

# Theoretical Study of Raman Spectra of C<sub>60</sub>S Isomers through Hartree-Fock Method

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**ABSTRACT:-** The Raman spectra of C<sub>60</sub>S have been calculated through Hartree-Fock Method. It has been also predicted that C<sub>60</sub>S having four isomers C<sub>60</sub>S [5, 6], C<sub>60</sub>S [5, 6], C<sub>60</sub>S [6, 6] and C<sub>60</sub>S [6, 6]. However this Hartree-Fock Method is not converging for open C<sub>60</sub>S [5, 6] and open C<sub>60</sub>S [6, 6] isomers. The simulated spectra of closed [5, 6] and C<sub>60</sub>S isomer C<sub>60</sub>S [6, 6] have been done. The Raman spectrum of C<sub>60</sub>S is calculated in between the range of frequencies 0 - 1650 cm<sup>-1</sup>. Each computed spectrum of closed C<sub>60</sub>S shown in **Figure 2** can be divided into four ranges of frequencies: 0 - 400 cm<sup>-1</sup>, 400 - 800 cm<sup>-1</sup>, 800 - 1200 cm<sup>-1</sup> and 1200 - 1650 cm<sup>-1</sup> and the results may be analyzed in each range separately. The strong intense lines of Raman spectra are appeared in closed [5, 6] than C<sub>60</sub>S isomer C<sub>60</sub>S [6, 6]. The calculated energy barriers for the conversion of the closed C<sub>60</sub>S [6, 6] isomer to the open C<sub>60</sub>S [5, 6] isomer are 233.2 kJ mol<sup>-1</sup> and 1.2 kJ mol<sup>-1</sup>. The opposite (reaction) conversion's barriers from open C<sub>60</sub>S [5, 6] to closed C<sub>60</sub>S [6, 6] isomer are 82.0 kJ mol<sup>-1</sup> and 150.5 kJ mol<sup>-1</sup>.

**KEYWORDS:** C<sub>60</sub>S, Raman spectra and Hartree-Fock Method

## I. INTRODUCTION

Presently large numbers of sulphur containing fullerene derivatives have been observed by researcher in the world [1-4]. They have been observing that these fullerenes are containing mostly with high sulphur content in their structures. It is very surprising that the simplest derivative of sulphur that containing fullerene C<sub>60</sub>S has not been synthesized so frequently. Although C<sub>60</sub>S are having great potential applications in the world of research and developed. Z. Slanina et al [5] had been calculated that C<sub>60</sub>S has three stable isomers, namely closed C<sub>60</sub>S [6, 6], closed C<sub>60</sub>S [5, 6], and open C<sub>60</sub>S [5, 6] isomers. Later X. Xu et al [6] found that there are four isomers of C<sub>60</sub>S namely closed C<sub>60</sub>S [6, 6], open C<sub>60</sub>S [6, 6], closed C<sub>60</sub>S [5, 6], and open C<sub>60</sub>S [5, 6] isomers. From then no further in information has been revealed in this field of research. It is observed that both researches had used semi-empirical AM1 and MNDO methods which are not very accurate for all types of calculations.

In the present study, all calculations have been done for two stable isomers C<sub>60</sub>S namely closed C<sub>60</sub>S [6, 6] and closed C<sub>60</sub>S [5, 6] isomers with the help of Hartree-Fock Method.

## II. COMPUTATIONAL DETAILS

### Structure of C<sub>60</sub>S Isomers:

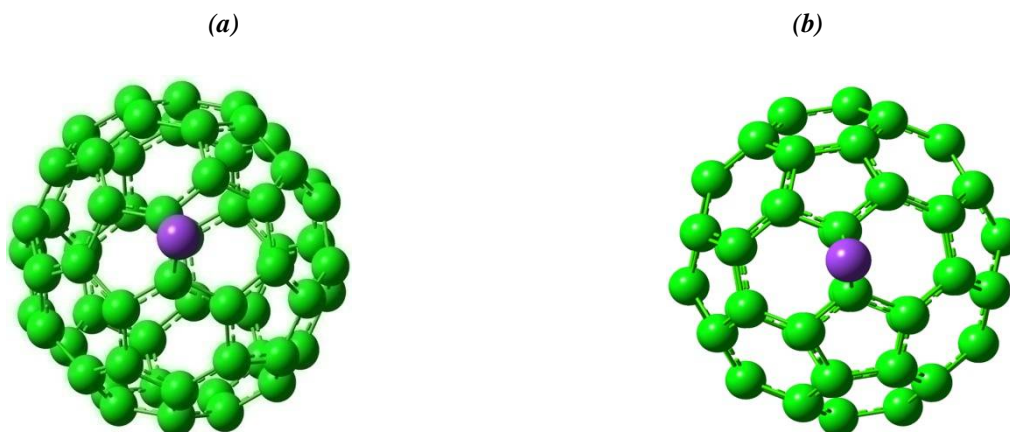
The structure of C<sub>60</sub>S consists of fullerene (C<sub>60</sub>) and a sulphur atom is connected with it. The structure has sixty carbon nuclei residing on a sphere with a sulphur atom such that sulphur atom connected with two carbon atoms of fullerene as sulphur atom has two valences. C<sub>60</sub>S has four isomers such that two open C<sub>60</sub>S [5, 6] and C<sub>60</sub>S [6, 6] and two closed isomers C<sub>60</sub>S [5, 6] and C<sub>60</sub>S [6, 6]. Two closed two isomers C<sub>60</sub>S [5, 6] and C<sub>60</sub>S [6, 6] as shown in **Figure 1 (a)** and **Figure 1 (b)** respectively. **Figure 1 (a)** displays the isomer [5, 6] with a sulphur atom bonded to two C atoms and out of the two bonds of sulphur atom one bond is shared with one pentagon carbon atom and the other bond shared with one hexagon carbon atom of C<sub>60</sub> cage. This type of C<sub>60</sub>S configuration is isomer C<sub>60</sub>S [5, 6]. C<sub>60</sub>S [6, 6] isomer is shown in **Figure 1 (b)** and in this case two bonds of sulphur atom are shared with the two hexagons of the carbon cage. The distance between carbon and sulphur atom is 2.13 Å and 2.14 Å.

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*Figure 1 (a) C<sub>60</sub>S configurations corresponding to (a) closed C<sub>60</sub>S [5, 6] (b) closed C<sub>60</sub>S [6, 6]. Sulphur atoms are shown in purple and green are carbon atoms.*

In the present work; the equilibrium structural geometry of C<sub>60</sub>S [5, 6] and C<sub>60</sub>S [6, 6] were determined through full optimization of geometrical parameters using the Hartree-Fock Method without any constraint. The optimized structural parameters of C<sub>60</sub>S [5, 6] and C<sub>60</sub>S [6, 6] are given in **Table 1** and **Table 2** respectively.

**Table 1 Results of calculation of C<sub>60</sub>O [5, 6]**

1.	2. Results of calculation [ref. 5]	3. Results of calculation [ref. 6]	4. Present calculation Results
	<b>C<sub>60</sub>S</b>	<b>C<sub>60</sub>S[5,6]</b>	<b>C<sub>60</sub>S [5,6]</b>
C – C hexagon	-	1.493 Å	1.365 -1.441 Å
C – C pentagon	-	1.493 Å	1.375 -1.464 Å
C - C*	-	-	1.463- 1.515 Å
C* - C*	2.296 Å	1.639 Å	1.3494Å
C* - S	1.695 Å	2.826 - 1.747 Å	2.145 Å
Angle (C* - S -C*)	-	55.9 °	36.7°
Angle (C-C*-C*) pentagon	-	-	108.0°
Angle (C-C*-C) hexagon	-	-	116.8°
Angle (C*-C*-C) hexagon	-	-	120.0°
Angle (C-C-C) pentagon	-	-	107.7 -108.9°
Angle (C-C-C) hexagon	-	-	118.4 -121.4°
Dipole moment	-	-	1.9205 D
Basis Set	3-21G	B3LYP/6-31G	STO-3G

**Table 1** and **Table 2** respectively show the results of optimized structure parameters of C<sub>60</sub>S [5, 6] and C<sub>60</sub>S [6, 6] as well as previous calculations of Z. Slanina et al [5] and X. Xu et al [6]. In **Table 1** these optimized parameters of calculations of Z. Slanina et al [5] are given in column (2) and those of X. Xu et al [6] for C<sub>60</sub>S [5, 6] isomer are in column (3) and column (4) shows the present optimized value of C<sub>60</sub>S. Similarly in **Table 2**, the

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optimized structure of  $C_{60}S$  [6, 6] isomer are presented in the same order. Here C represents a general carbon atom while  $C^*$  is the carbon atom bound with the sulphur atom and  $C^*-S-C^*$  is the angle between sulphur atom and its nearest two carbon atoms.  $C-C^*-C$  is the angle between the carbon atom (attached with sulphur atom) and its nearest two carbon atoms. Results of the present calculations are provided for angles  $C-C^*-C^*$  (pentagon),  $C-C^*-C$  (hexagon) and  $C^*-C^*-C$  (hexagon) for  $C_{60}S$  [5, 6] isomer. No clear the bond lengths of C-C hexagon as well as C-C pentagon are mentioned in the previous papers [5 - 6]. The angle  $C^*-S-C^*$  is quite different ( $55.9^\circ$ ) in the present calculations [6]. Additional geometry information is also provided for the present calculation in **Table 1 - 2** which are not available in [5] and [6].

**Table 2 Results of calculation of  $C_{60}O$  [6, 6]**

1.	2. Results of calculation [ref. 5]	3. Results of calculation [ref. 6]	4. Present calculation Results
	$C_{60}S$	$C_{60}S$ [6,6]	$C_{60}S$ [6,6]
C – C hexagon	-	1.497 Å	1.366 -1.379 Å
C – C pentagon	-	1.497 Å	1.375 -1.464 Å
C - $C^*$	-	-	1.463- 1.515 Å
$C^* - C^*$	1.594 Å	1.497 Å	1.3475 Å
$C^* - S$	1.729 Å	1.747 Å	2.147 Å
Angle ( $C^* - S - C^*$ )	-	$52.7^\circ$	$36.72^\circ$
Angle (C-C $^*$ -C) pentagon	-	-	$108.0^\circ$
Angle(C $^*$ -C $^*$ -C) hexagon	-	-	$120.0^\circ$
Angle (C-C-C) pentagon	-	-	$107.4 - 108.9^\circ$
Angle (C-C-C) hexagon	-	-	$120.0 - 121.7^\circ$
Dipole moment	-	-	1.1231 D
Basis Set	3-21G	B3LYP/6-31G	STO-3G

**Table 2** gives results of geometrical parameters for  $C_{60}S$  [6, 6] isomer after optimization in the present work and also calculations of others. It is seen that the results of the three calculations are comparable. Results of the present calculations are also given for angles  $C-C^*-C$  (pentagon) and  $C^*-C^*-C$  (hexagon) for  $C_{60}S$  [6, 6] isomer which are not available in [5, 6]. The bond lengths of C-C hexagon as well as C-C pentagon markedly vary for [6] in comparison with the present results as seen above. The angle  $C^*-S-C^*$  is quite different ( $52.7^\circ$ ) in present calculations with [6].

### III. METHODOLOGY

All calculations of the Raman spectra have been done according to [7]

The Raman spectra for only two isomers  $C_{60}S$  [5, 6] and  $C_{60}S$  [6, 6] are given in **Figures 2(a)-(b)** and **Table 1 - 2**. The variables used in the calculations of  $C_{60}S$  [5, 6] and  $C_{60}S$  [6, 6] for Raman spectra are same except nuclear repulsion energy. These are as follows: the rotational constants used in x, y, and z directions in the fullerenes derivative ( $C_{60}S$ ) are 0.09, 0.08 and 0.08 (GHz) respectively, the  $C_{60}S$  has 309 symmetry adapted basis functions, 927 primitive gaussians, 309 cartesian basis functions, 188 alpha electrons and 188 beta electrons. The variables of the nuclear repulsion energy used in the calculations of  $C_{60}S$  [5, 6] and  $C_{60}S$  [6, 6] are 9421.47 and 9418.98 Hartree respectively. The most significant change in the Raman spectrum induced by the substitution of sulphur in fullerene is the redistribution of the Raman intensity among the normal modes as shown in the **Table 1-2**. Starting with 183 total degrees of freedom for an isolated  $C_{60}S$  molecule and subtracting six degrees of freedom corresponding to three translations and three rotations, results in 177 vibration degrees of freedom. Although the fullerene derivatives  $C_{60}S$  [5, 6] and  $C_{60}S$  [6, 6] isomers have same number of 177 degrees of freedom yet they exhibit different spectra. The

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numerical results converged after 29 cycles and 21 cycles with density matrix = 0.1950D-08 and density matrix = 0.6887D-08 for C<sub>60</sub>S [5, 6] and [6, 6] respectively.

### IV. RESULTS OF RAMAN SPECTRA OF C<sub>60</sub>S [5, 6] and C<sub>60</sub>S [6, 6]

- 1) The Ab-Initio method used for calculation [8 - 10] overestimates Raman intensities. Thus all the calculated Raman intensities may show some error when compared with the available experimental data [11]. In the present case the calculated frequencies for C<sub>60</sub>S have been scaled down by a factor 0.855 uniformly throughout the range.
- 2) It should be noted that Hartree - Fock is the best method for the calculation of Raman spectra for C<sub>60</sub>S [5, 6] and C<sub>60</sub>S [6, 6]. However this method is not converging for open C<sub>60</sub>S [5, 6] and open C<sub>60</sub>S [6, 6] isomers.
- 3) The Raman spectrum of C<sub>60</sub>S is calculated in between the range of frequencies 0 - 1650 cm<sup>-1</sup>. Each computed spectrum of closed C<sub>60</sub>S shown in **Figure 2** can be divided into four ranges of frequencies: 0 - 400 cm<sup>-1</sup>, 400 - 800 cm<sup>-1</sup>, 800 - 1200 cm<sup>-1</sup> and 1200 - 1650 cm<sup>-1</sup> and the results may be analyzed in each range separately.
- 4) It is observed that low intensities of C<sub>60</sub>S [6, 6] are obtained than C<sub>60</sub>S [5, 6] throughout the range.
- 5) Five major peaks are seen in C<sub>60</sub>S [5, 6] while in C<sub>60</sub>S [6, 6] eight major peaks are seen in the given range of 0 - 400 cm<sup>-1</sup> as shown in **Figure 2**. Six major peaks are observed in both C<sub>60</sub>S [5, 6] and C<sub>60</sub>S [6, 6] in 400 - 800 cm<sup>-1</sup>. Three major peaks are calculated in both C<sub>60</sub>S [5, 6] and C<sub>60</sub>S [6, 6] in 800 - 1200 cm<sup>-1</sup>. Similarly in both C<sub>60</sub>S [5, 6] and C<sub>60</sub>S [6, 6] seven peaks are calculated in the last range of 1200 - 1650 cm<sup>-1</sup>.
- 6) **Figures 2** show that several intense peaks are observed in closed C<sub>60</sub>S [5, 6] isomer is more than closed C<sub>60</sub>S [6, 6] in Raman spectrum.
- 7) According to Z. Slanina et al [5] and X. Xu et al [6] accepted that closed C<sub>60</sub>S [6, 6] is the most stable isomer among all C<sub>60</sub>S isomers. The present calculations are also agreeing with the same idea. Therefore it is possible to calculate the Raman spectrum of C<sub>60</sub>S [6, 6] but lower intensities are calculated in it.
- 8) Raman spectrum of C<sub>60</sub>S may not be available through which C<sub>60</sub>S Raman spectra could be matched with the present Raman spectra of C<sub>60</sub>S [6, 6] result. Further, only Z. Slanina et al [5] did only calculate the Infrared spectrum for opened C<sub>60</sub>S [5, 6] isomer and here the present calculation of Raman spectrum has been for closed C<sub>60</sub>S [5, 6] isomer.
- 9) The number of Raman peaks observed in closed C<sub>60</sub>S [5, 6] isomer is more than closed C<sub>60</sub>S [6, 6] in Raman spectra as shown in **Table- 3** and **Table- 4**. Even the strong intense lines of Infrared spectra are appeared in closed C<sub>60</sub>S [5, 6] than closed C<sub>60</sub>S [6, 6] isomer. The Raman number and Raman intensity peaks spectrum of closed C<sub>60</sub>S [5, 6] is fading faster than closed C<sub>60</sub>S [6, 6] on increasing in temperature just like in Infrared spectrum of closed C<sub>60</sub>S [5, 6]. This shows that the closed C<sub>60</sub>S [5, 6] is less stable than closed C<sub>60</sub>S [6, 6] isomer.

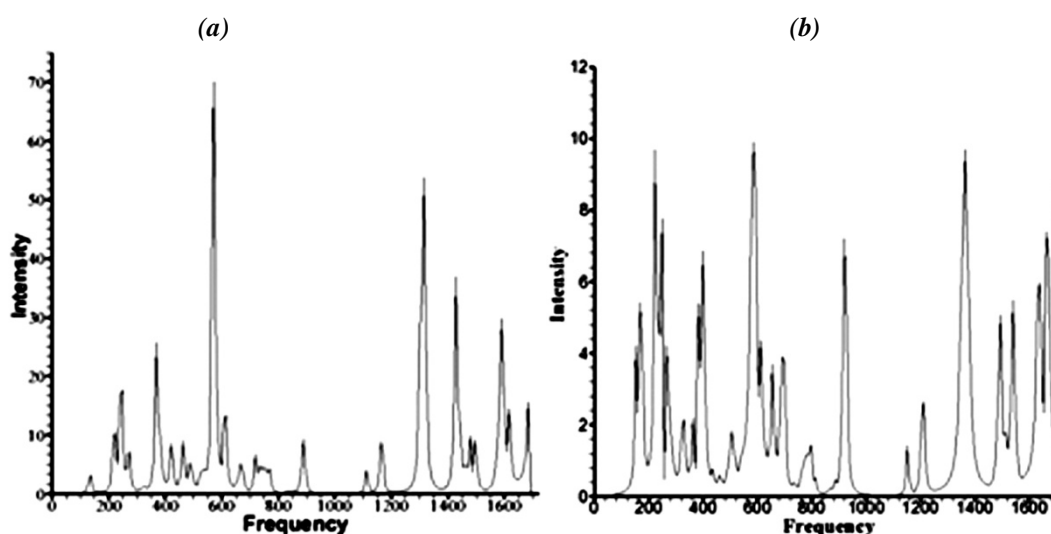


Figure 2 (a) Raman spectra of C<sub>60</sub>S [5, 6] and C<sub>60</sub>S [6, 6]

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- 10) It has been observed [5-6] and calculated that by changing temperature from lower to higher produces a more abrupt and substantial change in the Raman spectrum band shapes. It may be due to two barriers for the inter-conversion between the closed C<sub>60</sub>S [6, 6] and open C<sub>60</sub>S [5, 6] isomers. The calculated energy barriers for the conversion of the closed C<sub>60</sub>S [6, 6] isomer to the open C<sub>60</sub>S [5, 6] isomer are 233.2 kJ mol<sup>-1</sup> and 1.2 kJ mol<sup>-1</sup>. The opposite (reaction) conversion's barriers from open C<sub>60</sub>S [5, 6] to closed C<sub>60</sub>S [6, 6] isomer are 82.0 kJ mol<sup>-1</sup> and 150.5 kJ mol<sup>-1</sup>.
- 11) The present studies shows the Raman spectrum of closed C<sub>60</sub>S [5, 6] as given in **Figures 2**. It is not observed experimentally at room temperature due to its instability. Even there is lack of availability of Raman spectrum of C<sub>60</sub>S [5, 6] in the world.
- 12) Similarly the present Raman spectrum of closed C<sub>60</sub>S [6, 6] isomer also may not be available in the world. Although Z. Slanina et al [5] constructed fullerene with sulphur only for Infrared spectrum. He had not computed any Raman spectrum for any C<sub>60</sub>S [6, 6] isomer.
- 13) Moreover no attempted made by Z. Slanina et al [5] in scaling down of computed frequencies although they had accepted to be overestimates his calculations in Infrared spectra. The present computed Raman frequencies are different as they [5] had calculated Infrared spectrum for C<sub>60</sub>S. MNDO [5] energy having to its parameterizations corresponds to room temperature rather than to absolute zero. Therefore there may be chance of changing in calculated Infrared spectra frequencies of C<sub>60</sub>S.
- 14) The present studies have computed with accuracy the Raman spectrum of closed C<sub>60</sub>S [5, 6] and closed C<sub>60</sub>S [6, 6]. As the present studies are using better tool for computing Raman spectrum at room temperature.

### V. CONCLUSIONS

Large number of Raman spectrum peaks are observed in closed C<sub>60</sub>S [5, 6] isomer than closed C<sub>60</sub>S [6, 6] Raman spectrum. Even the strong intense lines of Raman spectrum are appeared in closed [5, 6] than C<sub>60</sub>S isomer C<sub>60</sub>S [6, 6].

**Table - 3 Raman spectrum of closed C<sub>60</sub>S [5, 6] isomer**

Frequency	Intensity [ 5, 6]	Frequency	Intensity [ 5, 6]	Frequency	Intensity [ 5, 6]	Frequency	Intensity [ 5, 6]
17.1	0.01	453.15	2.99	795.15	0.30	1231.2	0.37
25.65	0.01	461.7	8.98	803.7	0.21	1239.75	0.44
34.2	0.01	470.25	4.26	812.25	0.18	1248.3	0.55
42.75	0.01	478.8	2.55	820.8	0.18	1256.85	0.74
51.3	0.02v	487.35	5.41	829.35	0.32	1265.4	1.03
59.85	0.02	495.9	3.78	837.9	0.39	1273.95	1.58
68.4	0.03	504.45	1.58	846.45	0.30	1282.5	2.76
76.95	0.06	513	1.43	855	0.60	1291.05	6.34
85.5	0.07	521.55	2.67	863.55	0.48	1299.6	27.22
94.05	0.09	530.1	3.97	872.1	0.90	1308.15	36.39
102.6	0.13	538.65	4.12	880.65	3.27	1316.7	53.75
111.15	0.22	547.2	4.03	889.2	9.33	1325.25	20.15
119.7	0.55	555.75	8.44	897.75	3.70	1333.8	5.56
128.25	1.68	564.3	34.46	906.3	0.93	1342.35	2.58
136.8	3.25	572.85	69.98	914.85	0.41	1350.9	1.58
145.35	0.76	581.4	20.78	923.4	0.23	1359.45	1.14
153.9	0.35	589.95	6.71	931.95	0.15	1368	0.93
162.45	0.28	598.5	4.88	940.5	0.10	1376.55	0.86
171	0.30	607.05	11.78	949.05	0.08	1385.1	0.90
179.55	0.37	615.6	13.45	957.6	0.06	1393.65	1.09
188.1	0.52	624.15	3.23	966.15	0.06	1402.2	1.59
196.65	0.85	632.7	1.62	974.7	0.09	1410.75	3.02
205.2	1.83	641.25	1.23	983.25	0.06	1419.3	9.6
213.75	7.07	649.8	1.68	991.8	0.04	1427.85	36.90
222.3	10.49	658.35	2.54	1000.35	0.04	1436.4	15.43

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230.85	5.03	666.9	5.20	1008.9	0.04	1444.95	11.66
239.4	16.68	675.45	3.66	1017.45	0.04	1453.5	4.53
247.95	17.56	684	1.11	1026	0.04	1462.05	4.72
256.5	4.198	692.55	0.75	1034.55	0.04	1470.6	4.59
265.05	4.24	701.1	0.81	1043.1	0.04	1479.15	9.92
273.6	7.27	709.65	1.54	1051.65	0.05	1487.7	3.62
282.15	1.81	718.2	6.77	1060.2	0.06	1496.25	9.24
290.7	0.88	726.75	3.4	1068.75	0.07	1504.8	4.38
299.25	0.67	735.3	4.80	1077.3	0.10	1513.35	1.40
307.8	0.82	743.85	4.10	1085.85	0.15	1521.9	0.86
316.35	0.96	752.4	4.51	1094.4	0.28	1530.45	0.75
324.9	1.35	760.95	3.45	1102.95	0.76	1539	0.82
333.45	0.87	769.5	4.22	1111.5	4.07	1547.55	1.00
342	1.09	778.05	1.06	1120.05	1.56	1556.1	1.49
350.55	1.96	786.6	0.64	1128.6	0.53	1564.65	3.35
359.1	5.60	795.15	0.30	1137.15	0.46	1573.2	7.93
367.65	25.80	803.7	0.21	1145.7	0.72	1581.75	13.21
376.2	11.84	812.25	0.18	1154.25	1.95	1590.3	29.82
384.75	9.49	820.8	0.18	1162.8	8.82	1598.85	16.63
393.3	3.44	829.35	0.32	1171.35	6.67	1607.4	7.21
401.85	1.94	837.85	4.10	1179.9	1.52	1615.95	14.43
410.4	2.32	846.4	4.51	1188.45	0.64	1624.5	7.63
418.95	8.55	854.95	3.45	1197	0.41	1633.05	3.12
427.5	5.64	863.5	4.22	1205.55	0.34	1641.6	2.47
436.05	1.78	872.05	1.06	1214.1	0.32	1650.15	2.51
444.6	1.44	880.6	0.64	1222.65	0.33	1658.7	3.12

**Table - 4 Raman spectrum of closed  $C_{60}S$  [6, 6] isomer**

Frequency	Intensity [ 6, 6]	Frequency	Intensity [ 6, 6]	Frequency	Intensity [ 6, 6]	Frequency	Intensity [ 6, 6]
76.95	0.00	504.45	3.48	863.55	0.03	1291.05	0.03
85.5	0.01	513	2.12	872.1	0.03	1299.6	0.07
94.05	0.01	521.55	3.70	880.65	0.04	1308.15	0.21
102.6	0.01	530.1	2.26	889.2	0.11	1316.7	1.059
111.15	0.02	538.65	0.87	897.75	0.16	1325.25	0.45
119.7	0.03	547.2	0.56	906.3	0.04	1333.8	0.20
128.25	0.05	555.75	0.43	914.85	0.02	1342.35	0.14
136.8	0.14	564.3	0.41	923.4	0.01	1350.9	0.13
145.35	0.83	572.85	0.48	931.95	0.01	1359.45	0.13
153.9	0.29	581.4	0.38	940.5	0.00	1368	0.15
162.45	0.09	589.95	0.32	949.05	0.00	1376.55	0.16
171	0.05	598.5	0.35	957.6	0.00	1385.1	0.19
179.55	0.03	607.05	0.47	966.15	0.00	1393.65	0.21
188.1	0.03	615.6	0.78	974.7	0.00	1402.2	0.26
196.65	0.05	624.15	2.02	983.25	0.00	1410.75	0.33
205.2	0.13	632.7	10.60	991.8	0.00	1419.3	0.45
213.75	0.72	641.25	4.52	1000.35	0.00	1427.85	0.86
222.3	0.30	649.8	1.46	1008.9	0.00	1436.4	1.28
230.85	0.09	658.35	1.76	1017.45	0.00	1444.95	0.95
239.4	0.07	666.9	3.29	1026	0.00	1453.5	1.26
247.95	0.07	675.45	1.10	1034.55	0.00	1462.05	1.88

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256.5	0.07	684	0.43	1043.1	0.00	1470.6	2.76
265.05	0.24	692.55	0.32	1051.65	0.00	1479.15	5.44
273.6	0.15	701.1	0.40	1060.2	0.00	1487.7	14.70
282.15	0.15	709.65	1.31	1068.75	0.00	1496.25	72.35
290.7	0.08	718.2	0.79	1077.3	0.00	1504.8	54.03
299.25	0.08	726.75	0.85	1085.85	0.01	1513.35	11.39
307.8	0.14	735.3	3.36	1094.4	0.01	1521.9	4.76
316.35	0.41	743.85	3.38	1102.95	0.04	1530.45	4.12
324.9	0.43	752.4	2.72	1111.5	0.20	1539	2.07
333.45	0.22	760.95	2.29	1120.05	0.17	1547.55	1.31
342	0.24	769.5	3.20	1128.6	0.04	1556.1	0.99
350.55	0.36	778.05	0.81	1137.15	0.02	1564.65	0.87
359.1	0.88	786.6	0.61	1145.7	0.01	1573.2	0.92
367.65	2.99	795.15	0.22	1154.25	0.02	1581.75	1.41
376.2	1.76	803.7	0.13	1162.8	0.08	1590.3	1.75
384.75	0.71	812.25	0.09	1171.35	0.12	1598.85	1.03
393.3	0.68	820.8	0.07	1179.9	0.08	1607.4	0.87
401.85	0.76	829.35	0.11	1188.45	0.02	1615.95	0.90
410.4	1.03	837.9	0.15	1197	0.01	1624.5	1.29
418.95	3.03	846.45	0.05	1205.55	0.01	1633.05	1.50
427.5	2.41	855	0.05	1214.1	0.01	1641.6	3.19
436.05	4.12	504.45	3.48	1222.65	0.01	1650.15	4.46
444.6	16.48	513	2.12	1231.2	0.01		
453.15	8.63	521.55	3.70	1239.75	0.01		
461.7	5.95	530.1	2.26	1248.3	0.01		
470.25	16.77	538.65	0.87	1256.85	0.01		
478.8	42.00	547.2	0.56	1265.4	0.01		
487.35	27.07	555.75	0.43	1273.95	0.01		
495.9	10.94	564.3	0.41	1282.5	0.020		

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