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Normal Coordinates Analyses of Sucrose in the Crystalline State

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Abstract Combining a modified Urey-Bradley-Shimanouchi-intramolecular potential energy function with an intermolecular potential energy function that includes the Van der Walls interactions, the electrostatic terms, and an explicit hydrogen bond function, normal coordinate calculations has been performed for sucrose in the crystalline state. The infrared spectra in 4000 – 400 cm^{-1} and the Raman spectra in 3500 – 50 cm^{-1} range were recorded. These spectra constitute the experimental support that allows reproducing theoretically the vibrational frequencies and to establish a force field for this molecule through a normal coordinate analysis. The force constants were varied, so as to obtain an agreement between the observed vibrational frequencies and the calculated ones of sucrose. The initial force field parameters are derived from the sucrose and are fitted so as to obtain a good agreement between the calculated and the observed frequencies.

Keywords Sucrose, IR and Raman Spectra, Normal Coordinate Analysis

1. Introduction

The conformations of carbohydrate molecules have been the interest of a large number of normal coordinates calculations, using the several theoretical methods, such as molecular mechanics[1,2] , and ab-initio methods[2-7].Up to now, analogous computations have been performed on monosaccharides such as D-glucose[8], D-galactose[9], L-fucose[10] and d-fructose[11], on methylated monosaccharides such as methyl α-d-mannoside[12] and methyl α and β-d-galactoside[13], and also on several disaccharides having d-glucose, as a basic unit, with different glycosidic linkages such as cellobiose, maltose, sophorose,...[14,15]. In the present work, we report the force fields obtained from sucrose. They have been obtained using a modified Urey-Bradley-Shimanouchi force field (mUBSFF)[16] involving non-redundant symmetry coordinates, combined with a complete intermolecular potential energy function taking into account the Van der Waals and the electrostatic interactions and also a contribution of the hydrogen bonds.This force field provides a set of force constant characteristic of a chemical reality assigned to a group of atoms or molecule model in more complex systems[29]. It is the principle of transferability established by T. Shimanouchi[16].

With these potentials and on the basis of vibration data (infrared and Raman spectra of sucrose) and in accordance to previous works made on analogue molecules, we have fitted the set of parameters of both molecules in the crystalline state, they represent the force fields.

2. Experimental

2.1. IR and Raman spectrum

The sample of sucrose was supplied by Sigma-Aldrich (S 8501) and used to record infrared and Raman spectra without any further purification.

The IR spectrum of solid state compounds was recorded using a Brüker Fourier Transform IFS. 113V spectrometer. 100 scans have been accumulated at 2 cm^{-1} resolution for this compound. The Raman spectrum was recorded directly from the powder on a T 64000 ISA/ Jobin Yvon spectrometer with the 641.5 NM laser radiations and at 2 cm^{-1} resolution.

2.2.The Geometry

Sucrose is a disaccharide with the sequence as α-D-Glucopyranoside (1→2) β-D-Fructofuranosyl. Although, its crystal structure was reported in 1973 using neutron diffraction which allowed a thorough description of the essential structural features offered by crystalline sucrose[17]. The structural and conformational features of sucrose are illustrated in figure 1. This compound crystallizes in the monoclinic system.

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Table 1. Description of the hydrogen bonds in crystalline sucrose

O-H…O	Symmetry Operation	O-H	H…O	O…O	O-H…O(°)
Intermolecular hydrogen bond					
O(34)-H(45)...O(7)	I. 000	0.974	1.851	2.781	158.6
O(33)-H(44)...O(11)	I. 000	0.972	1.895	2.85	167.1
Intramolecular hydrogen bond					
O(7)-H(19)...O(33)	I. 001	0.972	1.892	2.855	170.2
O(8)-H(20)...O(32)	II. 001	0.959	1.907	2.862	172.8
O(10)-H(22)...O(8)	II. 111	0.956	1.921	2.848	162.9
O(32)-H(43)...O(30)	II. 000	0.969	1.908	2.864	168.5
O(30)-H(42)...O(34)	I. 001	0.976	1.760	2.716	165.4

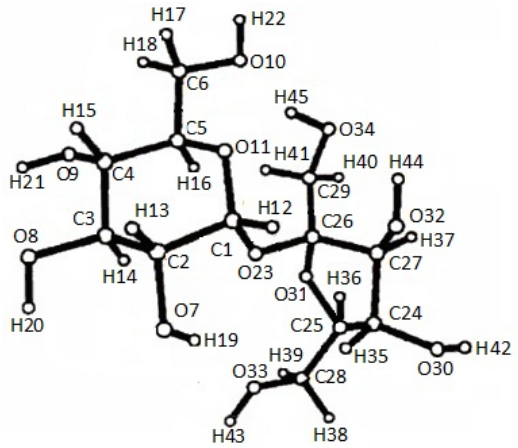

Figure 1. Molecular conformation and atom numbering for sucrose

The spatial group is then P_{21}, with two molecules per cell: (x, y, z), (-x, y+1, -z). The parameters of the unit cell are: a=10.8633Å, b= 8.7050 Å, c=7.7585 Å and β= 102.945°. Twenty-seven cells are needed to describe all of the 7 hydrogen bonds for sucrose which represented in Table 1.

The sucrose molecule is constituted by 45 atoms, then 153 internal coordinates are defined and 129 internal modes are expected. Therefore, there are 24 redundancies, 12 of them arise from the ring and 12 others are due to the tetrahedral groups. They were eliminated using the REDUND program[18].

The 129 internal vibration modes of the molecule are combined with the six external modes, (three translations and three rotations). The irreductible representation in the crystalline state is given by $\Gamma_{crystal} = 134\ A + 133B$, all of these modes are active in Raman and in IR.

3. Calculations Details

3.1. The Program

The normal coordinates calculations have been performed using the CVOA (crystalline vibrations optically active) program that has been written by Takeuchi[19]. The main goal of this program is to calculate the optically active vibrations of the molecule in the crystalline state as well as the frequencies of the normal modes of vibrations. The method here is derived from the Wilson GF method[20], and uses partly local symmetry coordinates developed by Shimanouchi[21].

3.2. Potential Energy Function

3.2.1. The Intermolecular Potential Function

As the calculations are performed in the solid state, the total potential energy function includes both an intramolecular potential and an intermolecular hydrogen bond potential function.

1. Title of the paper The potential due to the non-bonded atompair interaction, it is expressed by the Buckingham type function[22], $A_{ij}\ \exp(-B_{ij}\,R) - C_{ij}/r^6$, in this expression, the specific parameters A_{ij} ; B_{ij} and C_{ij} are specific parameters to each pair of atoms, here the values of the A, B and C parameters[23] are given in table 2. The interaction between the non-bonded atom pairs are taken into account between the cutoff distances r_{min} and r_{max} listed in table 2.

2. The electrostatic interaction term of coulombian, $q_i q_j/\xi r_{ij}$. In which q_i, q_j are the residual charges of the atoms $i\ and\ j$, j, ξ is the dielectric constant and r_{ij} is the distance separating two atoms.

The residual charges are computed by the DFT method employed using a (6-31 G (d,p)) basis function set in the GAUSSIAN 03/DFT program[24] (table 3). The exchanges functional are of the Becke type and the correlation effects determined according to the LYP (Lee- Yang-Parr) method[24].

3. The hydrogen bond potential is expressed by a potential energy function of the Urey-Bradley-Shimanouchi type[25]:

$$2V_H = \sum K_{O\ldots H}(\Delta r_{O\ldots H})^2 + \sum r_{O\ldots H} r_{H\ldots O} r_{O-H\ldots O}(\Delta \alpha_{O-H\ldots O})^2 + \sum r_{H\ldots O} r_{O\ldots C} r_{H\ldots O-C}(\Delta \alpha_{H\ldots O-C})^2 + \sum r_{O-H} r_{H\ldots O} r_{H-O\ldots H}(\Delta \alpha_{H-O\ldots H})^2 + \sum Y_{H\ldots O}(\Delta \tau_{O-H})^2 + \sum Y_{O-H}(\Delta \tau_{O-H})^2 \quad (1)$$

Therefore, each hydrogen bond involves new structural parameters: $K_{O\ldots H}$ are the force constants of the bond lengths, while $r_{O-H\ldots O}$, $r_{H\ldots O-C}$ and $r_{H-O\ldots H}$ are the force constants of the bond angles, and $Y_{H\ldots O}$ and Y_{O-H} are the force constants of the torsions.

Table 2. Van der Walls parameters for the Bückingham function, and cut-off distances of the sucrose

	A	B	C	$r_{min}<r<r_{max}$	
Type	Kcal/ mole	KcalÅ^{-1}	Kcal/mole	r_{min}(Å)	r_{max} (Å)
C…C	83630	3.600	568	2.297	2.29
C…O	63700	3.881	441	2.227	2.13
C…H	87660	3.670	125	1.936	2.00
O…O	96500	4.333	346	2.135	2.22
O…H	57500	4.727	122	1.887	1.93
H…H	26540	3.740	273	2.007	1.88

Table 3. Residual charges (in u.a.) used in the electrostatic potential

Atom	Charge sucrose	Atom	Charge sucrose
C1	0.390099	C24	0.145340
C2	0.130698	C25	0.155019
C3	0.143694	C26	0.482436
C4	0.181827	C27	0.127182
C5	0.139857	C28	0.056424
C6	0.021620	C29	0.060103
O7	-0.557922	O30	-0.558283
O8	-0.568464	O31	-0.551843
O9	-0.562481	O32	-0.551649
O10	-0.540751	O33	-0.564121
O11	-0.549484	O34	-0.547662
H12	0.109398	H35	0.101331
H13	0.109088	H36	0.107166
H14	0.100023	H37	0.115593
H15	0.104617	H38	0.090663
H16	0.110180	H39	0.118911
H17	0.134891	H40	0.115019
H18	0.124327	H41	0.067498
H19	0.327321	H42	0.317784
H20	0.320099	H43	0.317336
H21	0.324120	H44	0.328965
H22	0.309969	H45	0.323942
O23	-0.559883		

3.2.2. The Intramolecular Potential Function

The analytical expression for the intramolecular potential energy function is chosen that of modified Urey-Bradley-Shimanouchi[21].

$$V(r) = \frac{1}{2}\sum K_i(\Delta r_i)^2 + \frac{1}{2}\sum H_{ij}\left(\Delta\alpha_{ij}\right)^2 + \frac{1}{2}\sum F_{ij}\left(\Delta q_{ij}\right)^2 + \frac{1}{2}\sum Y_{ij}\left(\Delta\tau_{ij}\right)^2 + \frac{1}{2}\sum F'_{ij}\,W_{gij}\left(\Delta r_{ij} - \Delta\alpha ij2 + 12KtWt\Delta\alpha ij2\right) \quad (2)$$

The Δr_i are the variations of the bond lengths, the $\Delta\alpha_{ij}$ are the variations of the bond angles, the $\Delta\tau_{ij}$ are the variations of the bond torsions, the Δq_{ij} are the variations of the distances between non-bonded i and j atoms of (1-3) type, the K_i are the stretching constants, the H_{ij} are the constants of the angle deformations, the F_{ij} are the constants of the repulsion (1-3) type, the Y_{ij} are the torsional constants, the F'_{ij} are the constants due to the linear repulsion terms, the K_t are the internal constants of tetrahedral groups and the W_t are redundancy terms.

4. Results and Discussion

The initial force fields are those established previously for α-D-lactose[26] and α-melibiose[27]. These are represented in Table 4, 5, 6, 7, and 8.

The vibrational modes of the sucrose calculatedin this work has led to quite satisfying results.

A good agreement between calculated and observed frequencies is achieved after fitting theinitial force field, and the results are listed inTable 9.

Table 4. Final force field: intramolecular force constants for sucrose

Stretching	K_b(mdyn Å^{-1})	K_b(Kcal/ molÅ^2)
C-Ccy	2.950	212.200
Cc-Ce	2.650	190.620
Cc-Oe	2.830	203.568
Cc-Oc	2.900	208.603
Ce-Oe	3.600	258.955
C-O23	2.990	215.077
O-H	5.990	430.873
C-H	3.980	298.290

Table 5. Final force field: force constants of attractive and repulsive bending for sucrose

Bending	H (mdyn Å^{-1})	F (mdynÅ^{-1})	H (Kcal/mol rad²)	F (Kcal/mol rad²)
CcCOe	0.265	0.550	44.327	39.547
CcCcOc	0.336	0.650	60.219	46.738
CcCcO23	0.400	0.360	66.910	25.885
O23CO	0.370	0.680	61.891	48.895
CCCcy	0.360	0.210	60.219	15.100
HCeOe	0.224	0.675	37.469	48.535
HCcO23	0.200	0.600	33.455	43.142
CcOc	0.263	0.808	13.993	58.099
CcOeH	0.255	0.633	42.655	45.515
CeOeH	0.284	0.612	47.506	44.005
CcOcCc	0.600	0.420	87.910	30.200
CcO23Cc	0.650	0.330	108.72	23.728
CCH	0.187	0.410	31.280	29.480
CCeH	0.232	0.420	38.808	30.200
HCH	0.430	0.070	71.928	5.0330
CcCeOe	0.380	0.420	63.564	30.200
OeCcH	0.208	0.540	34.793	38.828
CeCcH	0.190	0.440	31.782	31.638
CeCcOc	0.360	0.675	60.219	48.535
CcCcCe	0.325	0.210	54.364	15.100
O23CcCe	0.300	0.625	50.182	44.940

4.1. 4000-2500 cm^{-1} region

The OH stretching modes are calculated and observed between 3578 and 3398 cm^{-1}. The intensities of these bands are weak in Raman and strong in IR. This OH stretching region is also strongly affected by the presence of the hydrogen bonds in the crystal structure.

Table 6. Final force field: force constant of the torsion coordinatesfor sucrose

Torsion	Y(mdynÅ^{-1})	Y (Kcal/mol)
C-Ccy	0.1000	3.200
C-Ocy	0.0615	1.968
Cc-Oe	0.0613	1.961
C-O23	0.0600	1.920
Ce-Oe	0.1050	3.360
Cc-Ce	0.1520	4.864

Table 7. Final force field: force constant of kappaand tension around the tetrahedral

Type	Y(mdynÅ^{-1})	Y (Kcal/mol)
Ka C6	0.045	1.44
Ka C28	0.045	1.44
Ka C29	0.045	1.44
l C-cy	0.095	3.04
l Cex	0.030	0.96

Table 8. Final force field: force constant in the hydrogen-bond potential

Type	Y(mdynÅ^{-1})	Y (Kcal/mol)
K Oc-H…O	0.248	7.936
K O-H…O	0.149	4.768
H O…H-O	0.070	2.240
H Oc…H-O	0.030	0.960
H C-O…H	0.030	0.960
H C-Oc…H	0.032	1.024
H H…O-H	0.026	0.832
Y Oc…H	0.000	0.000
Y O…H	0.000	0.000

The CH stretching region, unlike the area of OH, there bands observed intense Raman and IR low. The CH stretching modes are calculated between 3200 and 2800 cm^{-1}. In this range, we were interested in CH vibration of CH_2OH groups (symmetric and anti-symmetric vibration). The anti-symmetric modes coupled with the symmetric stretching mode of primary methylene group are calculated at 3076, 2983 and 2978 cm^{-1}.

The PEDs show that the OH and the CH stretching modes are almost pure modes.

4.2. 1900-1200 cm^{-1} region

This zone has very many bands utilizing much coupled movements, bringing into play the different deformations of CH_2OH groups, but also the angular deformations of CCH, OCH, HCH and COH type. The scissoring modes of the methylene groups are calculated at 1480, 1476 and 1437 cm^{-1} .These results are in a good agreement with those proposed by Dauchez et al.[15]. The wagging mode contributes to different calculated frequencies at 1509 and 1219 cm^{-1} .The twisting modes of the hydroxyl groups are calculated at 1509, 1166 and 1121 cm^{-1}. Other bands are calculated for sucrose, at 1597, 1543, 1531 and 1437 cm^{-1} and assigned to HCO bending deformations. Between 1600 and 1200 cm^{-1} the calculated bands due to movements of CCH andOCH.

In this region, the modes CCH and OCH are coupled between them and with other modes like the elongations of CO and the deformations of COH [28].

4.3. 1200-900 cm^{-1} region

In this region, the calculated frequencies are due to highly coupled modes that endocyclic and exocyclic CO and CCstretching vibrations with theCOH, HCO, HCH and CCH bending modes[29, 30]. The calculated frequencies at 1253 and 1240 cm^{-1} are assigned to the CO stretching modes. The obtained PED in this region are also in agreement with the assignments made previously for disaccharides[14, 15, 31].

4.4. 900-700 cm^{-1} region

This region of frequencies generally called the "fingerprint" or the anarmonic region[32] is the most discussed in the literature. The band observed at 920-915 cm^{-1} in the different disaccharides was attributed by Vasko et al.[34] to COH deformations 916 cm^{-1} correspond to the $C28-O33-H$ deformation coupled with the CO stretching mode.

The bands corresponding to the contribution of CC and CO torsional modes are calculated at 855 to 732 cm^{-1}.

4.5. 700-200 cm^{-1}and below regions

In this part of the spectrum, mainly the movement of angular deformation of the heavy atoms CCC,CCO, OCO and COC is involved. This range is characteristic of each saccharide[33] and[29]. The observed bands at 503 cm^{-1} and calculated at 502 cm^{-1} with PEDs due to deformation modes of the heavy atoms involved in the hemi-acetal group.

The domain below 100 cm^{-1} corresponds to the overall movements of the lattice due to the modes of translation (T_x, T_y, T_z) and rotation around the axes of inertias (R_a, R_b, R_c). These modes are coupled with CCC and CCO bending vibrations and to torsion around CC and CO bond. This result follows the trend previously observed in the sucrose[35].

5. Conclusions

The vibrational spectroscopic data of sucrose molecule have been well reproduced from the modified Urey-Bradley-Shimanouchi force field. In this work, the principle of transferability established by Shimanouchi has been validated since the difference between the initial and final force constants are not significant. Moreover, the force field obtained for this molecule may now be taken the study of vibrational normal modes of other molecules of bigger size and more complex structures such as the disaccharides, oligosaccharide and glycoproteins.

Table 9. Final force field: force constant in the hydrogen-bond potential

Observedfrequencies		Calculatedfrequencies (cm^{-1})		Assignements
IR	Raman	A	B	Potential energy distribution (%)
-	3578	3573	3573	77 % (O7-H19)
3563	3545	3550	3549	78 % (O30-H42)
-	3502	3499	3499	67 % (O8-H20)
-	3445	3446	3446	76 % (O10-H22)
-	3441	3445	3444	73 % (O9-H21)
-	3426	3423	3422	98 % (O32-H43)
-	3403	3402	3402	64 % (O34-H45) + 12 % (O33+H44)
3386	3398	3401	3401	65 % (O33-H44) + 12 % (O34+H45)
-	3184	3191	3191	81 % (C6-H17) + 15 % (C6+H18)
-	3127	3126	3125	26 % (C29-H40) + 20 % (C1+H12)
-	3123	3123	3123	82 % (C1-H12) + 10 % (C3+H14)
-	3118	3122	3122	45 % (C28-H39) + 11 % (C28+H38)
3074	3070	3076	3074	78 % as" + 19 % ss"
-	3053	3051	3050	59 % (C1-H16) + 13 % as' + 12 % ss"
-	3042	3043	3042	64 % (C3-H14) + 33 % (C2+H13)
3040	3030	3033	3031	36 % (C6-H18) + 12 % (C6+H17)
-	3023	3021	3023	30 % (C25-H36) + 19 % ss + 19 % ss'
3011	3017	3016	3014	67 % (C4-H15) + 10 % ss
2983	2994	2984	2985	30 % (C24-H35) + 14 % ss
2978	2976	2971	2973	25 % (C3-H14) + 21 % (C4+H15)
2958	2963	2966	2965	45 % (C28-H38) + 10 % (C28+H39)
2942	2943	2947	2976	53 % (C29-H41)
2763	2765	2760	2763	21 % (H40CH41)+ 12 % (H17C6H18) + 20 %Sci''
-	2733	2735	2744	20 % (H17C6H18)+ 12 % (H40C29H41) + 26 %Sci
2724	2723	2724	2723	19 % (H38CH39)+ 12 % (H38C28H39) + 24%Sci'
1802	1895	1900	1901	50 % (C27CO31)+ 38 % (C25O31C)
1844	1858	1852	1841	42 % (O11C1C2)+ 29 % (O11C5C4)
1919	1811	1816	1816	25 % (C24C25O)+ 28 % (C27CO31)
1766	1768	1778	1780	79 % (C27CO31)
1700	1696	1698	1700	31 % (C4C5O11)+ 24 % (C2C1O11)
1680	1676	1680	1683	96 % (C3O8H20)
1656	1652	1657	1658	72 % Wag"+26 % Twi"
1610	1612	1613	1614	34 % (C4C3H14)+ 25 % (H13C2O7)
1604	1559	1597	1601	61 % (H13C2O7)+ 15 % τ(C3-O8)
-	1546	1543	1552	52 % (OC24H35) + 18 % (HC24C25) + 17 % (C27C24H)
-	1538	1537	1536	96 % (C6O10H22)
-	1532	1531	1533	85 % (O31C25H) + 14 % (HC25C28)
-	1513	1530	1516	49 % τ(C27O32) + 33 % (HC27C24)
-	1509	1509	1512	66 % Twi"+32 % Wag"
1461	1480	1485	1584	47 % (C3C4H15) + 22 % \tau(C4-C9)
-	1476	1478	1543	56 % (H12C1C2) + 40 % (OH12C1O11)
1433	1439	1437	1436	62 % (O11C5H16) + 35 % (C6C5H16)
1420	1429	1424	1423	89 %τ(O23C26)
1411	1414	1415	1416	18 % (H16C5C4) + 23 % (H15C4HO9)
1404	1407	1413	1412	28 %τ(C3O8) + 26 % (O8C3H14) + 23 % τ(O23-C26)
-	1387	1368	1489	96 % τ(O23C26)
1378	1375	1375	1483	44 % τ(C2O7) + 28 % (H13C2C3) + 62 % (C1C2H13)
1368	1369	1360	1365	24 % (H15C4O9) + 21 % (H16C5C4) + 11 % (O11C5H16)
1348	1347	1341	1344	70 % (C24O30H)
1323	1323	1320	1320	76 % (O23C1H12) + 20 % (H12C1O11)
-	1305	1308	1310	20 % τ(O23-C26) + 18 % (O23C1H12) + 13 % (HC27C26)
1303	1295	1295	1299	32 % τ(O23C26) + 55 % (C29O34H)
-	1290	1292	1295	25 % τ(C24C30) + 18 % (HC24C25) + 16 % (C27C24H)
-	1286	1287	1289	72 % (C28O33H) + 14 % Roc'
1278	1280	1277	1280	38 % τ(O23C26)
1262	1267	1262	1266	42 % τ(O23C26)+ 23 % (HC25C28) + 15 % (O31CC29)
-	1248	1253	1255	15 % τ(C25C28)+ 10 % (C24-C25)+ 10 % (C28-O33)
-	1238	1240	1243	77 % τ(O23C26)
-	1233	1237	1236	12 % (H15C4C5) + 11 % (C5-O11)+ 10 % (C4-C5)
1238	1239	1236	1229	27 % (C27O32H)
-	1219	1219	1222	24 % Wag + 22 % (C1-C2)

-	1215	1214	1217	51 % (O31CC29)+ 36 % (C27CO23) + 18 % (C27O32H)
-	1205	1201	1210	32 % (O31CC29)+ 12 % (C11C1O23) + 18 %
1209	1208	1204	1205	89 % (O31CC29)
-	1993	1192	1196	43 % (C29-O34)
-	1182	1182	1181	40 % (O31CC29)
1172	1163	1166	1163	26 % Twi + 10 % (H15C4C5)
1161	1154	1159	1160	62 %(O23CC29)
-	1140	1141	1144	22%(C2O7H19)
1137	1137	1134	1136	15 % (C25-C28)
1129	1128	1122	1121	28 % (C6-O10)
1118	1115	1121	1122	26 % Roc +26 % Twi
1106	1106	1110	1109	30 % (C6-O10) + 17 % (C3-O8)
-	1096	1094	1098	15 % (C25-C28)
-	1083	1087	1086	44 % (O23C1H12)+ 37 %Wa
1069	1068	1075	1075	62 % (O23CC29)+ 24% (HC27C24)
-	1047	1047	1046	42 % τ(O23-C26)+10 % Ro' + 14 % (C25-C28)
1041	1043	1043	1044	10 % (C4-C5)
1038	1032	1030	1030	68 %τ(O23-C26)
-	1025	1027	1026	33 % τ(O23-C26)+ 11 % (C2-C3)+ 10 % (C5-C6)
1014	1014	1013	1014	24 % (C2-O7) + 19 % (C3-C4)
993	992	995	995	37 % (O23-C27) + 24 % (C24-O30) + 11 % (C27C24H)
970	975	975	975	25 % (C26O23C1) + 21 % (C1-O23) + 12 % (C2C1O23)
-	967	965	965	66 % Ro"+ 33 % τ(O23-C26)
-	949	959	959	22 % (O31CC29) + 11 % (C25O31C) + 21 % Ro'
943	943	942	942	51 % Ro + 25 % (C5-O11)
915	917	916	917	30 % (C26-O23)+ 13 % (C26O23C1)+ 11 % (C26-O31)
868	864	955	956	89 % τ(O23-C26)
848	849	953	954	56 % τ(O23-C26) + 17 % (C29-O34)
-	823	821	822	61 % τ(O23-C26) + 27 % (C29-O34)
794	806	800	801	65 % τ(C6-O10) + 15 % Def
-	754	748	749	60 % τ(O23-C26) + 16 % Def + 24 % (C2C1O23)
734	737	732	733	53 % τ(O23-C26) + 13 % Def
-	712	714	712	91 % (O23CC29)
684	687	689	687	79 % (O31CC29) + 21 % Def'
-	662	657	658	89 % (C27CO23)
644	640	637	637	53 %τ(C1-O23)+ 23 % Def
-	613	613	614	59 % (O31CC29) + 11 % Def'
596	586	587	588	19 %τ(C1-O23)+ 19 % τ(O23-C26) + 24 % (O31C26O)
-	578	574	576	38 % (O31C26O) + 32 % (C26O23C1) + 10 % (C2C1O23)
555	562	561	561	40 % (O31C26O) + 23 % τ(C25-O31)
524	527	530	530	22 % (O11C1O23) + 13 % (C27CO23) + 23 %τ(C25-O31)
503	502	502	509	88 % τ(C26-O31)
-	483	481	483	62 % τ(C26-O23) + 34 % τ(C26-C29)
475	476	476	476	25 % (O31CC29)
-	450	454	456	46 % (C27CO23) + 17 % (C26-O31) + 16 % τ(C25-C28)
-	-	438	439	55 %τ(C1-O23) + 40 % τ(O23-C26)
-	-	424	423	25 % (O11C1O23)
-	418	414	412	41 %τ(C26-O31) + 32 % τ(C26-O31) + 28 % (C26-C27)
-	-	393	394	34 % (C27CO23) + 24 % τ(C1-O11) + 21 % τ(C25-C28)
-	-	381	382	69 % τ(C26-O31) + 31 % τ(C1-O23)
-	368	369	370	48 % τ(C25-O31) + 18 % τ(C26-C29)+ 16 % τ(C26-O31)
-	357	361	362	30 % (C27CO23) + 28 % (C25C24O) + 25 % (O31C26O)
-	350	349	346	23 % (C26O23C1) + 29 % (O8C3C4) + 14 % (C2C3O8)
-	315	318	319	79 % (C27CO23)
-	308	309	306	88 % τ(C26-O31)
-	286	289	281	62 % τ(C26-O23) + 34 % τ(C26-C29)
-	-	276	277	25 % (O31CC29)
-	-	270	265	46 % (C27CO23) + 17 % (C26-O31) + 16 % τ(C25-C28)
-	257	253	254	55 % τ(C1-O23) + 40 % τ(O23-C26)
-	-	240	240	25 % (O11C1O23)
-	231	232	233	41 % τ(C26-O31) + 32 % τ(C26-O31) + 28 % (C26-C27)
-	-	219	227	34 % (C27CO23) + 24 % τ(C1-O11) + 21 % τ(C25-C28)
-	-	208	209	69 % τ(C26-O31) + 31 % τ(C1-O23)
-	199	195	197	48 % τ(C25-O31) + 18 %τ(C26-C29)+ 16 % τ(C26-O31)
-	-	184	185	60 % τ(C5-C6) + 25 %τ(O23-C26)

-	-	174	174	47 % τ(C4-C5) + 23 % τ (C26-O31) + 37 % τ (C27-C23)
-	-	160	165	79 % τ(O23-C26)
-	-	150	150	45 % τ (C1-O23)
-	-	139	127	20 % T_y + 10 % R_a
-	-	105	107	30 % T_y + 10 % R_a
-	-	98	97	20 % T_y + 9 % T_x
-	-	86	85	19 % R_a + 16 % R_c
-	-	57	59	22 % R_a + 13 % R_b
-	-	28	26	22 % T_z + 9 % R_b

As: antisymmetry CH_2 stretching mode; ss, symmetric CH_2 stretching mode; Sci:CH_2 scissoring mode; Wag: CH_2wagging mode; Tw: CH_2 twisting mode; Ro: CH_2 rocking mode; To: torsional modes; Def. CH_2 deformation mode; Tx, Tyand Tz are translational lattice vibrations along x, y and z crystallographic axes, respectively. Ra, Rb and Rc are rotational lattice vibrations around the principal axes a, b,c of the molecule,respectively

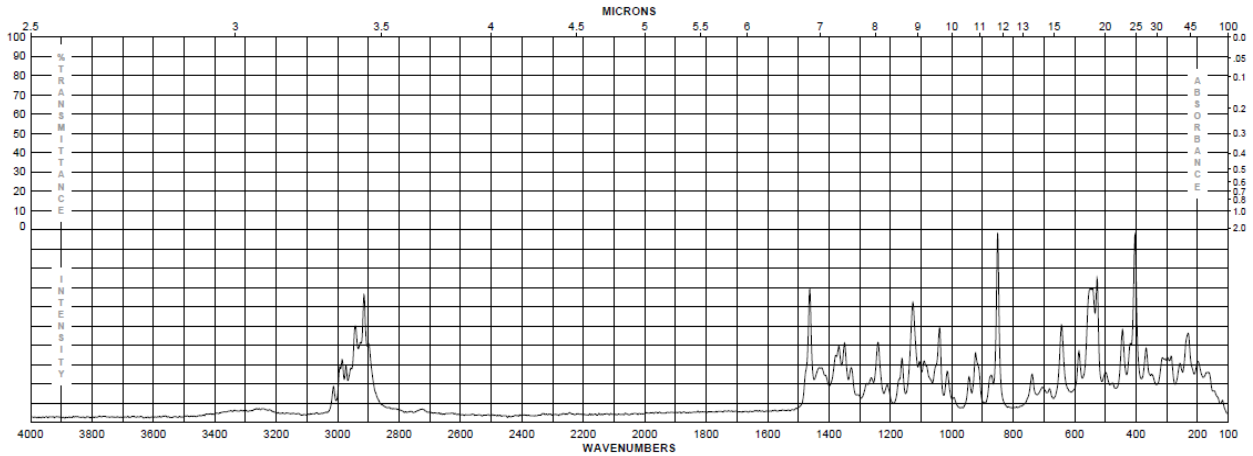

Figure 2. The Raman spectrum ofsucrose

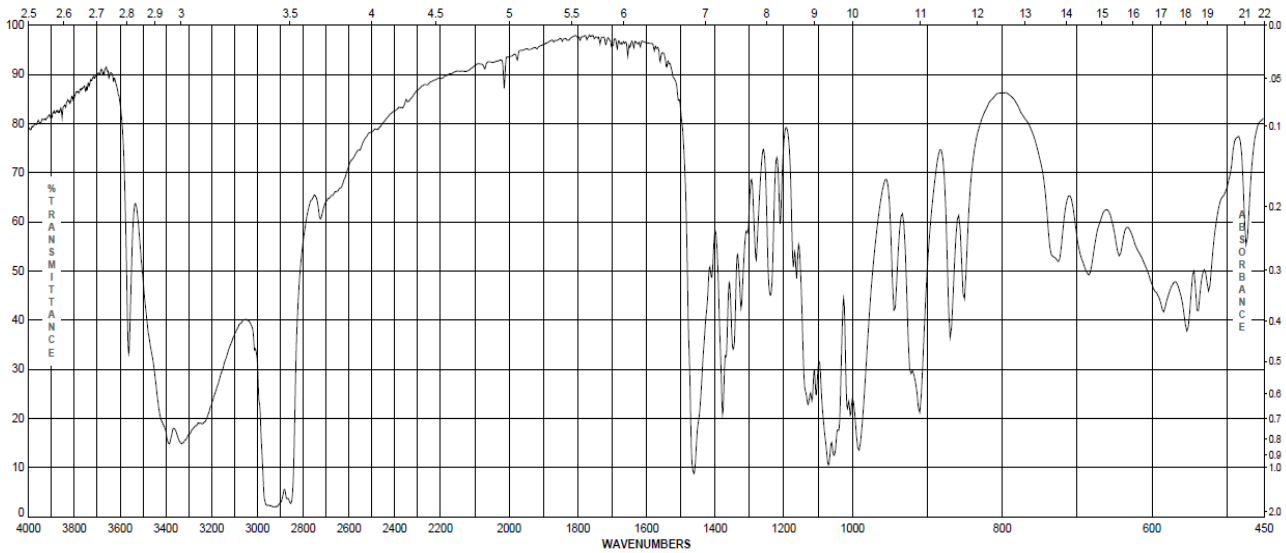

Figure 3. The IR spectrum ofsucrose

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