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Theoretical Study of Infrared Spectra of $C_{60}S$ Isomers through Hartree-Fock Method

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Abstract: ***The Infrared spectra of $C_{60}S$ have been calculated through Hartree-Fock Method. It has been also predicted that $C_{60}S$ having four isomers $C_{60}S$ [5, 6], $C_{60}S$ [5, 6] $C_{60}S$ [6, 6] and $C_{60}S$ [6, 6]. However this Hartree-Fock Method is not converging for opened $C_{60}S$ [5, 6] and opened $C_{60}S$ [6, 6] isomers. The simulated spectra of closed $C_{60}S$ [5, 6] and closed $C_{60}S$ [6, 6] isomer have been done. Each computed spectrum of closed $C_{60}S$ can be divided into four ranges of frequencies: 0-600 cm^{-1}, 600-800 cm^{-1}, 800-1200 cm^{-1} and 1200-1650 cm^{-1} and the results may be analyzed in each range separately. The strong intense lines of infrared spectra are appeared in closed [5, 6] than $C_{60}S$ isomer $C_{60}S$ [6, 6]. The calculated energy barriers for the conversion of the closed $C_{60}S$ [6, 6] isomer to the opened $C_{60}S$ [5, 6] isomer are 233.2 kJ mol^{-1} and 1.2 kJ mol^{-1}. The opposite (reaction) conversion's barriers from opened $C_{60}S$ [5, 6] to closed $C_{60}S$ [6, 6] isomer are 82.0 kJ mol^{-1} and 150.5 kJ mol^{-1}.***

Keywords: $C_{60}S$, Infrared spectra and Hartree-Fock Method

1. Introduction

Large numbers of sulphur containing fullerene derivatives have been observed, [1-4]. These fullerenes are containing mostly with high sulphur content in their structures. It is very surprising that the simplest derivative of sulphur containing fullerene $C_{60}S$ has not been synthesized. Although $C_{60}S$ are having potential applications in the world of research and developed. Z. Slanina et al [5] had been calculated that $C_{60}S$ has three stable isomers, namely closed $C_{60}S$ [6, 6], closed $C_{60}S$ [5, 6], and open $C_{60}S$ [5, 6] isomers. Later X. Xu et al [6] found that there are four isomers of $C_{60}S$ namely closed $C_{60}S$ [6, 6], open $C_{60}S$ [6, 6], closed $C_{60}S$ [5, 6], and open $C_{60}S$ [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 four isomers $C_{60}S$ namely closed $C_{60}S$ [6, 6] and closed $C_{60}S$ [5, 6] isomers with the help of Hartree-Fock Method. However this method is not converging for open $C_{60}S$ [5, 6] and open $C_{60}S$ [6, 6] isomers.

2. Computational Details

2.1 Structure of $C_{60}S$ Isomers:

The structure of $C_{60}S$ consists of C_{60} and a sulphur atom is connected with it. The structure has sixty carbon nuclei residing on a sphere with a sulphur atom such that connected with two carbon atoms as sulphur atom has two valences. $C_{60}S$ has two isomers $C_{60}S$ [5, 6] and $C_{60}S$ [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_{60} cage. This type of $C_{60}S$ configuration is isomer $C_{60}S$ [5, 6]. $C_{60}S$ [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. In the present work; the equilibrium structural geometry of $C_{60}S$ [5, 6] and $C_{60}S$ [6, 6] were determined through full optimization of geometrical parameters using the Hartree-Fock Method without any constraint. The optimized structural parameters of $C_{60}S$ [5, 6] and $C_{60}S$ [6, 6] are given in ***Table 1*** and ***Table 2*** respectively.

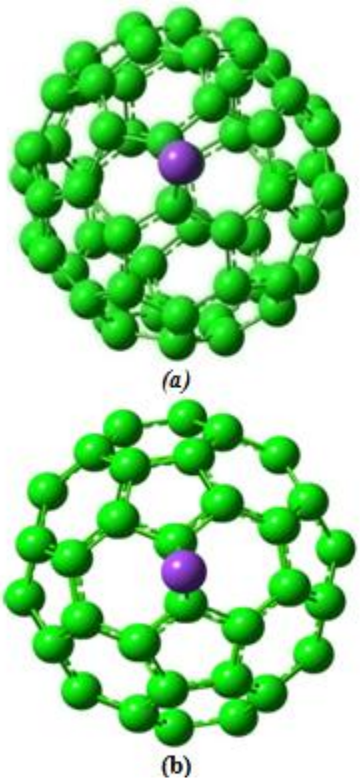

Figure 1 (a) $C_{60}S$ configurations corresponding to (a) closed $C_{60}S$ [5, 6] (b) closed $C_{60}S$ [6, 6]. Sulphur atoms are shown in purple and green are carbon atoms.

Table 1 and ***Table 2*** respectively show the results of optimized structure parameters of $C_{60}S$ [5, 6] and $C_{60}S$ [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 $C_{60}S$ [5, 6] isomer are in column (3) and column (4) show the present optimized value of $C_{60}S$. Similarly in ***Table 2***, the optimized structure of $C_{60}S$ [6, 6] isomer are presented in the same order.

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°) in present calculations with [6].

3. Methodology

All calculations of the Infrared spectra have been done according to [7]. The Infrared spectra for the two isomers $C_{60}S$ [5, 6] and $C_{60}S$ [6, 6] are given in ***Figures 2(a)-(b)***. The variables used in the calculations of $C_{60}S$ [5, 6] and $C_{60}S$ [6, 6] for Infrared 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. 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 numerical results converged after 29 cycles and 21 cycles with density matrix = 0.1950D-08 and density matrix = 0.6887D-08 for $C_{60}S$ [5, 6] and [6, 6] respectively.

Table 1 Results of calculation of $C_{60}O$ [5, 6]

	2. Results of calculation [ref. 5]	***3. Results of calculation [ref. 6]***	***4. Present calculation Results***
	$C_{60}S$	**$C_{60}S$[5,6]**	**$C_{60}S$ [5,6]**
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 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°	36.72°
Angle (C-C^*-C) pentagon	-	-	108.0°
Angle(C^*-C^*-C) hexagon	-	-	120.0°
Angle (C-C-C) pentagon	-	-	107.4 - 108.9°
Angle (C-C-C) hexagon	-	-	120.0 - 121.7°
Dipole moment	-	-	1.1231 D
Basis Set	3-21G	B3LYP/6-31G	STO-3G

4. Calculation Results of $C_{60}S$ [5, 6] and $C_{60}S$ [6, 6]

1) The Ab-Initio method used for calculation [8 - 10] overestimates Infrared intensities. Thus all the calculated Infrared intensities may show some error when compared with the available experimental data [11]. In the present case the calculated frequencies for $C_{60}S$ 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 Infrared spectra for $C_{60}S$ [5, 6] and $C_{60}S$ [6, 6]. However this method is not converging for opened $C_{60}S$ [5, 6] and opened $C_{60}S$ [6, 6] isomers.

3) The Infrared spectrum of $C_{60}S$ is calculated in between the range of frequencies 0 - 1650 cm^{-1}. Each computed spectrum of closed $C_{60}S$ shown in ***Figure 2***. It can be divided into four ranges of frequencies: 0-600 cm^{-1}, 600-800 cm^{-1}, 800-1200 cm^{-1} and 1200-1650 cm^{-1} and the results may be analyzed in each range separately.
4) Few numbers of peaks is seen in: 0-600 cm^{-1} as shown in figure 2. All lowest peaks are seen in 600-800 cm^{-1}. No peaks have been calculated in 800-1200 cm^{-1} range. The numbers of highest peaks are seen in 1200-1650 cm^{-1}. In the first range it appears that carbon atoms of fullerene show only movement keeping sulphur atom stationary. Cage movement includes radial breathing mode, twisted mode, carbon atoms zig-zag modes etc.
5) According to Z. Slanina et al [5] and X. Xu et al [6] accepted that closed $C_{60}S$ [6, 6] is the most stable isomer among all $C_{60}S$ isomers. The present calculations are also agreeing with the same idea. Therefore it is possible to calculate the Infrared spectrum of closed $C_{60}S$ [6, 6].

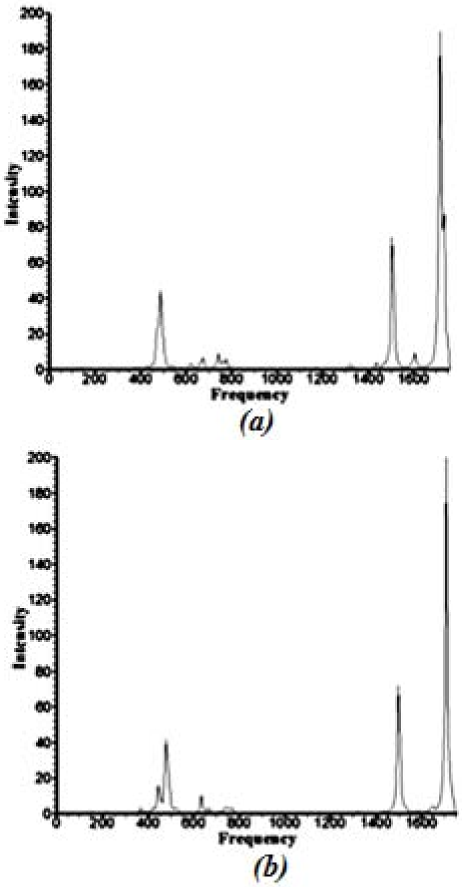

Figure 2: (a) Infrared spectra of $C_{60}S$ [5, 6] and $C_{60}S$ [6, 6]

6) Semi-Empirical studies [5] suggesting that $C_{60}S$ isomers may be overestimating its Infrared spectra therefore $C_{60}S$ [6, 6] Infrared spectrum of is not matching with the present Infrared $C_{60}S$ [6, 6] spectrum result. Further to Z. Slanina et al [5] did calculate the Infrared spectrum for opened $C_{60}S$ [5, 6] isomer and here the present calculation has been done for closed $C_{60}S$ [5, 6] isomer. No calculations might be done for Infrared spectrum opened $C_{60}S$ [5, 6] isomer as opened $C_{60}S$ [5, 6] isomer is not converging in Hatree-Fock method. .
7) ***Figures 2*** show that several intense peaks are observed in closed $C_{60}S$ [5, 6] isomer than closed $C_{60}S$ [6, 6] in Infrared spectrum.
8) Large number of Infrared peaks are observed in closed $C_{60}S$ [5, 6] isomer more than closed $C_{60}S$ [6, 6] in Infrared spectra as shown in ***Table-3*** and ***Table-4***. Even the strong intense lines of Infrared spectra are appeared in closed $C_{60}S$ [5, 6] than closed $C_{60}S$ [6, 6] isomer. The Infrared number and Infrared intensity peaks spectrum of closed $C_{60}S$ [5, 6] is fading faster than closed $C_{60}S$ [6, 6] on increasing in temperature. This shows that the closed $C_{60}S$ [5, 6] is less stable than closed $C_{60}S$ [6, 6] isomer.
9) It has been observed [5-6, 13] and calculated that by changing temperature from lower to higher produces a more abrupt and substantial change in the Infrared band shapes. It may be due to two barriers for the inter-conversion between the closed $C_{60}S$ [6, 6] and open $C_{60}S$ [5, 6] isomers. The calculated energy barriers for the conversion of the closed $C_{60}S$ [6, 6] isomer to the opened $C_{60}S$ [5, 6] isomer are 233.2 kJ mol^{-1} and 1.2 kJ mol^{-1}. The opposite (reaction) conversion's barriers from opened $C_{60}S$ [5, 6] to closed $C_{60}S$ [6, 6] isomer are 82.0 kJ mol^{-1} and 150.5 kJ mol^{-1}.
10) The present studies shows the Infrared of closed $C_{60}S$ [5, 6] as given in ***Figures 2***. It is not matching with the Infrared of Z. Slanina et al [5] as they have computed for open $C_{60}S$ [5, 6]. This is isomer of $C_{60}S$ [5, 6]. However, it was observed [6] that it is impossible for the closed [5, 6] isomer of $C_{60}S$ to be observed in experiment at room temperature due to its instability.
11) Similarly the present Infrared closed $C_{60}S$ [6, 6] isomer is not fully matching with Z. Slanina et al [5]. The reason is that the parameters used by Z. Slanina et al [5] for construction of fullerene are very different than present studies. The carbon – carbon distance in present studies are 1.375 -1.464 Å. and Z. Slanina et al [5] used 1.594 Å - 2.296 Å which is wrong distance for carbon – carbon. According to M D. Newton et al [12] C_{60} cage carbon- carbon distances approximately 1.40 Å.
12) 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. The computed frequencies are come out slightly different at different temperatures. 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 frequencies of $C_{60}S$.
13) The present studies IR of $C_{60}S$ [6, 6] is better predicted of I.R. than Z. Slanina et al [5]. As the present studies are using better tool for computing IR at room temperature.

5. Conclusions

Large number of Infrared peaks are observed in closed $C_{60}S$ [5, 6] isomer than closed $C_{60}S$ [6, 6] Infrared spectrum. Even the strong intense lines of Infrared spectra are appeared in closed [5, 6] than $C_{60}S$ isomer $C_{60}S$ [6, 6].

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Table 3: Infrared spectrum of closed C_{60}S [5, 6] isomer

Frequency	*Intensity [5, 6]*	*Frequency*	*Intensity [5, 6]*	*Frequency*	*Intensity [5, 6]*	*Frequency*	*Intensity [5, 6]*
76.95	0.01	504.45	11.08	863.55	0.09	1291.05	0.16
85.5	0.01	513	3.30	872.1	0.06	1299.6	0.37
94.05	0.01	521.55	1.80	880.65	0.05	1308.15	1.58
102.6	0.02	530.1	1.86	889.2	0.08	1316.7	2.54
111.15	0.03	538.65	2.58	897.75	0.26	1325.25	2.26
119.7	0.05	547.2	1.76	906.3	0.24	1333.8	1.29
128.25	0.17	555.75	0.68	914.85	0.06	1342.35	0.42
136.8	0.57	564.3	0.48	923.4	0.03	1350.9	0.25
145.35	0.86	572.85	0.52	931.95	0.02	1359.45	0.20
153.9	0.18	581.4	0.75	940.5	0.01	1368	0.19
162.45	0.06	589.95	0.52	949.05	0.01	1376.55	0.19
171	0.03	598.5	0.45	957.6	0.00	1385.1	0.21
179.55	0.02	607.05	0.73	966.15	0.00	1393.65	0.24
188.1	0.02	615.6	2.65	974.7	0.00	1402.2	0.29
196.65	0.02	624.15	3.19	983.25	0.00	1410.75	0.38
205.2	0.02	632.7	0.86	991.8	0.00	1419.3	0.56
213.75	0.04	641.25	0.64	1000.35	0.00	1427.85	1.18
222.3	0.14	649.8	0.97	1008.9	0.00	1436.4	3.83
230.85	0.21	658.35	3.65	1017.45	0.00	1444.95	2.16
239.4	0.06	666.9	4.21	1026	0.00	1453.5	1.46
247.95	0.10	675.45	6.51	1034.55	0.00	1462.05	1.83
256.5	0.10	684	1.87	1043.1	0.00	1470.6	3.39
265.05	0.05	692.55	0.68	1051.65	0.00	1479.15	4.05
273.6	0.10	701.1	0.47	1060.2	0.00	1487.7	8.65
282.15	0.15	709.65	0.49	1068.75	0.00	1496.25	14.65
290.7	0.17	718.2	0.77	1077.3	0.01	1504.8	74.56
299.25	0.06	726.75	2.24	1085.85	0.01	1513.35	52.07
307.8	0.06	735.3	4.20	1094.4	0.02	1521.9	11.20
316.35	0.13	743.85	9.28	1102.95	0.05	1530.45	4.48
324.9	0.19	752.4	3.41	1111.5	0.14	1539	2.44
333.45	0.22	760.95	4.01	1120.05	0.76	1547.55	1.65
342	0.14	769.5	4.08	1128.6	0.28	1556.1	1.31
350.55	0.15	778.05	6.06	1137.15	0.08	1564.65	1.199
359.1	0.21	786.6	1.62	1145.7	0.05	1573.2	1.35
367.65	0.49	795.15	1.42	1154.25	0.06	1581.75	1.88
376.2	1.00	436.05	2.15	1162.8	0.19	1590.3	3.57
384.75	0.46	444.6	2.01	1171.35	0.72	1598.85	6.05
393.3	0.78	453.15	2.51	1179.9	0.39	1607.4	9.36
401.85	0.53	461.7	6.16	1188.45	0.09	1615.95	3.59
410.4	0.55	470.25	20.73	1197	0.04	1624.5	1.80
418.95	0.71	478.8	24.79	1205.55	0.03	1633.05	1.39
427.5	1.83	487.35	44.70	1214.1	0.02	1641.6	1.36
436.05	2.15	795.15	1.42	1222.65	0.02	1650.15	1.53
444.6	2.01	803.7	0.44	1231.2	0.02		
453.15	2.51	812.25	0.24	1239.75	0.02		
461.7	6.16	820.8	0.16	1248.3	0.03		
470.25	20.73	829.35	0.13	1256.85	0.03		
478.8	24.79	837.9	0.15	1265.4	0.04		
487.35	44.70	846.45	0.17	1273.95	0.06		
495.9	21.64	855	0.08	1282.5	0.09		

Table 4: Infrared 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
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		