

Calculations of Raman Spectra for C₆₀O isomers using Hartree-Fock Method

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ABSTRACT: The Raman spectra of C₆₀O have been calculated through Hartree-Fock Method. It has been also predicted the simulated spectra of C₆₀O isomer. 14 major Raman peaks in addition to certain weak peaks are seen in the spectra of C₆₀O [5, 6] while 11 major Raman peaks with weak peaks are observed in C₆₀O [6, 6]. Four significant Raman lines are seen for [5, 6] in the range of frequencies of 1400-1701 cm⁻¹ (1436 cm⁻¹, 1496 cm⁻¹, 1590 cm⁻¹ and 1633 cm⁻¹). The strongest line appeared at 1436 cm⁻¹. In addition to the above another smaller strong line is observed at 1633 cm⁻¹ and rest two lines are also of high intensities for [5, 6]. For C₆₀O [6, 6] three significant Raman lines are observed at 1436 cm⁻¹, 1462 cm⁻¹ and 1633 cm⁻¹. All these lines are of high intensities with the line at 1436 cm⁻¹ being the strongest among these three. It should be noted that the two lines at 1436 cm⁻¹ and 1633 cm⁻¹ are found in both spectra of C₆₀O. Between these two lines, the line at 1436 cm⁻¹ for C₆₀O [5, 6] is stronger than C₆₀O [6, 6] while at 1633 cm⁻¹ the line for [6, 6] has higher intensity than [5, 6].

KEYWORDS: C₆₀O, Raman spectra and Hartree-Fock Method

I. INTRODUCTION

The simplest fullerene oxide, C₆₀O is an interesting chemical species. This simple fullerene derivative C₆₀O serves as a starting material for more complex fullerene oxides [1, 2] in addition to an important ingredient in the synthesis of a range of chemical compounds. [1-10] C₆₀O has an improved antioxidant activity [11] along with much shorter lifetime in its triplet state when compared to fullerene [12]. It was interesting suggestion from theoretical calculations that the oxygen atom could also be encapsulated inside the fullerene cage if it acquires enough energy to overcome both the bond formation of exohedral C₆₀O in addition to the potential barrier to endohedral O@C₆₀ complex. It was estimated to be about 89 kcal/mol at the B3LYP/3-21G level [13]. Creegan et al [14] was the first reported the synthesis of C₆₀O in 1992. Many experiments [12, 15-18] along with the theoretical [19-25] research have been focus studied the structure and stability of C₆₀O where the oxygen can bridge either to the carbon atoms adjacent two six-membered rings ([6,6] epoxide form) or one five- plus one six-membered ring ([5,6] open form). However it has been found from ¹³C NMR and IR measurements [14] that C₆₀O should be the epoxide C_{2v} structure with an oxygen atom connecting two six-membered rings but later it was confirmed using fullerene ozonide by Weisman et al. [16] experimentally that both the epoxide [6, 6] and open (annulene-like) [5, 6] isomeric form can be prepared, depending on how C₆₀O is synthesized. He found that such fullerene ozonide C₆₀O₃ can be separated into either the [6, 6] form (in the case of thermolysis) or the [5, 6] form (in the case of photolysis) [16].

In theory, there have been numerous ab initio and semiempirical studies suggesting that the [5,6] isomer is slightly more stable than the [6,6] isomer [18-21] and reorganize between the two isomers involves two transition states and an intermediate state corresponding to local minimum, [19, 21] it has to be note down that the methodologies utilized for these studies could not account for the precise electron correlation or basis set effect on the equilibrium geometries and relative stability between the two isomers for this molecule, particularly considering apparently small energy difference between the two isomers predicted from previous studies. It is interestingly that, a couple of molecular dynamics [22, 23] as well as atomic force calculation [24] studies predicted the epoxide [6, 6] form as the more stable species than the open [5, 6] structure. Thus, in apparent of disagreement between a range of theoretical calculation results and experimental findings, it appears necessary to examine this molecule employing more

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sophisticated methods that should incorporate sufficient electron correlation treatment with large basis set effect as well as investigating vibrational and thermal contributions to the stability of the molecule.

In this paper systematically compute raman spectra of $C_{60}O$ ([6, 6] and [5, 6] isomers) using Hartree-Fock method.

II. COMPUTATIONAL DETAILS

Structure of $C_{60}O$ Isomers: $C_{60}O$ [5, 6] and $C_{60}O$ [6, 6]

The simplest structure of $C_{60}O$ molecule model has sixty carbon nuclei reside on a sphere with an oxygen atom connected two carbon atoms. In the given paper $C_{60}O$ has two isomers $C_{60}O$ [5, 6] and $C_{60}O$ [6, 6] as shown in **Figure 1(a)** and **1(b)**. $C_{60}O$ [5, 6] has oxygen atom sharing with one hexagon and one pentagon of the fullerene (**Figure 1(a)**) and the other isomer $C_{60}O$ [6, 6] shares an oxygen atom with two hexagons (carbon atoms) of fullerene as shown in **Figure 1(b)**. The average bond length of C-C bond lengths of the structure $C_{60}O$ may be taken to be same and π electrons are evenly delocalized all over bonds except those at carbon with an oxygen atom.

In earlier work Cardini *et.al* [27] the experimental and result of calculations for IR spectra were presented for $C_{60}O$ molecule without distinguishing between two isomers $C_{60}O$ [5, 6] and $C_{60}O$ [6, 6]. Later in Sohn *et al* [28] two isomers $C_{60}O$ [5, 6] and $C_{60}O$ [6, 6] were reported to exist. Calculations of Raman spectra for these two isomers are carried out and presented here.

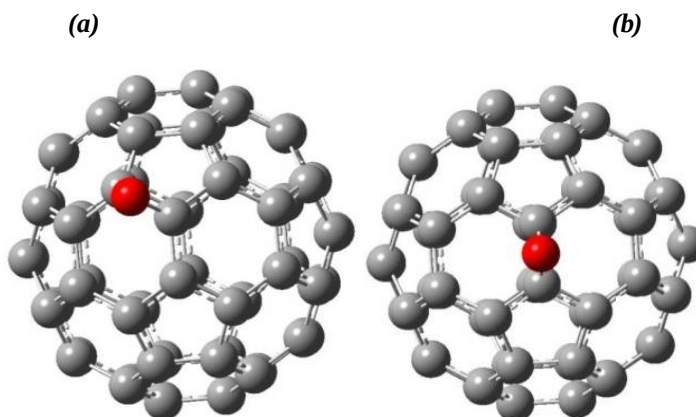


Figure 1 (a) $C_{60}O$ configurations corresponding to [5, 6] (b) $C_{60}O$ [6, 6]. Oxygen atoms are shown in red and grey are carbon atoms.

Despite the symmetry of $C_{60}O$ molecule, the eigenvectors are, in general, somewhat difficult to visualize. In the present work the equilibrium structural geometry of $C_{60}O$ [5, 6] and $C_{60}O$ [6, 6] were determined through full optimization of geometrical parameters using the Hartree-Fock Method without any constraint. The optimized structural parameters of $C_{60}O$ [5, 6] and $C_{60}O$ [6, 6] are given in **Table 1** and **Table 2** respectively.

Table 1 and **Table 2** respectively show the results of optimized structure parameters of $C_{60}O$ [5, 6] and $C_{60}O$ [6, 6] as well as previous calculations of Cardini *et al* and Sohn *et al* [27, 28]. In **Table 1** these optimized parameters of calculations of Cardini *et al* are given in column (2) and those of Sohn *et al* for $C_{60}O$ [5, 6] isomer are in column (3) and column (4) show the present optimized value of $C_{60}O$. Similarly in **Table 2**, the optimized structure of $C_{60}O$ [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 oxygen atom and C'-O-C' is the angle between oxygen atom and its nearest two carbon atoms. C-C'-C is the angle between the carbon atom (attached with oxygen 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 $C_{60}O$ [5, 6] isomer. It may be seen that results of [27] generally compare with the present results while the results of [28] do not compare for isomer $C_{60}O$ [5, 6]. The bond lengths of C-C hexagon as well as C-C pentagon markedly vary for [27] in comparison with the present results. The angle C'-O-C' is quite different (67.7°) in the present calculations in

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comparison with [28] (104.2°) while it compares with [27] (65°). Additional geometry information is also provided for the present calculation in **Table 1** which are not available in [27] and [28].

Table 1 gives results of geometrical parameters for C₆₀O [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 C₆₀O [6, 6] isomer which are not available in [27, 28].

Table 1 Results of calculation of C₆₀O [5, 6]

1.	2. Results of calculation [ref. 27]	3. Results of calculation [ref. 28]	4. Present calculation Results
	C ₆₀ O	C ₆₀ O [5,6]	C ₆₀ O [5,6]
C – C hexagon	1.407-1.479 Å	2.193 Å	1.365 -1.441 Å
C – C pentagon	1.407-1.479 Å	2.193 Å	1.375 -1.464 Å
C - C'	1.468 Å	-	1.463- 1.515 Å
C' - C'	1.538 Å	-	1.600Å
C' - O	1.430 Å	1.390 Å	1.43616 Å
Angle (C'-O-C')	65°	104.2°	67.7°
Angle (C-C'-C') pentagon	-	-	105.2°
Angle (C-C'-C) hexagon	-	-	116.8°
Angle (C'-C'-C) hexagon	-	-	115.8°
Angle (C-C-C) pentagon	107.6 - 108.5°	-	107.7 -108.9°
Angle (C-C-C) hexagon	118.8 - 121.4°	-	118.4 -121.4°
Dipole moment	-	-	1.159 D
Basis Set	-	6-31G	STO-3G

Table 2 Results of calculation of C₆₀O [6, 6]

1.	2. Results of calculation [ref. 27]	3. Results of calculation [ref. 28]	4. Present calculation Results
	C ₆₀ O	C ₆₀ O [6,6]	C ₆₀ O [6,6]
C – C hexagon	1.407-1.479 Å	1.511 Å	1.366 -1.379 Å
C – C pentagon	1.407-1.479 Å	1.511 Å	1.450 -1.492 Å
C - C'	1.468 Å	-	1.509 - 1.509Å
C' - C'	1.538 Å	-	1.533 Å
C' - O	1.430 Å	1.447 Å	1.434 Å
Angle (C'-O-C')	65°	63.1°	64.6°
Angle (C-C'-C) pentagon	-	-	105.7°
Angle(C'-C'-C) hexagon	-	-	117.0°
Angle (C-C-C) pentagon	107.6 - 108.5°	-	107.4 - 108.9°
Angle (C-C-C) hexagon	118.8 - 121.4°	-	120.0 - 121.7°
Dipole moment	-	-	1.159 D
Basis Set	-	6-31G	STO-3G

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The bond lengths of C-C hexagon as well as C-C pentagon markedly vary for [27] in comparison with the present results. The angle C'-O-C' is comparable (64.6°) in present calculations with [27] (65°) and [28] (63.1°). It may be seen that in the present results pentagon angles and hexagons angle for C₆₀O [5, 6] and C₆₀O [6, 6] compare very well with the result of [27].

The raman spectra for the two isomers C₆₀O [5, 6] and C₆₀O [6, 6] are given in **Figures 2(a)-(b)**. The variables used in the calculations of raman of C₆₀O by the program are: the rotational constants used in x, y, and z directions in the fullerenes derivative (C₆₀O) are 0.09, 0.08 and 0.08 (GHz) respectively, the C₆₀O has 305 symmetry adapted basis functions, 915 primitive gaussians, 305 cartesian basis functions, 184 alpha electrons and 184 beta electrons with the nuclear repulsion energy of 9190.52 Hartree. The most significant change in the raman spectrum induced by the substitution of oxygen in fullerene is the redistribution of the raman intensity among the normal modes as shown in the **Table 3-4**. Starting with 183 total degrees of freedom for an isolated C₆₀O 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 C₆₀O [5, 6] and C₆₀O [6, 6] isomers have same number of 177 degrees of freedom yet they exhibit different spectra

III. METHODOLOGY:

All calculation of Raman Spectrum has been done according to [26]. The values of variables used in the calculations for the program are as follows: the rotational constants in x, y and z axes in the C₆₀O [5, 6] and C₆₀O [6, 6] are 0.09, 0.08 and 0.08 (GHz) respectively. The C₆₀O [5, 6] and C₆₀O [6, 6] have same number of 305 basis functions, 915, primitive gaussians, 305 cartesian basis functions, 184 alpha electrons and 184 beta electrons with the nuclear repulsion energy as 9191.80 Hartree for C₆₀O [5, 6] and is 9190.52 Hartree in the case of C₆₀O [6, 6]. The numerical results converged after 17 cycles and 15 cycles with density matrix = 0.6764D-08 and density matrix = 0.5915 D-08 for C₆₀O [5, 6] and [6, 6] respectively.

IV. RESULTS OF RAMAN SPECTRA OF C₆₀O [5, 6] and C₆₀O [6, 6]

Using the experience gained from the above prediction of C₆₀ the results of C₆₀O have also been scaled down by the same factor of 0.855. The results of calculations of Raman Spectrum for C₆₀O [5, 6] and [6, 6] are displayed in **Figure 2 (a)-(b)** and in **Table 3-4** and are given below:

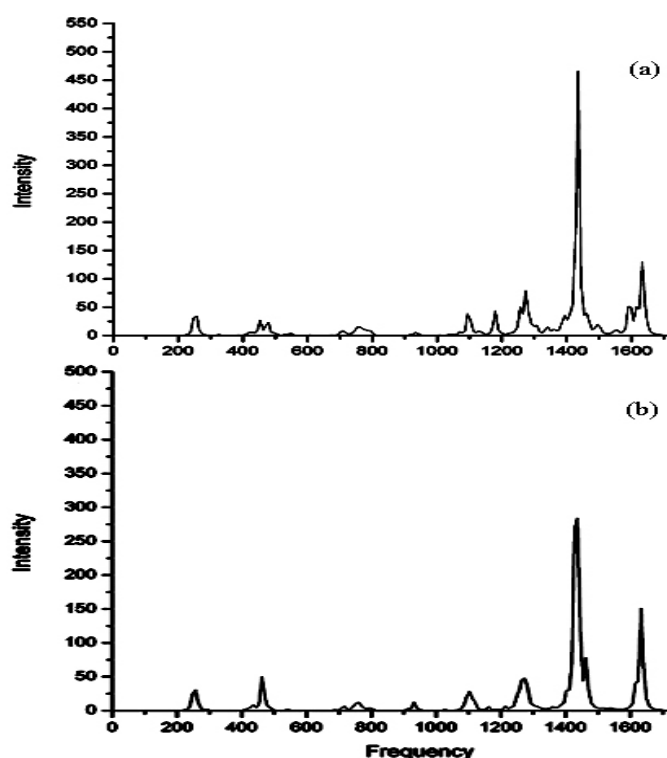


Figure 2 Raman spectrum of (a) C₆₀O [5, 6] (b) C₆₀O [6, 6].

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The Raman spectra optimized structural parameters of $C_{60}O$ provided in **Table 3-4** are used in carrying out the calculations of Raman spectra for $C_{60}O$. The notable change in the Raman spectra are seen by addition of oxygen atom in C_{60} when compared with the spectrum of C_{60} in **Figure 2(a)-(b)**. It may be seen that only 10 Raman peaks are observed in the spectrum of C_{60} while greater number of peaks are seen in the spectra of $C_{60}O$ by addition of an oxygen atom to C_{60} . The redistribution in the case of $C_{60}O$ [5, 6] and [6, 6] of the Raman intensity is given in **Tables 3 - 4** and in **Figure 2 (a)-(b)**. 14 major Raman peaks in addition to certain weak peaks are seen in the spectra of $C_{60}O$ [5, 6] while 11 major Raman peaks with weak peaks are observed in $C_{60}O$ [6, 6] in **Tables 3 - 4** and **Figure 2 (a)-(b)**. The Raman spectra of $C_{60}O$ [5, 6] and [6, 6] may be mainly divided into four regions namely: 200 - 600 cm^{-1} ; 600 - 1000 cm^{-1} ; 1000 - 1400 cm^{-1} and; 1400 - 1701 cm^{-1} . The highest intensity in the case of $C_{60}O$ [5, 6] and [6, 6] are calculated in the range 1400 - 1701 cm^{-1} and the lowest intensity in 600 - 1000 cm^{-1} range. In the range of 200 - 600 cm^{-1} for $C_{60}O$ [5, 6] and [6, 6], each spectrum has 3 significant peaks. The first two peaks in the case of $C_{60}O$ [5, 6] occur at 257 cm^{-1} , 453 cm^{-1} and in the case of $C_{60}O$ [6, 6] at the frequencies 257 cm^{-1} , 436 cm^{-1} . The third significant peak for $C_{60}O$ [5, 6] at 479 cm^{-1} occurs and in case of $C_{60}O$ [6, 6] is seen at 462 cm^{-1} .

Each spectrum of $C_{60}O$ [5, 6] and [6, 6] in the range of 600 - 1000 cm^{-1} has two significant peaks. In case of $C_{60}O$ [5, 6] at 710 cm^{-1} , 761 cm^{-1} and for $C_{60}O$ [6, 6] at 718 cm^{-1} , 761 cm^{-1} with $C_{60}O$ [5, 6] having higher intensities than $C_{60}O$ [6, 6]. Five major Raman lines are obtained for $C_{60}O$ [5, 6] while only two lines are calculated in the frequency range 1000 - 1400 cm^{-1} for $C_{60}O$ [6, 6]. First-three and fifth Raman lines of $C_{60}O$ [5, 6] show high intensities (1094 cm^{-1} , 1180 cm^{-1} , 1257 cm^{-1} and 1394 cm^{-1}) while the fourth Raman line (1342 cm^{-1}) appears with lower intensity. Raman lines of $C_{60}O$ [6, 6] at 1103 cm^{-1} and 1274 cm^{-1} appear with higher intensities than those of [5, 6].

Four significant Raman lines are seen for [5, 6] in the range of frequencies of 1400-1701 cm^{-1} (1436 cm^{-1} , 1496 cm^{-1} , 1590 cm^{-1} and 1633 cm^{-1}). The strongest line appeared at 1436 cm^{-1} . In addition to the above another smaller strong line is observed at 1633 cm^{-1} and rest two lines are also of high intensities for [5, 6]. For $C_{60}O$ [6, 6] three significant Raman lines are observed at 1436 cm^{-1} , 1462 cm^{-1} and 1633 cm^{-1} . All these lines are of high intensities with the line at 1436 cm^{-1} being the strongest among these three. It should be noted that the two lines at 1436 cm^{-1} and 1633 cm^{-1} are found in both spectra of $C_{60}O$. Between these two lines, the line at 1436 cm^{-1} for $C_{60}O$ [5, 6] is stronger than $C_{60}O$ [6, 6] while at 1633 cm^{-1} the line for [6, 6] has higher intensity than [5, 6].

V. CONCLUSIONS

It may be observed that only 10 Raman peaks are observed in the spectrum of C_{60} while greater number of peaks is seen in the spectra of $C_{60}O$ by addition of an oxygen atom to C_{60} . The highest intensity in the case of $C_{60}O$ [5, 6] and [6, 6] are calculated in the range 1400 - 1701 cm^{-1} and the lowest intensity in 600 - 1000 cm^{-1} range. Four significant Raman lines are seen for [5, 6] in the range of frequencies of 1400-1701 cm^{-1} (1436 cm^{-1} , 1496 cm^{-1} , 1590 cm^{-1} and 1633 cm^{-1}). The strongest line appeared at 1436 cm^{-1} . In addition to the above another smaller strong line is observed at 1633 cm^{-1} and rest two lines are also of high intensities for [5, 6]. For $C_{60}O$ [6, 6] three significant Raman lines are observed at 1436 cm^{-1} , 1462 cm^{-1} and 1633 cm^{-1} . All these lines are of high intensities with the line at 1436 cm^{-1} being the strongest among these three. It should be noted that the two lines at 1436 cm^{-1} and 1633 cm^{-1} are found in both spectra of $C_{60}O$. Between these two lines, the line at 1436 cm^{-1} for $C_{60}O$ [5, 6] is stronger than $C_{60}O$ [6, 6] while at 1633 cm^{-1} the line for [6, 6] has higher intensity than [5, 6].

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Table 3 Raman Spectrum of $C_{60}O$ [5, 6]

Frequency	Intensity	Frequency	Intensity	Frequency	Intensity	Frequency	Intensity
171	0.2	556	1.6	941	3.6	1325	5.1
180	0.2	564	0.7	949	1.2	1334	10.3
188	0.3	573	0.5	958	0.9	1342	15.4
197	0.4	581	0.7	966	0.4	1351	7.9
205	0.5	590	0.5	975	0.3	1359	11
214	0.7	599	0.4	983	0.3	1368	8.8
222	1.2	607	1.3	992	0.4	1377	9.7
231	2.4	616	0.5	1000	1.1	1385	22.6
239	6.7	624	0.3	1009	1.3	1394	35.8
248	31.6	633	0.2	1017	0.7	1402	27.2
257	34.5	641	0.2	1026	0.7	1411	40
265	10.7	650	0.3	1035	1.8	1419	55.4
274	3.2	658	0.6	1043	2.4	1428	189.9
282	1.5	667	1	1052	1.3	1436	466
291	1	675	1.2	1060	2	1445	87.4
299	1	684	1.1	1069	6.6	1454	35.7
308	0.7	693	1.7	1077	4.9	1462	39.7
316	0.7	701	6.4	1086	7.9	1471	22.1
325	2	710	8.4	1094	38.9	1479	10.7
333	1	718	4.9	1103	26.9	1488	13.7
342	0.6	727	2.5	1112	7.2	1496	20
351	0.5	735	3.5	1120	5.4	1505	13.5
359	0.7	744	7.6	1129	7.8	1513	5.1
368	0.5	752	14.5	1137	6	1522	3.6
376	0.5	761	15.3	1146	2.6	1530	3.3
385	1.4	770	12.5	1154	2.5	1539	4.5
393	0.9	778	10	1163	4.3	1548	8.4
402	1.3	787	8.9	1171	14	1556	10.2
410	2.2	795	8.6	1180	43.6	1565	5.3
419	5.9	804	2.1	1188	10.7	1573	6.1
428	5.6	812	1	1197	5.1	1582	12.1
436	4.3	821	0.7	1206	2.7	1590	51.1
445	9.2	829	0.5	1214	2.6	1599	50.2
453	27.3	838	0.3	1223	4.3	1607	25.8
462	9.5	846	0.2	1231	4.7	1616	51
470	16.7	855	0.2	1240	8	1625	47
479	23.1	864	0.2	1248	15.3	1633	130.3
487	6.1	872	0.2	1257	50.5	1642	57.5
496	4.7	881	0.2	1265	37.6	1650	20.4
504	3.1	889	0.3	1274	79	1659	7.1
513	1.3	898	0.7	1283	38.8	1667	3.8
522	1.1	906	0.5	1291	20.5	1676	2.4
530	2.1	915	1.6	1300	16.5	1684	1.7
539	2.1	923	2.2	1308	17.8	1693	1.3
547	4.3	932	5.1	1317	6.6	1701	1

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Table 4 Raman Spectrum of $C_{60}O$ [6, 6]

Frequency	Intensity	Frequency	Intensity	Frequency	Intensity	Frequency	Intensity
171	0.2	556	0.7	941	3	1325	3.4
180	0.2	564	0.3	949	2.4	1334	2.5
188	0.3	573	0.2	958	0.8	1342	2.5
197	0.3	581	0.2	966	0.4	1351	3
205	0.5	590	0.2	975	0.3	1359	5.8
214	0.7	599	0.1	983	0.2	1368	4.8
222	1.1	607	0.1	992	0.2	1377	5.1
231	2	616	0.1	1000	0.2	1385	8
239	5.1	624	0.1	1009	0.3	1394	11.2
248	24.4	633	0.1	1017	0.4	1402	29.2
257	31	641	0.1	1026	1.4	1411	30.2
265	12.3	650	0.2	1035	1	1419	67.9
274	3.4	658	0.4	1043	0.5	1428	268
282	1.7	667	0.3	1052	0.7	1436	284.1
291	2	675	0.4	1060	0.9	1445	123.7
299	1	684	1.3	1069	1.3	1454	43.5
308	0.6	693	0.9	1077	2.6	1462	78.2
316	0.4	701	1.3	1086	8.4	1471	32.1
325	0.5	710	5.1	1094	20.4	1479	11.6
333	0.4	718	6.1	1103	28.3	1488	6.7
342	0.6	727	1.8	1112	17.3	1496	4.6
351	0.7	735	2.3	1120	13.2	1505	3.5
359	0.4	744	6.5	1129	3.4	1513	3.3
368	0.3	752	10.4	1137	1.8	1522	3.4
376	0.3	761	12.3	1146	1.4	1530	2.5
385	0.4	770	6.6	1154	1.9	1539	3.8
393	0.6	778	3.7	1163	6.1	1548	2.5
402	0.8	787	3.1	1171	1.8	1556	2.3
410	1.7	795	3.8	1180	1.1	1565	2
419	3.2	804	2.5	1188	1.2	1573	2.1
428	5.3	812	0.8	1197	1.5	1582	2.4
436	8.7	821	0.6	1206	2.1	1590	3.3
445	4.4	829	0.5	1214	6.4	1599	5.1
453	9.2	838	0.3	1223	3.2	1607	10.6
462	50.1	846	0.2	1231	4.9	1616	40
470	21.7	855	0.2	1240	6.2	1625	43.9
479	7.2	864	0.2	1248	20.5	1633	151.1
487	4.6	872	0.2	1257	29	1642	62
496	1.7	881	0.2	1265	45.3	1650	17.8
504	1	889	0.3	1274	48.1	1659	6.9
513	0.7	898	0.5	1283	34	1667	3.7
522	0.5	906	1.4	1291	11.8	1676	2.4
530	0.6	915	3	1300	8.5	1684	1.6
539	1.4	923	2.9	1308	6.3	1693	1.2
547	1.1	932	12.8	1317	5.6	1701	0.9

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