.0000 \\ \hline \end{array}$

of dosage, compactness, portability, blandness of taste and ease of administration²². Quantitative spectrometry is an extension of calorimetry and many pharmacopical substances are assayed spectrophotometrically²³.

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TABLE 6
INTERNAL STANDARD EVALUATION FOR OLANZAPINE

Condition of	Internal standard of specific modes of vibration at 2933 cm ⁻¹							
exposure	A _{2933/2933}	A _{2933/2933}	A _{1412/2933}	A _{1223/2933}	A _{1142/2933}	A _{964/2933}	A _{846/2933}	A _{745/2933}
Labeled condition	1.0000	1.6530	1.3952	1.1395	1.1902	1.0041	0.6801	1.2329
Exposed to sunlight	1.0000	2.1164	1.8694	1.4682	1.6210	1.3487	0.8149	1.7051
At ice point	1.0000	1.8919	1.4725	1.2469	1.2378	0.9234	0.7039	1.1580
L	Ir	nternal sta	undard of	specific m	odes of v	ibration a	t 1585 cm	-1
	A _{2933/1585}	A _{2933/2933}	A _{1412/2933}	A _{1223/2933}	A _{1142/2933}	A _{964/2933}	A _{846/2933}	A _{745/2933}
Labeled condition	0.6049	1.0000	0.8441	0.6894	0.7197	0.6074	0.4115	0.7458
Exposed to sunlight	0.4725	1.0000	0.8833	0.6937	0.7659	0.6373	0.3850	0.8057
At ice point	0.5286	1.0000	0.7783	0.6591	0.6543	0.4881	0.3721	0.6121
X	Ir	nternal sta	undard of	specific m	odes of v	ibration a	t 1412 cm	-1
	A _{2933/1412}	A _{2933/1412}	A _{1412/1412}	A _{1223/1412}	A _{1142/1412}	A _{964/1412}	A _{846/1412}	A _{745/1412}
Labeled condition	0.7167	1.1847	1.0000	0.8167	0.8531	0.7197	0.4875	0.8836
Exposed to sunlight	0.5349	1.1321	1.0000	0.7854	0.8671	0.7215	0.3252	0.9121
At ice point	0.6791	1.2848	1.0000	0.8468	0.8407	0.4642	0.4780	0.7864
	Ir	nternal sta	undard of	specific m	odes of v	ibration a	t 1223 cm	l ⁻¹
	A _{2933/1223}	A _{2933/1223}	A _{1412/1223}	A _{1223/1223}	A _{1142/1223}	A _{964/1223}	A _{846/1223}	A _{745/1223}
Labeled condition	0.8776	1.4506	1.2244	1.0000	1.0445	0.8812	0.5968	1.0819
Exposed to sunlight	0.6811	1.4414	1.2732	1.0000	1.1041	0.9186	0.5550	1.1613
At ice point	0.8019	1.5172	1.1809	1.0000	0.9927	0.7405	0.5645	0.9287
L	Internal standard of specific modes of vibration at 1142 cm ⁻¹							
	A _{2933/1142}	A _{2933/1142}	A _{1412/1142}	A _{1223/1142}	A _{1142/1142}	A _{964/1142}	A _{846/1142}	A _{745/1142}
Labeled condition	0.8402	1.3895	1.1722	0.9574	1.0000	0.8436	0.5714	1.0358
Exposed to sunlight	0.6169	1.3055	1.1532	0.9057	1.0000	0.8320	0.5027	1.0519
At ice point	0.8079	1.5284	1.1895	1.0074	1.0000	0.7460	0.5686	0.9355
^	Ι	nternal st	andard of	specific n	nodes of v	vibration a	t 964 cm	1
	A _{2933/964}	A _{2933/964}	A _{1412/964}	A _{1223/964}	A _{1142/964}	A _{964/964}	A _{846/964}	A _{745/964}
Labeled condition	0.9959	1.6462	1.3895	1.1349	1.1854	1.0000	0.6773	1.2278
Exposed to sunlight	0.7414	1.5691	1.3860	1.0886	1.2019	1.0000	0.6042	1.2642
At ice point	1.0830	2.0489	2.1542	1.3504	1.3406	1.0000	0.7623	1.2541
^	Ι	nternal st	andard of	specific n	nodes of v	vibration a	t 846 cm	1
	A _{2933/846}	A _{2933/846}	A _{1412/846}	A _{1223/846}	A _{1142/846}	A _{964/846}	A _{846/846}	A _{745/846}
Labeled condition	1.4704	2.4304	2.0514	1.6755	1.7500	1.4763	1.0000	1.8127
Exposed to sunlight	1.2272	2.5972	1.7112	1.8018	1.9893	1.6552	1.0000	2.0925
At ice point	1.4207	2.6877	2.0919	1.7715	1.7586	1.3118	1.0000	1.6451
*	Ι	nternal st	andard of	specific n	nodes of v	vibration a	ut 745 cm ⁻	1
	A _{2933/745}	A _{2933/745}	A _{1412/745}	A _{1223/745}	A _{1142/745}	A _{964/745}	A _{846/745}	A _{745/745}
Labeled condition	0.8111	1.3408	1.1317	0.9243	0.9654	0.8144	0.5517	1.0000
Exposed to sunlight	0.5865	1.2412	1.0964	0.8611	0.9507	0.7910	0.4779	1.0000
At ice point	0.8636	1.6337	1.2716	1.0768	1.0689	0.7974	0.6079	1.0000

In the present work medicines of sertraline and olanzapine in the form of tablets were subjected to quantitative estimation (Tables 7 and 8) of the drug substance in the tablet using UV-visible spectroscopic technique. The tablets Serta 25 mg and

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				e	
Wavelength	Concentration	Average ab wavelengtl	sorbance of n maximum	Estimation of	Percentage of the labeled
(1111)	(incg)	Pure	Serta	- Selta (ling)	amount
273	50	0.2146	0.2098	24.64	98.56
273	100	0.3004	0.2946	24.72	98.87
273	150	0.4066	0.3993	24.75	99.00
273	200	0.5007	0.4939	24.86	99.45
273	250	0.6085	0.6002	24.86	99.44

TABLE-7 ESTIMATION OF ASSAY IN SERTA 25 mg

TABLE-8 ESTIMATION OF ASSAY IN OLEANZ 10 mg

Wavelength	Concentration	Average ab wavelengtl	sorbance of n maximum	Estimation of	Percentage of the labeled
(1111)	(incg) –	Pure	Oleanz	- Oleanz (Ing)	amount
259	10.0	0.6794	0.6747	10.07	100.68
259	12.5	0.7813	0.7768	10.08	100.79
259	15.0	0.8907	0.8838	10.08	100.83
259	17.5	0.9253	0.9203	10.08	100.84
259	20.0	0.9967	0.9919	10.09	100.89

Oleanz 10 mg containing sertraline and olanzapine as the active ingredient were obtained from a leading pharmaceutical company. The drug content is determined by preparing a stock solution of the test sample and the solution is diluted to the same concentration as that of the standard sample and the absorbance of the resulting solution under UV-visible radiation was measured²⁴. The drugs were found to obey Beer's law. The drug content of the tablet is calculated as given below:

Drug content of	Test absorption		Standard weight		Average weight
the tablet/assay	Standard absorption	X	Test weight	x	of one tablet

The UV spectral recording of the pure samples sertraline and tablets Serta 25 mg was carried out for concentrations of 50, 100, 150, 200 and 250 mcg. The UV spectral recording of the pure samples olanzapine and tablets Oleanz 10 mg was carried out for concentrations of 10.0, 12.5, 15.0, 17.5 and 20.0 mcg. The UV-visible spectra of sertraline exhibits wavelength maximum at 273 nm. The average weight of one tablet was found to be 114.7 mg. Fig. 3 presents an overlaid spectrum of the tablet Serta 25 mg for various concentrations. The UV-visible spectra of olanzapine exhibits wavelength maximum at 259 nm. The average weight of one tablet it found to be 173.2 mg.



Fig. 3. Overlaid UV-visible spectra of Serta 25 mg for various concentrations

Conclusion

FTIR and FT-Raman spectroscopic technique have been employed for the qualitative analysis of the two antipsychotic drugs sertraline and olanzapine. A satisfactory vibrational assignment of the two drugs has been done from the FTIR and FT-Raman spectra of the drugs. They confirm the basic functional groups present in the compound. The intensity ratio calculated among specific modes of vibrations clearly shows that some vibrational bands are more altered due to sunlight exposure and storage at ice point. This clearly denotes that a change in the quality of the drugs has taken place due to the change in storage condition. The UV-visible spectroscopic method was used to find the amount of drug present in tablet formulations. Tablets Serta 25 mg and Oleanz 10 mg were found to contain 24.77 mg of sertraline and 10.08 mg of olanzapine as the active substance.

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