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Calculations of Infrared Spectrum for C₆₀Br₆ using Hartree-Fock Method

Rashid Nizam¹, A. M. Safwan Ahmad²

Assistant Professor, Department of Physics, IFTM University, Moradabad, India¹

B. Tech Student, Department of Mechanical Engineering, Aligarh Muslim University, Aligarh, India²

ABSTRACT: The Infrared spectra of C_{60} and $C_{60}Br_6$ have been calculated through Hartree-Fock Method. There are 25 significant peaks are observed in the Infrared spectrum of $C_{60}Br_6$. The bending vibrations of C-Br atoms are seen in the range of 60 - 170 cm⁻¹ in the spectrum. Carbon - bromine stretching vibrations are found in the range of 150-900 cm⁻¹ and combine powerfully with the radial vibrations of the carbon cage. It important to note that the carbon atoms do not contribute in the low-frequency modes, while above 250-300 cm⁻¹ frequency the vibrations are in turn localized mostly on the carbon skeleton of the molecules without significant displacements of bromine atoms. The intense IR spectrum of $C_{60}Br_6$ at 550-620 cm⁻¹ region originates from radial motions of carbon skeleton with partially localized on the bromine fragments of $C_{60}Br_6$ molecule. The medium IR spectrum of $C_{60}Br_6$ is seen in a 700-800 cm⁻¹ region is due to vibrations in the $C_{60}Br_6$ molecule yield the strong IR spectrum at 750-850 cm⁻¹ region. It is further seen that the stretching vibrations of the C-C atoms fall into 1000-1530 cm⁻¹ interval of IR spectrum. While the deformation of Infrared peaks among carbon - bromine atoms and among the carbon - carbon atoms of $C_{60}Br_6$ structure occur around 1000-1200 cm⁻¹ and 1200-1400 cm⁻¹ respectively and are seen with low intensity.

KEY WORDS: C₆₀, C₆₀Br₆, Infrared Spectrum and Hartree-Fock Method

I. INTRODUCTION

A fullerene is one of the molecules composed entirely of carbon in the form of a hollow sphere, ellipsoid or tube. Spherical fullerenes are known as buckyballs and look like football [1]. The cylindrical fullerenes are called carbon nanotubes or buckytubes. Fullerenes are also similar to graphene structure composed of stacked graphene sheets of linked hexagonal rings but may also sometimes contain pentagonal or heptagonal rings [2].

The physical techniques have been employed on fullerene and its derivatives to measure the vibrational spectra and Infrared spectra. The production of $C_{60}Br_6$ [3], $C_{60}Br_8$ [4] and $C_{60}Br_{24}$ [3, 4] have been attained recently along with their single crystal X-ray structures determined [3, 4]. It should be noted that neither experimental nor predicted results of Infrared of $C_{60}Br_6$ are extensively available in the literature.

II. COMPUTATIONAL DETAILS

Structure of C₆₀Br₆

The configuration $C_{60}Br_6$ consists of C_{60} and six Br atoms as shown in *Figure 1*. The structure of C_{60} has 12 pentagonal and 20 hexagonal faces and six Br atoms are attached to six carbon atoms on the fullerene shell through a single radial covalent bond. These six isolated Br atoms are attached to one of the carbon atoms on a pentagonal ring on the C_{60} shell, with one Br per pyracylene unit shown in *Figure 1*. The C-Br bond length is 2.07 and one electron is shared between the carbon atom and the Br atom [5, 6].



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Figure 1 Bromine doped fullerene $C_{60}Br_6$

III. METHODOLOGY

All calculation of $C_{60}Br_6$ has been done to [7]

Numerical Calculations for C₆₀Br₆

It should be noted that neither experimental nor predicted results of Infrared of $C_{60}Br_6$ are extensively available in the literature. The predicted results of Infrared spectrum of $C_{60}Br_6$ are presented below. This method has already been validated in the above section. After optimizating the structure of $C_{60}Br_6$, calculations for Infrared spectrum start. *Table 1* shows results of optimized structure of $C_{60}Br_6$ molecule and the notations used are explained below. Here C again represents a general carbon atom of C_{60} and the carbon atoms that are bonded with the bromine atom in $C_{60}Br_6$ are represented by C''. The optimized structure of $C_{60}Br_6$ has 20 hexagons and 12 pentagons. It is found that the bond lengths of C-C hexagon as well as C-C pentagon in the cage of $C_{60}Br_6$ do not markedly vary from one another after optimization. The angle of these 20 hexagons and 12 pentagons faces are represented by (C-C-C) and the optimized values are given in *Table 1*.

 $C_{60}Br_6$ has C_1 symmetry and has 192 degrees of freedom that included normal degrees of freedom for C_{60} and for additional six bromine atoms. The important parameters chosen for the program package to calculate the Infrared of $C_{60}Br_6$ are: the rotational constants of $C_{60}Br_6$ in x, y and z axes of the fullerenes derivative are 0.04, 0.03 and 0.03 (GHz) respectively. The $C_{60}Br_6$ structure has 408 symmetry adapted basis functions, 1242 primitive 12376aussians, 414 cartesian basis functions, 285 alpha electrons and 285 beta electrons with the nuclear repulsion energy of 18390.92 Hartree.

1.	2. Calculation Results - C ₆₀ Br ₆			
C – C hexagon	1.348-1.350 Å			
C – C pentagon	1.348 -1.351 Å			
C'' – Br	2.076 Å			
Angle (C-C-C) pentagon	107.9 -108.1°			
Angle (C-C-C) hexagon	120.0°			
Dipole moment	5.571 D			
Basis Set	STO-3G			

Table 1 Calculated results of Bond lengths, Angles and other Parameters for $C_{60}Br_6$

The calculation of Infrared spectrum of C₆₀Br₆ took 12 steps to converge after the optimization.



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IV. RESULTS OF C₆₀Br₆ INFRARED SPECTRUM

It is a known fact that the theoretical based calculations invariably overestimate frequencies by 10-30% [8] and, therefore, the calculation results do not compare well with the experimental data. Taking the above fact in mind a scaling factor (0.855) has been used for the purposes of comparison with experimental data. In the present calculations the predicted frequencies as shown in *Table 2* as well as in *Figure 2* have been scaled down by a factor of 0.855 uniformly across the range.

The predicted for IR spectrum of $C_{60}Br_6$ are given in *Figure 2* and on *Table 2*. Following conclusions may be drawn from the results obtained for IR calculations of $C_{60}Br_6$. There are 25 significant peaks in the Infrared spectrum of $C_{60}Br_6$ from 0 to 1530 cm⁻¹ as shown in *Figure 2* and *Table 2*. The bending vibrations of C-Br atoms are seen in the range of 60 – 170 cm⁻¹ in the spectrum. Carbon – bromine stretching vibrations are found in the range of 150-900 cm⁻¹ and combine powerfully with the radial vibrations of the carbon cage. It should be noted that the carbon atoms do not contribute in the low-frequency modes, whereas above 250-300 cm⁻¹ frequency the vibrations are in turn localized mostly on the carbon skeleton of the molecules without significant displacements of bromine atoms. The intense IR spectrum of $C_{60}Br_6$ at 550-620 cm⁻¹ region originates from radial motions of carbon skeleton with partially localized on the bromine fragments of $C_{60}Br_6$ molecule. The medium IR spectrum of $C_{60}Br_6$ in a 700-800 cm⁻¹ region is due to vibrations of the un-substituted fragments of bromine molecule. The strong IR spectrum observed at 750-850 cm⁻¹ region is caused by the deformations due to carbon- carbon atoms and carbon- bromine in the $C_{60}Br_6$ molecule. It is further seen that the stretching vibrations of the C-C atoms fall into 1000-1530 cm⁻¹ interval of IR spectrum. While the deformation of Infrared peaks among carbon – bromine atoms and among the carbon – carbon atoms of $C_{60}Br_6$ structure occur around 1000-1200 cm⁻¹ and 1200-1400 cm⁻¹ respectively and are seen with low intensity.



Figure 2 Infrared spectrum of C₆₀Br₆



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Table 2 Infrared spectrum of $C_{60}Br_6$

Frequency	Intensity	Frequency	Intensity	Frequency	Intensity	Frequency	Intensity
34	1	410	18	787	10	1163	4
43	1	419	16	795	8	1171	19
51	2	428	24	804	2	1180	6
60	6	436	51	812	1	1188	3
68	9	445	15	821	1	1197	1
77	2	453	15	829	1	1206	1
86	1	462	6	838	1	1214	-
94	1	470	6	846	1	1223	-
103	0	479	5	855	1	1231	-
111	1	487	12	864	1	1240	1
120	1	496	13	872	1	1248	1
128	3	504	28	881	2	1257	1
137	2	513	41	889	5	1265	1
145	8	522	12	898	13	1274	2
154	3	530	5	906	11	1283	3
162	8	539	4	915	2	1291	6
171	4	547	7	923	1	1300	22
180	1	556	7	932	-	1308	66
188	2	564	3	941	-	1317	39
197	1	573	3	949	-	1325	19
205	1	581	5	958	-	1334	7
214	2	590	8	966	-	1342	10
222	5	599	5	975	-	1351	4
231	2	607	6	983	-	1359	2
239	4	616	17	992	-	1368	2
248	3	624	23	1000	-	1377	3
257	3	633	9	1009	-	1385	8
265	4	641	5	1017	-	1394	37
274	8	650	10	1026	-	1402	17
282	27	658	15	1035	-	1411	25
291	26	667	11	1043	-	1419	33
299	12	675	10	1052	-	1428	22
308	4	684	15	1060	-	1436	8
316	3	693	7	1069	-	1445	4
325	6	701	8	1077	-	1454	7
333	21	710	3	1086	-	1462	14
342	11	718	2	1094	1	1471	5
351	15	727	4	1103	3	1479	8
359	54	735	13	1112	5	1488	16
368	53	744	15	1120	2	1496	44
376	15	752	7	1129	1	1505	23
385	14	761	4	1137	1	1513	7
393	15	770	11	1146	1	1530	5
402	15	778	12	1154	1	-	-



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V. CONCLUSIONS

There are 25 significant peaks are observed in the Infrared spectrum of $C_{60}Br_6$ from 0 to 1530 cm⁻¹. The bending vibrations of C-Br atoms are seen in the range of 60 - 170 cm⁻¹ in the spectrum. Carbon - bromine stretching vibrations are found in the range of 150-900 cm⁻¹ and combine powerfully with the radial vibrations of the carbon cage. It should be noted that the carbon atoms do not contribute in the low-frequency modes, whereas above 250-300 cm⁻¹ frequency the vibrations are in turn localized mostly on the carbon skeleton of the molecules without significant displacements of bromine atoms.

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