

Vibrational analysis of 1-bromooctane

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Fourier transform infrared and Raman spectra of the organic compound 1-bromooctane have been recorded in the range 4000-400 cm^{-1} and 3500-100 cm^{-1} , respectively. A detailed vibrational analysis in terms of assignment of the observed frequencies of this molecule for its four most probable conformations in liquid phase, having symmetries C_s and C_1 , has been done using normal co-ordinate calculations. The force-field transferred from already studied lower chain bromo-alkanes is subjected to refinement so as to fit the observed infrared and Raman frequencies with those of the calculated ones. The potential energy distribution has also been calculated for each mode of vibration of the molecule for the most probable conformations present in its liquid phase.

Keywords: FT-IR, Raman, Normal co-ordinate calculations, 1-Bromooctane

1 Introduction

1-Bromooctane (1-BMO) is a colourless and transparent liquid at ambient temperatures and has numerous synthetic applications. It is used to provide alkyl chain in the synthesis of compounds which have potential use in pharmaceuticals^{1,2}. It acts as an intermediate in polymer industry specially to provide alkyl backbone³ and has applications in the fabrication of semiconductor devices in electronic sector. It finds use in synthesizing brominated organic molecules which are used as, flame retardant in fire extinguishing media, fumigants and industrial biocides⁴. As vibrational spectroscopy plays a vital role in the characterization of drug substances in pharmaceutical industry. Therefore, keeping in view the chemical and pharmaceutical importance of 1-BMO it is considered worthwhile to carry out its vibrational analysis using normal co-ordinate calculations to get an insight into structural features, conformational state, molecular symmetry and molecular force-field of this molecule.

Normal co-ordinate calculations have been employed in the vibrational spectral analyses of polyatomic molecules during the past few decades⁵ and now-a-days are commonly used to study complex molecules⁶⁻¹². Experimental considerations alone cannot not yield the unique assignment of observed vibrational frequencies to specific modes of vibration

of complex molecules such as 1-BMO. Thus normal co-ordinate analysis is chosen as a great help in the analysis of their vibrational spectra and elucidation of their structure. Although several halo-alkanes have been studied in the past extensively by several researchers¹³⁻¹⁹, no detailed study of 1-BMO is available in literature.

In the present study, Fourier transform infrared (FT-IR) and Raman spectra of 1-BMO are recorded in its liquid state at ambient temperature. Assignments of the observed infrared and Raman bands of this molecule to various modes of vibrations for its different conformations expected to be present in the liquid state have been made using normal co-ordinate calculations.

2 Experimental Details

The spectroscopic grade pure sample of 1-BMO with stated purity of 98% has been procured from Sigma-Aldrich Company, USA and used as such without further purification. The FT-IR measurements were performed in the wavelength region 4000-400 cm^{-1} on Perkin-Elmer Spectrum RX-I Fourier transform infrared spectrometer. The resolution of spectrometer was maintained at 2 cm^{-1} . The Raman measurements were performed in the wavelength region 3500-100 cm^{-1} using a Lab Ram HR 800 Micro-Raman instrument with Argon 15 mW

(488 nm) laser as an excitation source focused into a ~ 1 micron diameter spot in a back scattering geometry, where the incident beam is linearly polarized and the spectral detection unpolarised. A Mplan 50 \times lens was used during the entire measurements and a Peltier cooled CCD for spectral detection. The overall spectral resolution was ~ 1 cm^{-1} . The FT-IR and Raman spectra of 1-BMO are shown in Figs 1 and 2(a,b), respectively.

3 Normal Co-ordinate Calculations

The normal co-ordinate calculations were carried out for the four most probable conformations of 1-BMO present in its liquid phase, as are found in several similar halogenated alkanes¹³. Among these, the most symmetric conformation I has a *trans* configuration. This conformation of 1-BMO has Br atom co-planar with C-C skeleton and belongs to C_s point group as shown in Fig. 3(a). The other conformations II, III and IV as shown in Figs 3(b, c and d) possess C_1 symmetry. In the conformation II called gauche, the Br atom lies above the C-C skeletal plane, while in the conformation III the methyl group attached to the C_7 atom has been rotated about C_6-C_7 bond to occupy the position of H_{13} . In conformation IV, the Br atom is above (or below) the C-C skeletal plane and the methyl group attached to C_7 is rotated about the C_6-C_7 bond to occupy the positions of H_{13} (or H_{14}).

The molecular parameters used are C-C = 1.54 Å, C-H = 1.09 Å, C-Br = 1.94 Å and all the bond angles assumed as 109.47°. Internal co-ordinates and symmetry co-ordinates of the molecule for the four conformations were constructed utilizing the approach of Schachtschneider and Snyder⁵.

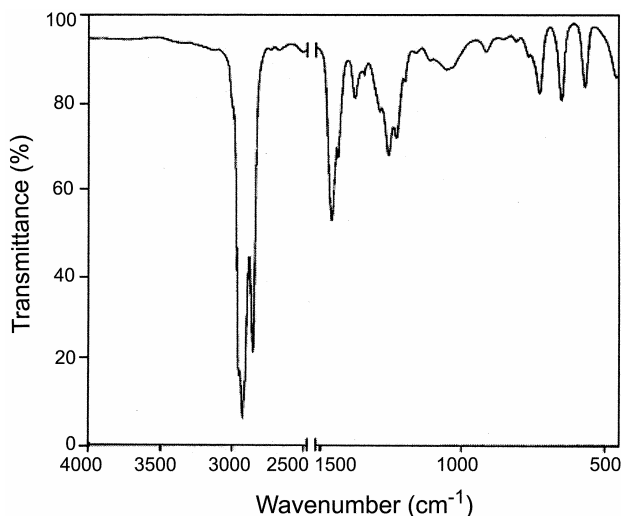


Fig. 1 — FT-IR spectrum of 1-bromooctane

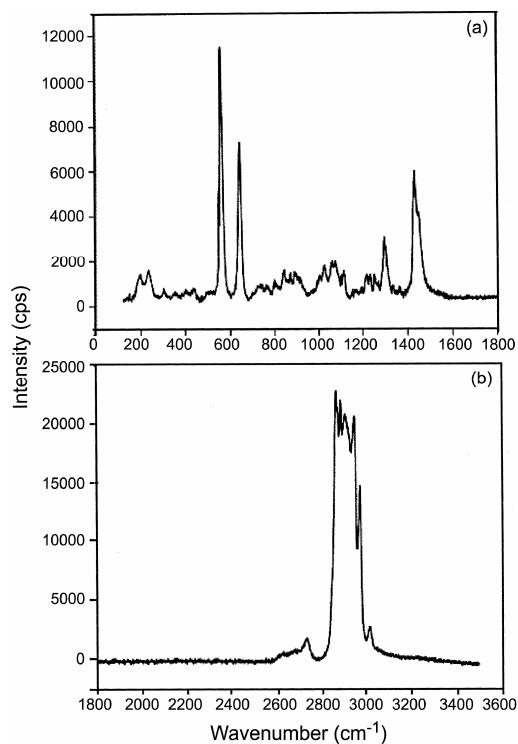


Fig. 2 — Raman spectra of 1-bromooctane (a) in the range 100-1800 cm^{-1} and (b) in the range of 1800-3500 cm^{-1}

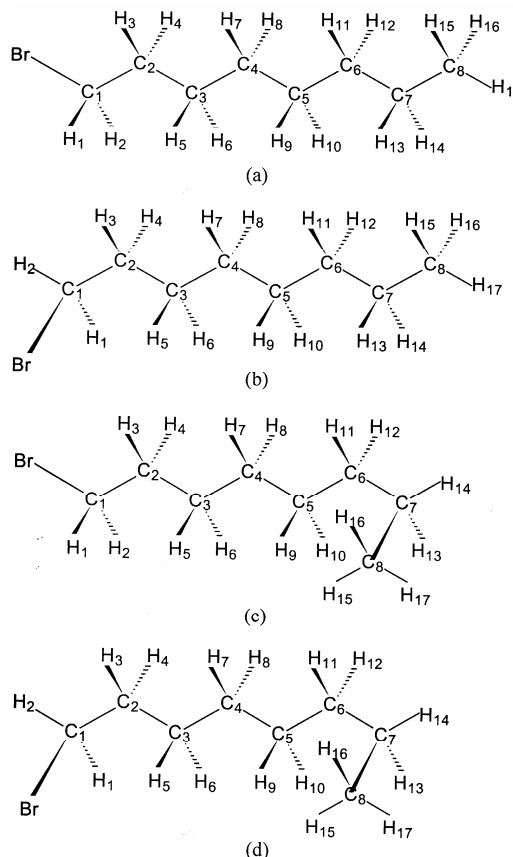


Fig. 3 — Structures of different conformers of 1-bromooctane

The total number of modes of vibration for the molecule 1-BMO corresponding to the 26 atoms present in it, is 72. The number of genuine normal modes of vibrations present in two symmetry species a' and a'' of conformation I with C_s symmetry has been calculated as 41 and 31, respectively. These modes are both Raman active as well as infrared active. For the conformations II, III and IV with symmetry C_1 all the vibrational modes belong to only one symmetry species i.e. a . These are allowed in both, infrared and Raman spectra.

The normal co-ordinate calculations were carried out utilizing a modified version of the computer program²⁰ MOLVIB. The initial force constants for 1-BMO were transferred from the study of 2-bromo-4-methylpentane²¹ and 1,2-dihaloalkanes²². The force-

field was then refined to fit the calculated frequencies with the observed frequencies for this molecule using the computer program²⁰ MOLFIT. The force-field after a number of iterations generated frequencies in close agreement with the observed ones within an average error of $\pm 5.9 \text{ cm}^{-1}$. The percentage potential energy distribution (PED) over the symmetry co-ordinates for the calculated frequencies has also been calculated. The final refined force-field of the molecule is given in Table 1.

4 Results and Discussion

The observed infrared and Raman frequencies of 1-BMO, their relative intensities and the calculated frequencies for all the four conformers and the modes of vibration along with their PED are presented in Table 2.

Table 1 — Force-constants of 1-bromooctane

Force constant	Group	Co-ordinate (s) involved	Atom (s) common	Value	Force constant	Group	Co-ordinate (s) involved	Atom (s) common	Value
Stretch					$F_{R\Xi}$	C-C-Br	CC, CCB	C-C	0.058
K_r	CH ₃	C-H	-	4.687	$F_{Br\omega}$	C-CH ₂ Br	CBr, CCC	C	-0.041
$K_r(\text{Br})$	CH ₂ Br	C-H	-	4.758	$F_{Br\xi}$	C-CH ₂ Br-C	CBr, CCH	C	0.226
K_d	CH ₂	C-H	-	4.572	$F_{Br\theta}$	CH ₂ Br	CBr, BrCH	C-Br	0.333
K_R	C-CH ₃	C-C	-	4.764	$F_{Br\Xi}$	C-CH ₂ Br	CBr, CCB	C-Br	0.601
$K_{R'}$	C-C	C-C	-	4.705	Bend-bend				
$K_R(\text{Br})$	C-C-Br	C-C	-	4.228	F_β	C-CH ₃	CCH, CCH	C-C	-0.019
K_{Br}	C-Br	C-Br	-	2.696	$F_\beta(\text{Br})$	C-CH ₂ Br	CCH, CCH	C-C	0.014
Stretch-stretch					F_γ	C-CH _{1,2} -C	CCH, CCH	C-C	-0.054
F_r	CH ₃	CH, CH	C	0.031	$F'_\gamma = F'_\xi$	C-CH _{1,2} -C	CCH, CCH	C-H	-0.019
$F_r(\text{Br})$	CH ₂ Br	CH, CH	C	-0.062	$F_{\gamma\omega}$	C-CH ₃	CCH, CCC	C-C	0.016
F_d	CH ₂	CH, CH	C	0.0009	$F_{\gamma\omega'}$	C-CH _{1,2} -C	CCH, CCC	C-C	0.042
F_R	C-C-C	CC, CC	C	0.511	$F_{\gamma\omega''}$	C-CH ₂ Br	CCH, CCC	C-C	0.066
$F_d(\text{Br})$	C-C-C	CC, CC	C	0.348	F_θ	C-CH ₂ Br	BrCH, BrCH	C-Br	-0.025
$F_{R'}$	C-C-C	CC, CC	C	0.407	F_ω	C-C-C	CCC, CCC	C	0.110
F_{RBr}	C-C-Br	CC, CBr	C	0.585	$F_{\gamma\theta}$	C-CH ₂ Br	CCH, BrCH	C-H	0.025
Bend					$F_{\Xi\theta}$	C-CH ₂ Br	CBr, BrCH	C-Br	0.048
H_α	CH ₃	HCH	-	0.537	f^t_β	C-CH ₃	HCC, CCH	C-C	0.049
$H_\alpha(\text{Br})$	CH ₂ Br	HCH	-	0.510	f^g_β	C-CH ₃	HCC, CCH	C-C	0.011
H_δ	CH ₂	HCH	-	0.552	f^t_γ	CH _{1,2} -CH _{2,3}	HCC, CCH	C-C	0.020
H_β	CH ₃	CCH	-	0.614	f^g_γ	CH _{1,2} -CH _{2,3}	HCC, CCH	C-C	-0.010
$H_\beta(\text{Br})$	C-CH ₂ Br	CCH	-	0.579	$f^t_{\gamma\omega}$	C*-CH _{1,2} C*H _{2,3}	HCC*, CCH	C	0.088
H_γ	C-CH ₂ -C	CCH	-	0.634	$f^g_{\gamma\omega}$	C*-CH _{1,2} C*H _{2,3}	HCC*, CCH	C	0.048
H_θ	CH ₂ Br	BrCH	-	0.668	$f^t_{\gamma\omega\omega}$	C-CH ₂ -CH ₂ -C	CCC, CCH	C-C	0.049
H_ω	C-C-C	CCC	-	1.378	$f^g_{\gamma\omega\omega}$	C-CH ₂ -CH ₂ -C	CCC, CH	C-C	-0.135
H_Ξ	C-C-Br	CCBr	-	0.954	f^t_{ω}	C-CH ₂ -CH ₂ -C	CCC, CCC	C-C	-0.024
Stretch-bend					f^g_{ω}	C-CH ₂ -CH ₂ -C	CCC, CCC	C-C	0.011
$F_{R\beta}$	C-CH ₃	CC, CCH	C-C	0.325	$f^t_{\omega\Xi}$	C-C-C-Br	CCC, CCB	C-C	0.042
$F_{R\beta}(\text{Br})$	C-CH ₂ Br	CC, CCH	C-C	0.413	$f^g_{\omega\Xi}$	C-C-C-Br	CCC, CCB	C-C	-0.014
$F_{R\gamma}$	C-CH ₂ -C	CC, CCH	C-C	0.425	$f^t_{\gamma\Xi}$	Br-CH ₂ -CH ₂ -C	HCC, CCB	C-C	0.041
$F'_{R\gamma}$	C-CH ₂ -C	CC, CCH	C	0.053	$f^g_{\gamma\Xi}$	Br-CH ₂ -CH ₂ -C	HCC, CCB	C-C	0.044
$F_{R\omega}$	C-CH ₃	CC, CCC	C-C	0.661	Torsion				
$F_{R\omega}(\text{Br})$	C-C-C	CC, CCC	C-C	0.502	H_ζ	C-C	C-C	-	0.0095
$F_{R\omega'}$	C-C-C	CC, CCC	C-C	0.423					

Stretching constants are in units of $\text{mdyn } \text{\AA}^{-1}$, stretch-bend constants are in units of $\text{mdyne } \text{\AA} \text{ rad}^{-2}$.

Table 2 — Observed and calculated frequencies, modes of vibrations and potential energy distribution of 1-BMO^a

Observed frequencies (cm ⁻¹)		Calculated frequencies (cm ⁻¹)	Modes of vibrations and PED (%)
Infrared	Raman		
1-Bromooctane (I) C _s <i>a'</i> symmetry species			
2960 vvs	2961 vs	2961	CH ₃ as(99)
	2894 vvs	2896	CH ₂ Brss(98)
	2872 vvs	2972	CH ₃ ss(92)
	2872 vvs	2870	CH ₂ ss(27) CH ₂ ss(26) CH ₂ ss(18) CH ₂ ss(15)
		2866	CH ₂ ss(28) CH ₂ ss(27) CH ₂ ss(17) CH ₂ ss(14)
2858 vvs		2862	CH ₂ ss(28) CH ₂ ss(25) CH ₂ ss(19) CH ₂ ss(15)
2858 vvs		2858	CH ₂ ss(28) CH ₂ ss(27) CH ₂ ss(19) CH ₂ ss(15)
2858 vvs		2856	CH ₂ ss(27) CH ₂ ss(26) CH ₂ ss(20) CH ₂ ss(16)
	2852 vvs	2855	CH ₂ ss(28) CH ₂ ss(27) CH ₂ ss(18) CH ₂ ss(16)
1461 vvs		1462	CH ₃ aδ (78) CH ₂ δ(12)
	1456 vs sh	1458	CH ₂ δ(74) R ₃ (17)
	1436 vvs	1448	CH ₂ δ(67) R ₆ (16) CH ₃ aδ (14)
1431 w sh		1428	CH ₂ δ(29) CH ₂ δ(27) CH ₂ δ(14) CH ₂ δ(11)
1431 w sh		1425	CH ₂ δ(42) CH ₂ δ(37)
		1422	CH ₂ δ(42) CH ₂ δ(39)
		1420	CH ₂ δ(28) CH ₂ δ(27) CH ₂ δ(15)
		1413	CH ₂ Brδ(71) R ₁ (20)
1377 ms		1382	CH ₂ w(26) CH ₂ w(26) CH ₂ w(26)
1377 ms		1379	CH ₂ w(52) CH ₂ w(33) CCs(10)
	1365 vw	1361	CH ₂ w(33) CH ₂ w(33)
1340 w		1344	CH ₃ sδ(83)
	1337 vw	1328	CH ₂ w(17) CH ₂ w(13) CH ₂ w(11) CH ₃ sδ(11)
	1301 vs	1299	CH ₂ w(28)
		1204	CH ₂ Brw(81) CH ₂ w(13)
	1172 vvw	1176	CH ₂ w(43) CH ₃ r(17) CCs(15)
		1124	CH ₂ w(46) CH ₂ w(12) CCs(11) CH ₂ w(10)
	1077 ms	1075	CCs(29) CCs(26) CCs(15) CCs(15)
	1077 ms	1072	CCs(45) CCs(20) CCs(15) CCs(10)
1051 m		1055	CCs(59) CCs(16) CCs(11)
	1029 m	1032	CCs(67) CCs(22) CCs(12)
1022 w		1019	CCs(57) CCs(10)
		976	CCs(88) CCs(16) CH ₂ w(10)
911 m	910 vw	910	CH ₃ r(53) CCs(35) CH ₂ w(14)
647 vvs	646 vvs	646	CBrδ(77) CCCδ(17) CCBrd(10)
	495 vvw	491	CCCδ(24) CCCδ(23) CCCδ(20) CCCδ(12) CH ₂ w(11)
	438 w	428	CCCδ(42) CCCδ(25) CCCδ(15) CH ₂ w(13) CCCδ(10)
		362	CCCδ(21) CCBrd(13) CCCδ(11) CCCδ(10) CCs(10)
		289	CCCδ(33) CCCδ(20) CCCδ(17) CCCδ(16) CCBrd(11)
	198 s	191	CCCδ(21) CCCδ(15) CBrδ(12) CCCδ(10)
		144	CCBrδ(34) CCCδ(22) CCCδ(15) CCCδ(10)
		60	CCCδ(31) CCCδ(23) CCCδ (17) CCCδ(15) CCBrd(14)
<i>a''</i> symmetry species			
	3009 m	3009	CH ₂ Bras(100)
2960 vvs	2961 vs	2961	CH ₃ as(98)
	2934 vs	2940	CH ₂ as(28) CH ₂ as(28) CH ₂ as(17) CH ₂ as(17)
	2934 vs	2938	CH ₂ as(28) CH ₂ as(28) CH ₂ as(15) CH ₂ as(15)
	2934 vs	2935	CH ₂ as(25) CH ₂ as(25) CH ₂ as(18) CH ₂ as(17)
2928 vvs		2932	CH ₂ as(28) CH ₂ as(27) CH ₂ as(19) CH ₂ as(18)
2928 vvs		2929	CH ₂ as(26) CH ₂ as(25) CH ₂ as(20) CH ₂ as(19)
2928 vvs		2927	CH ₂ as(26) CH ₂ as(25) CH ₂ as(18) CH ₂ as(17)
1461 vvs		1459	CH ₃ aδ (93)
	1301 vs	1299	CH ₂ t(31) CH ₂ t(26) CH ₂ t(22) CH ₂ t(15)
		1297	CH ₂ t(37) CH ₂ t(25) CH ₂ t(18)
1288 m		1281	CH ₂ t(33) CH ₂ t(31) CH ₂ t(16) CH ₂ t(14)

Contd

Table 2 — Observed and calculated frequencies, modes of vibrations and potential energy distribution of 1-BMO^a — *Contd*

Observed frequencies (cm ⁻¹)		Calculated frequencies (cm ⁻¹)	Modes of vibrations and PED (%)
Infrared	Raman		
1258 vs		1262	CH ₂ t(20) CH ₂ t(16) CH ₂ t(16) CH ₂ t(16) CH ₂ t(10)
	1220 m	1218	CH ₂ t(69)
	1196 w	1199	CH ₂ Br(79) CH ₂ t(18)
1188 vw		1183	CH ₂ t(52) CH ₂ Br(15)
	1077 ms	1077	CH ₃ r(35) CH ₂ r(21) CH ₂ r(14)
	1006 w	1006	CH ₂ r(20) CH ₂ r(19) CH ₃ r(15) CH ₂ r(12) CH ₂ r(10)
		931	CH ₂ r(22) CH ₂ r(18) CH ₂ r(14) CH ₂ Brr(13) CH ₃ r(13)
	873 w	856	CH ₂ r(21) CH ₂ r(19) CH ₂ Brr(16) CH ₃ r(12) CH ₂ r(12)
		788	CH ₂ r(25) CH ₂ r(24) CH ₂ r(24) CH ₂ Brr(16)
	736 vw	734	CH ₂ r(26) CH ₂ r(24) CH ₂ r(16) CH ₂ Brr(14) CH ₂ r(14)
	701 vw	699	CH ₂ r(29) CH ₂ r(28) CH ₂ Brr(12) CH ₂ r(12) CH ₂ r(11) CH ₂ r(10)
		681	CH ₂ r(37) CH ₂ Brr(24) CH ₂ r(22) CH ₂ r(12)
		78	CH ₃ τ(96)
		51	CCτ(35) CCτ(23) CCτ(17) CH ₂ Brr(11) CCτ(11)
		48	CCτ(32) CCτ(27) CCτ(23) CCτ(11)
		38	CCτ(46) CH ₂ Brr(29) CCτ(17)
		29	CCτ(49) CCτ(31) CH ₂ Br(13)
		20	CCτ(35) CCτ(24) CH ₂ Brr(24) CCτ(10)
		10	CCτ(33) CH ₂ Brr(18) CCτ(17) CCτ(14) CCτ(12)
1-Bromooctane (II) C ₁ 'a' symmetry species			
	3009 m	3009	CH ₂ Bras(100)
2960 vvs	2961 vs	2961	CH ₃ as(99)
2960 vvs	2961 vs	2961	CH ₃ as(98)
	2934 vs	2940	CH ₂ as(28) CH ₂ as(27) CH ₂ as(18) CH ₂ as(17)
	2934 vs	2938	CH ₂ as(28) CH ₂ as(28) CH ₂ as(17) CH ₂ as(15)
	2934 vs	2935	CH ₂ as(26) CH ₂ as(25) CH ₂ as(18) CH ₂ as(17)
2928 vvs		2932	CH ₂ as(27) CH ₂ as(27) CH ₂ as(19) CH ₂ as(18)
2928 vvs		2929	CH ₂ as(26) CH ₂ as(26) CH ₂ as(20) CH ₂ as(19)
2928 vvs		2927	CH ₂ as(26) CH ₂ as(26) CH ₂ as(18) CH ₂ as(18)
	2894 vvs	2896	CH ₂ Brss(99)
	2872 vvs	2972	CH ₃ ss(92)
	2872 vvs	2870	CH ₂ ss(27) CH ₂ ss(27) CH ₂ ss(17) CH ₂ ss(16)
		2865	CH ₂ ss(28) CH ₂ ss(28) CH ₂ ss(15) CH ₂ ss(14)
2858 vvs		2861	CH ₂ ss(25) CH ₂ ss(25) CH ₂ ss(17) CH ₂ ss(17)
2858 vvs		2858	CH ₂ ss(28) CH ₂ ss(28) CH ₂ ss(18) CH ₂ ss(17)
2858 vvs		2856	CH ₂ ss(26) CH ₂ ss(25) CH ₂ ss(20) CH ₂ ss(19)
	2852 vvs	2855	CH ₂ ss(27) CH ₂ ss(26) CH ₂ ss(18) CH ₂ ss(17)
1461 vvs		1462	CH ₃ aδ (78) CH ₂ δ(12)
	1456 vs sh	1459	CH ₃ aδ (93)
	1456 vs sh	1452	CH ₂ δ(75) R ₃ (18)
	1436 vvs	1448	CH ₂ δ(67) R ₆ (16) CH ₃ aδ (14)
1431 w sh		1428	CH ₂ δ(29) CH ₂ δ(27) CH ₂ δ(13) CH ₂ δ(12)
1431 w sh		1425	CH ₂ δ(40) CH ₂ δ(40)
		1422	CH ₂ δ(43) CH ₂ δ(40)
		1420	CH ₂ δ(28) CH ₂ δ(27) CH ₂ δ(12) CH ₂ δ(12)
		1415	CH ₂ Brδ(73) R ₁ (21)
1377 ms		1381	CH ₂ w(32) CH ₂ w(30) CH ₂ w(19)
1377 ms		1380	CH ₂ w(56) CH ₂ w(27)
		1358	CH ₂ w(35) CH ₂ w(30) CH ₃ sδ(14)
1340 w		1343	CH ₃ sδ(82)
	1337 vw	1327	CH ₂ w(21) CH ₂ w(13) CH ₂ w(12)
	1301 vs	1302	CH ₂ w(22)
	1301 vs	1298	CH ₂ t(25) CH ₂ t(19) CH ₂ t(18) CH ₂ t(16)
		1296	CH ₂ t(32) CH ₂ t(31) CH ₂ t(12) CH ₂ t(12)

Contd —

Table 2 — Observed and calculated frequencies, modes of vibrations and potential energy distribution of 1-BMO^a — *Contd*

Observed frequencies (cm ⁻¹)		Calculated frequencies (cm ⁻¹)	Modes of vibrations and PED (%)
Infrared	Raman		
1288 m		1281	CH ₂ t(33) CH ₂ t(31) CH ₂ t(15) CH ₂ t(14)
1258 vs		1262	CH ₂ t(20) CH ₂ t(16) CH ₂ t(16) CH ₂ t(15) CH ₂ t(15)
1232 m sh	1236 m	1239	CH ₂ Brw (47) CH ₂ Br(10)
	1220 m	1218	CH ₂ t(68)
	1196 w	1203	CH ₂ Br(70) CH ₂ t(13)
1188 vw		1179	CH ₂ t(39) CH ₂ w(11)
	1172 vvw	1173	CH ₂ w(31) CH ₃ r(15) CCs(13) CH ₂ t(10)
	1117 m	1114	CH ₂ w(39) CH ₂ w(10)
	1077 ms	1076	CH ₃ r(35) CH ₂ r(21) CH ₂ r(13)
	1077 ms	1073	CCs(50) CCs(16) CCs(11)
	1077 ms	1070	CCs(59) CCs(17) CCs(10)
1051 m		1055	CCs(63) CCs(13) CCs(10)
	1029 m	1034	CCs(54) CCs(23) CCs(18) CCs(12)
1022 w		1015	CCs(52) CCs(11) CCs(11)
	1006 w	1001	CH ₂ r(19) CH ₂ r(17) CH ₃ r(14) CH ₂ r(11)
		973	CCs(70) CCs(13)
	917 vvw	917	CH ₂ r(19) CH ₂ r(16) CH ₂ r(14) CH ₂ r(14) CH ₃ r(12)
	894 m	909	CH ₃ r(49) CCs(32) CH ₂ w(14)
	846 m	843	CH ₂ r(21) CH ₂ r(21) CH ₂ r(16) CH ₂ r(11) CH ₃ r(11) CH ₂ r(11)
		786	CH ₂ Br(35) CH ₂ r(18) CH ₂ r(17) CH ₂ r(16)
		754	CH ₂ Br(32) CH ₂ r(17) CH ₂ r(12)
724 vvs	723 vvw	718	CH ₂ r(25) CH ₂ r(24) CH ₂ r(20) CH ₂ r(14)
		692	CH ₂ r(29) CH ₂ r(28) CH ₂ r(19) CH ₂ r(15)
565 vvs	564 vvs	565	CBr(89) CCBrd(13)
	495 vvw	491	CCCδ(19) CCCδ(14) CCCδ(11) CBr(11)
	473 vvw	470	CCCδ(32) CCCδ(25) CCCδ(17) CCCδ(16) CH ₂ w(11)
	356 w	354	CCCδ(31) CCCδ(24) CCCδ(17) CCCδ(14) CCCδ(10)
	304 ms	305	CCCδ(18) CCCδ(11) CCs(11)
		226	CCCδ(36) CCCδ(31) CCBrd(19) CCCδ(12)
		181	CCBrδ(35) CCCδ(29)
		92	CCCδ(33) CCCδ(32) CCCδ(19) CCCδ(16)
		78	CH ₃ τ(96)
		50	CCτ(37) CCτ(29) CCτ(18)
		45	CCτ(40) CCτ(28) CCτ(15) CCτ(10)
		34	CCτ(47) CH ₂ Br(22) CCτ(13) CCτ(10)
		24	CCτ(35) CCτ(28) CH ₂ Br(18)
		14	CH ₂ Brτ(45) CCτ(25)
		10	CCτ(34) CCτ(33) CCτ(13)
1-Bromooctane (III) C ₁ 'a' symmetry species			
	3009 m	3009	CH ₂ Bras(100)
2960 vvs	2961 vs	2961	CH ₃ as(97)
2960 vvs	2961 vs	2961	CH ₃ as(96)
	2934 vs	2940	CH ₂ as(30) CH ₂ as(28) CH ₂ as(19) CH ₂ as(15)
	2934 vs	2938	CH ₂ as(30) CH ₂ as(28) CH ₂ as(17) CH ₂ as(11)
	2934 vs	2935	CH ₂ as(40) CH ₂ as(20) CH ₂ as(15) CH ₂ as(12)
2928 vvs		2932	CH ₂ as(39) CH ₂ as(20) CH ₂ as(20) CH ₂ as(15)
2928 vvs		2930	CH ₂ as(26) CH ₂ as(24) CH ₂ as(23) CH ₂ as(20)
2928 vvs		2927	CH ₂ as(31) CH ₂ as(27) CH ₂ as(22) CH ₂ as(12)
	2894 vvs	2896	CH ₂ Brss(98)
	2872 vvs	2972	CH ₃ ss(96)
	2872 vvs	2869	CH ₂ ss(32) CH ₂ ss(25) CH ₂ ss(24)
		2864	CH ₂ ss(26) CH ₂ ss(25) CH ₂ ss(23) CH ₂ ss(22)
2858 vvs		2860	CH ₂ ss(34) CH ₂ ss(22) CH ₂ ss(20) CH ₂ ss(20)
2858 vvs		2859	CH ₂ ss(59) CH ₂ ss(14) CH ₂ ss(13) CH ₂ ss(10)

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Table 2 — Observed and calculated frequencies, modes of vibrations and potential energy distribution of 1-BMO^a — *Contd*

Observed frequencies (cm ⁻¹)		Calculated frequencies (cm ⁻¹)	Modes of vibrations and PED (%)
Infrared	Raman		
2858 vvs		2857	CH ₂ ss(25) CH ₂ ss(25) CH ₂ ss(24) CH ₂ ss(23)
	2852 vvs	2855	CH ₂ ss(34) CH ₂ ss(26) CH ₂ ss(24)
1461 vvs		1465	CH ₃ aδ (48) CH ₂ δ(38)
	1456 vs sh	1459	CH ₃ aδ (92)
	1456 vs sh	1458	CH ₂ δ(74) R ₃ (17)
	1456 vs sh	1454	CH ₃ aδ (44) CH ₂ δ(41)
	1436 vvs	1434	CH ₂ δ(65) R ₄ (13)
1431 w sh		1425	CH ₂ δ(46) CH ₂ δ(35) R ₇ (10)
1431 w sh		1424	CH ₂ δ(62) R ₅ (13) CH ₂ δ(11)
		1420	CH ₂ δ(36) CH ₂ δ(25) CH ₂ δ(12)
		1413	CH ₂ Brsδ(71) R ₁ (20)
1377 ms		1380	CH ₂ w(36) CH ₂ w(18) CH ₂ w(16) CH ₂ w(15)
1377 ms		1378	CH ₂ w(45) CH ₂ w(41)
		1357	CH ₂ w(32) CH ₂ w(23)
1340 w		1343	CH ₃ sδ(99)
		1317	CH ₂ w(17) CH ₂ w(16)
	1301 vs	1304	CH ₂ t(56) CH ₂ t(27)
	1301 vs	1298	CH ₂ t(47) CH ₂ t(41)
1288 m		1284	CH ₂ t(41) CH ₂ t(19) CH ₂ t(18) CH ₂ t(13)
	1273 vw	1271	CH ₂ t(26) CH ₂ t(21) CH ₂ t(12) CH ₂ t(11)
	1255 m	1250	CH ₂ t(30) CH ₂ t(19)
		1206	CH ₂ w(58) CH ₂ Brw(22)
		1204	CH ₂ Brw(60) CH ₂ w(21) CH ₂ w(11)
	1196 w	1199	CH ₂ Br(79) CH ₂ t(17)
1188 vw		1184	CH ₂ t(51) CH ₂ Br(15)
	1166 vw	1169	CH ₂ t(20) CH ₂ w(20) CH ₂ w(15) CH ₂ w(10)
	1117 m	1121	CH ₂ w(29) CCs(23)
1111 w		1108	CCs(23) CCs(21) CH ₂ w(11)
	1063 ms	1067	CCs(17) CCs(12) CH ₂ r(10)
	1063 ms	1062	CCs(51) CCs(37)
1051 m		1055	CCs(52) CCs(26) CCs(10)
	1029 m	1037	CCs(22) CCs(21) CH ₃ r(13) CH ₂ w(10)
	993 vw	999	CCs(32) CH ₂ r(17) CH ₂ r(14) CH ₂ r(11)
	993 vw	994	CCs(25) CCs(21) CH ₃ r(14)
		975	CCs(71) CCs(10) CCs(10)
		930	CH ₂ r(22) CH ₂ r(18) CCs(13) CH ₂ Brr(12) CH ₂ r(12)
	917 vvw	915	CH ₃ r(45) CCs(36)
849 w		851	CH ₂ r(23) CH ₂ r(22) CH ₂ Brr(18) CH ₂ r(13)
805 w	802 w	791	CH ₂ r(48) CH ₃ r(18)
764 m	763 w	761	CH ₂ r(24) CH ₂ r(20) CH ₂ Brr(16) CH ₂ r(12) CH ₂ r(11)
	701 vw	708	CH ₂ r(35) CH ₂ r(28) CH ₂ Brr(17)
		681	CH ₂ r(39) CH ₂ Brr(26) CH ₂ r(22) CH ₂ r(11)
647 vvs	646 vvs	646	CBr(76) CCCδ(17) CCBrd(10)
	495 vvw	485	CCCδ(32) CCCδ(30) CCCδ(14) CCCδ(10)
		414	CCCδ(27) CCCδ(13) CCCδ(12) CCBrd(11)
	404 w	407	CCCδ(22) CCCδ(22) CCCδ(20) CCCδ(10)
		283	CCCδ(34) CCCδ(18) CCBrd(17) CCCδ(12)
		227	CCCδ(35) CCCδ(33) CBr(15)
		153	CCBrδ(30) CCCδ(19) CCCδ(14) CCCδ(13)
		77	CH ₃ τ(49) CCCδ(20) CCCδ(11) CCBrd(11)
		67	CH ₃ τ(48) CCCδ(17) CCCδ(12)
		50	CCτ(36) CCτ(19) CH ₂ Brr(15) CCτ(15) CCτ(14)
		47	CCτ(38) CCτ(23) CCτ(22)
		35	CCτ(51) CCτ(23) CH ₂ Brr(21)

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Table 2 — Observed and calculated frequencies, modes of vibrations and potential energy distribution of 1-BMO^a — *Contd*

Observed frequencies (cm ⁻¹)		Calculated frequencies (cm ⁻¹)	Modes of vibrations and PED (%)
Infrared	Raman		
		27	CCτ(50) CH ₂ Brτ(32) CCτ(12)
		19	CCτ(46) CCτ(26) CCτ(19)
		9	CCτ(41) CH ₂ Brτ (24) CCτ(22)
1-Bromooctane (IV) C ₁			
<i>'a' symmetry species</i>			
	3009 m	3009	CH ₂ Bras(100)
2960 vvs	2961 vs	2961	CH ₃ as(97)
2960 vvs	2961 vs	2961	CH ₃ as(96)
	2934 vs	2940	CH ₂ as(30) CH ₂ as(27) CH ₂ as(20) CH ₂ as(14)
	2934 vs	2938	CH ₂ as(30) CH ₂ as(27) CH ₂ as(18) CH ₂ as(12)
	2934 vs	2935	CH ₂ as(38) CH ₂ as(21) CH ₂ as(16) CH ₂ as(11)
2928 vvs		2933	CH ₂ as(41) CH ₂ as(20) CH ₂ as(19) CH ₂ as(14)
2928 vvs		2930	CH ₂ as(25) CH ₂ as(24) CH ₂ as(22) CH ₂ as(22)
2928 vvs		2927	CH ₂ as(32) CH ₂ as(26) CH ₂ as(23) CH ₂ as(10)
	2894 vvs	2896	CH ₂ Brss(99)
	2872 vvs	2972	CH ₃ ss(96)
	2872 vvs	2869	CH ₂ ss(33) CH ₂ ss(26) CH ₂ ss(24)
		2864	CH ₂ ss(28) CH ₂ ss(27) CH ₂ ss(22) CH ₂ ss(20)
2858 vvs		2860	CH ₂ ss(43) CH ₂ ss(18) CH ₂ ss(17) CH ₂ ss(17)
2858 vvs		2859	CH ₂ ss(50) CH ₂ ss(17) CH ₂ ss(17) CH ₂ ss(14)
2858 vvs		2857	CH ₂ ss(28) CH ₂ ss(25) CH ₂ ss(23) CH ₂ ss(22)
	2852 vvs	2855	CH ₂ ss(32) CH ₂ ss(25) CH ₂ ss(24)
1461 vvs		1465	CH ₃ aδ(48) CH ₂ δ(38)
	1456 vs sh	1459	CH ₃ aδ(92)
	1456 vs sh	1454	CH ₃ aδ(44) CH ₂ δ(41)
	1456 vs sh	1452	CH ₂ δ(76) R ₃ (18)
	1436 vvs	1434	CH ₂ δ(64) R ₄ (13)
1431 w sh		1425	CH ₂ δ(49) CH ₂ δ(32) R ₇ (10)
1431 w sh		1424	CH ₂ δ(62) R ₅ (13) CH ₂ δ(12)
		1420	CH ₂ δ(34) CH ₂ δ(25) CH ₂ δ(15)
		1415	CH ₂ Brδ(73) R ₁ (21)
1377 ms		1379	CH ₂ w(38) CH ₂ w(32) CH ₂ w(13)
1377 ms		1379	CH ₂ w(57) CH ₂ w(24) CH ₂ w (10)
		1353	CH ₂ w(37) CH ₂ w(21) CH ₃ sδ(10)
1340 w		1343	CH ₃ sδ(94)
		1318	CH ₂ w(30) CH ₂ Brw (12) CH ₂ w(12)
	1301 vs	1304	CH ₂ t(56) CH ₂ t(27)
	1301 vs	1298	CH ₂ t(48) CH ₂ t(39)
1288 m		1284	CH ₂ t(42) CH ₂ t(18) CH ₂ t(18) CH ₂ t(12)
	1273 vw	1271	CH ₂ t(26) CH ₂ t(24) CH ₂ t(10)
	1255 m	1251	CH ₂ t(25) CH ₂ t(20)
1232 m sh	1236 m	1240	CH ₂ Brw (45) CH ₂ Brτ(10)
		1206	CH ₂ w(60) CH ₂ t(14) CH ₂ Brτ(12)
	1196 w	1203	CH ₂ Brτ(59) CH ₂ w(20)
	1172 vvw	1179	CH ₂ t(45) CH ₂ Brτ(10)
1155 w	1154 w	1164	CH ₂ w(19) CH ₂ w(18)
	1117 m	1118	CCs(33) CH ₂ w(17) CH ₃ r(12)
1111 w		1103	CH ₂ w(20) CCs(18) CH ₃ r(12) CCs(11)
	1063 ms	1067	CCs(31) CCs(10)
	1063 ms	1063	CCs(46) CCs(32)
1051 m		1048	CCs(26) CCs(25) CCs(23)
	1029 m	1033	CCs(40) CH ₃ r(12)CH ₂ w(12)
	1006 w	1003	CCs(40) CCs(30) CH ₃ r(15)
	993 vw	994	CCs(33) CH ₂ r(15) CH ₂ r(15)
		965	CCs(47) CCs(15) CH ₃ r(10)

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Table 2 — Observed and calculated frequencies, modes of vibrations and potential energy distribution of 1-BMO^a — *Contd*

Observed frequencies (cm ⁻¹)		Calculated frequencies (cm ⁻¹)	Modes of vibrations and PED (%)
Infrared	Raman		
	917 vvw	916	CH ₃ r(34) CCs(16) CH ₂ r(10)
	917 vvw	915	CCs(21) CCs(14) CH ₃ r(12) CH ₂ r(10)
		838	CH ₂ r(23) CH ₂ r(22) CH ₂ r(19) CH ₂ Brr(11)
		788	CH ₂ r(44) CH ₃ r(16) CH ₂ Brr(13)
764 m	763 w	769	CH ₂ Brr(42) CH ₂ r(12) CH ₂ r(10)
	736 vw	736	CH ₂ r(23) CH ₂ r(23) CH ₂ r(16) CH ₂ Brr(13) CH ₂ r(12)
	701 vw	697	CH ₂ r(36) CH ₂ r(26) CH ₂ r(25)
565 vvs	564 vvs	565	CBrS(87)
	495 vvw	501	CCCδ(17) CCCδ(16) CCCδ(14) CCCδ(14) CBrS(12) CCCδ(11)
	455 vvw	450	CCCδ(34) CCCδ(20) CCCδ(17) CCCδ(15)
	384 vvw	374	CCCδ(38) CCCδ(20) CCCδ(14)
		328	CCCδ(33) CCBrd(17)
	235 s	235	CCCδ(40) CCCδ(33) CCCδ(12) CCCδ(10) CCs(10)
	198 s	192	CCBrδ(51) CCCδ(25)
		114	CCCδ(39) CCCδ(26) CCCδ(24)
		71	CH ₃ τ(93)
		48	CCτ(39) CCτ(22) CCτ(21)
		43	CCτ(36) CCτ(35) CCτ(12) CCτ(11)
		32	CCτ(60) CCτ(26)
		24	CH ₂ Brrτ(47) CCτ(35)
		12	CCτ(43) CCτ(32) CCτ(12)
		11	CCτ(36) CH ₂ Brrτ(27) CCτ(21)

^a Very very strong (vvs), very strong (vs), strong (s), medium (m), weak (w), very weak (vw), shoulder (sh), asymmetric stretch (as), symmetric stretch (ss), stretch (s), asymmetric bending (aδ), symmetric bending (sδ), wagging (w), twisting (t), rocking (r), torsional (τ).

The assignments of the observed frequencies to different modes of vibration have been made on the basis of normal co-ordinate calculations and the PED. Table 2 clearly depicts that while most of the prominent infrared and Raman bands could be correlated with the calculated frequencies of the molecule with *C_s* symmetric conformation yet some other strong Raman bands at 1063, 564 and 235 cm⁻¹ and intense infrared bands at 1232, 724 and 565 cm⁻¹ could be correlated only with the calculated frequencies for other conformations of the molecule. This shows that 1-BMO exists in different conformations in its liquid state at ambient temperatures. However, all the infrared and Raman bands of the molecule in the liquid phase could be correlated with the calculated frequencies for the four conformers belonging to *C_s* and *C₁* symmetries. Four Raman bands at 1365, 910, 873 and 438 cm⁻¹ and an infrared band at 911 cm⁻¹ solely belong to calculated frequencies of conformation I while an infrared band at 724 cm⁻¹ and six Raman bands at 894, 846, 723, 473, 356 and 304 cm⁻¹ belong to conformation II only (Table 2). Similarly two infrared bands at 849 and 805 cm⁻¹ and three Raman bands at 1166, 802 and 404 cm⁻¹ are found to correspond to the calculated

frequencies of the conformation III. Furthermore, an infrared band at 1155 cm⁻¹ and four Raman bands at 1154, 455, 384 and 235 cm⁻¹ are assigned to conformation IV only.

The C-H stretch modes of vibration for all the four conformations of the molecule either belonging to the CH₂Br or CH₃ or CH₂ groups have been calculated in the frequency range 3009 -2855 cm⁻¹ as pure modes. Among these the asymmetric modes of vibration appear with relatively higher values in the order CH₂Br > CH₃ > CH₂ followed by symmetric C-H vibrations occupying lower positions in the spectra in the same order. Most of these calculated frequencies find a correlation with the strongly observed infrared and Raman bands in the range 3009-2852 cm⁻¹. These results are the same as those for other similar molecules already studied^{14,16,23-26}.

The bending vibrational frequencies for the CH₂Br, CH₃ and CH₂ groups have been calculated in the range 1465-1413 cm⁻¹ for each conformation as nearly pure modes and most of these are assigned to observed infrared and Raman bands in the range 1461-1431 cm⁻¹ except the CH₃ symmetric bending mode of vibration which has been calculated at 1344 cm⁻¹ for conformation I and at 1343 cm⁻¹ for

conformations II-IV, this mode has been assigned to an infrared band at 1340 cm^{-1} . The above values are almost the same as those reported earlier for similar molecules^{13-16,23,27}.

The next lower range of frequencies consists of wagging, twisting and rocking modes of vibration. It is observed from Table 2 that most of the modes of vibrations calculated in the finger print region of the molecule are sensitive towards conformational changes in the structure. The wagging modes of vibration calculated at 1361 , 1169 and 1164 cm^{-1} are assigned to different observed Raman bands at 1365 , 1166 and 1154 cm^{-1} (infrared band at 1155 cm^{-1}) uniquely for different conformations, respectively. Similarly the rocking modes of vibration calculated at 910 , 909 , 856 , 843 , 791 and 718 cm^{-1} are assigned to observed Raman bands at 910 , 894 , 873 , 846 , 802 and 723 cm^{-1} , respectively and those calculated at 910 , 791 and 718 cm^{-1} are assigned to infrared bands at 911 , 805 and 724 cm^{-1} uniquely for different conformations, respectively.

The seven C-C stretch modes of vibration of the molecule have been calculated mostly in the range 1121 - 909 cm^{-1} for all the conformations as slightly mixed modes and are assigned to observed infrared and Raman bands in the range 1117 - 894 cm^{-1} . These values are consistent with those reported in literature for similar molecules^{21,22}. It is noticed from the Table 2 that these modes of vibrations are sensitive towards conformational changes.

The C-Br stretch vibrations show sensitivity towards conformational changes. The C-Br stretch mode of vibration for conformation I with symmetry C_s and conformation III with symmetry C_1 has been calculated at 646 cm^{-1} as almost pure mode, as expected an intense Raman band at 646 cm^{-1} and a strong infrared band at 647 cm^{-1} are related to this mode. For conformation II and conformation IV with symmetry C_1 the C-Br stretch mode of vibration has been calculated at 565 cm^{-1} . A very strong Raman band at 564 cm^{-1} and an intense infrared band at 565 cm^{-1} are related with this mode. These calculations are in full agreement with their values for similar molecules reported in the literature^{13,15,21,22,26}. This justifies the final force-field obtained for the molecule as well as the existence of more than one conformation in the liquid state of 1-BMO.

The CCC and CCB_r bending vibrational modes for all the four conformations have been calculated within a wide range 501 - 60 cm^{-1} . This is in accordance with

the values obtained for similar molecules^{13,18}. It is seen from Table 2 that in this region some conformational sensitive frequencies have been calculated most of which are assigned uniquely to different observed bands.

The lowest frequencies calculated for all the four conformers with values below 78 cm^{-1} consist of torsional modes. These modes also show conformational sensitivity however, no measurements are done in the infrared and Raman spectra in this range and the refinement of the torsional force constant could not be made and it was transferred as such from the initial force-field.

5 Conclusions

In the present study, a detailed vibrational analysis of 1-BMO has been carried out by normal co-ordinate calculations. The observed FT-IR and Raman bands have been assigned to different modes of vibrations of all the four most probable conformations of the molecule. It has been established that these conformations co-exist in the liquid state of the compound under study at ambient temperatures, as some specific bands have been assigned uniquely to each of these conformations. The force-field has been refined for this molecule for all the four conformations simultaneously. This force-field of the molecule is quite reliable as the calculated frequencies of the molecule fit the observed ones within an average error of $\pm 5.9\text{ cm}^{-1}$ and with a decent potential energy distribution.

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