

Modelling and Vibrational Structure of C_{60} and C_{80}

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Abstract

Fullerene derivatives have been shown to contribute in many applications. As a result, both structural and vibrational properties of C_{60} and C_{80} fullerenes and their epoxides are studied by quantum mechanical semiempirical PM3 method. Results indicate a similarity between the structures of fullerenes as compared with their epoxides in one hand and the studied dimers on the other hand. The final heat of formation is higher in case of C_{80} and its epoxide as compared with that of C_{60} . Results showed that, the calculated C_{60} spectra are higher than experimental spectra in terms of both anharmonicity effects and electron correlation.

Key words: PM3, C_{60} , C_{80} , fullerene epoxide, vibrational spectra

Introduction

The structure of C_{60} was discovered, in 1985 by Harold Kroto et al.¹ Five years later, Krätschmer et al.² investigated a technique for synthesizing C_{60} as a bulk solid. Later on, C_{60} was prepared in both powder form and bulk quantities.³ The vibrational Raman spectra for both C_{60} and C_{70} were obtained.⁴ The fine intramolecular vibrational modes of crystalline C_{60} were elucidated using high-resolution FT Raman spectroscopy.⁵ The surface morphology, optical absorption characteristics and structure of C_{60} cluster thin films which were obtained by thermal evaporation have been investigated.⁶ C_{60} solid film was irradiated with pulsed UV-laser-light, as a result, a surface transformation of the irradiated films has been observed. A new carbon phase has been formed with diamond-like sp^3 bonding through an oxygen-assisted fullerene cage opening.⁷ A modified method of Raman scattering study for C_{60} dimer was described by Lededkin et al.⁸ The vibrational spectrum of C_{60} has been obtained through quantum chemical calculations.⁹ The equilibrium geometry of C_{60} has been calculated.¹⁰ Electron correlations are shown to have a significant influence on the calculated bond distances (1.446 and 1.406 Å). A program package for solving the vibrational Schrödinger equation in one and two dimensions was developed by Stare and Mavri.¹¹ Accordingly, the IR spectra can be calculated beyond the limit of electrical harmonicity. Furthermore, the Raman spectra can replace the dipole moment function by the corresponding polarizability function. It is demonstrated that, the Grid basis set has several advantages over the Gaussian basis set for realistic, anharmonic systems.

Using a tight-binding potential model both structural and vibrational properties of C_{60} and C_{70} fullerenes were studied.¹² It is shown that this tight-binding molecular-dynamics scheme has accuracy comparable to ab initio techniques. The structure, energetic, and vibrational properties of five different $[C_{60}]_N$ oligomers ($N=2, 3,$ and 4) were studied using Density Functional based nonorthogonal tight-binding (DF-TB).¹³ Quantum molecular dynamics are used to assign the predominant $I_h C_{60}$ symmetries of observed modes. The vibrational structure in the phosphorescence spectrum of C_{60} is studied using molecular modelling.¹⁴ The spectral studies of the molecular dynamics of some adducts of C_{60} to TTF was investigated.¹⁵ Using ab initio calculations it is found that, g- C_{80} and g- C_{240} cages are less stable than their graphite isomers and have smaller HOMO-LUMO gaps.¹⁶ Terso potential molecular dynamics was used to investigate the interaction between C_{60} molecules and a diamond substrate. It is observed that the impact of C_{60} molecules on the diamond substrate seldom results in the formation of an sp^3 structure.¹⁷ The C_{60} structure dependence on the C_{60} fullerene concentration in water was studied using UV-VIS, Raman, IR-spectroscopy and small-angle neutron scattering (SANS) as well as PM3 semiempirical calculations.¹⁸ Using AM1 (UHF) type calculations the substitutionally B, N and P doped C_{80} structures were found to be stable.¹⁹ Finally, either C_{60} or C_{80} are linked into polymeric chains, and as a result nanotubes are produced.^{20–22} The potential acute and sub chronic toxic effects of fullerenes (C_{60}) applied in benzene on the mouse skin were studied. The obtained data indicate that fullerenes applied in benzene at a likely industrial exposure level do not cause acute toxic

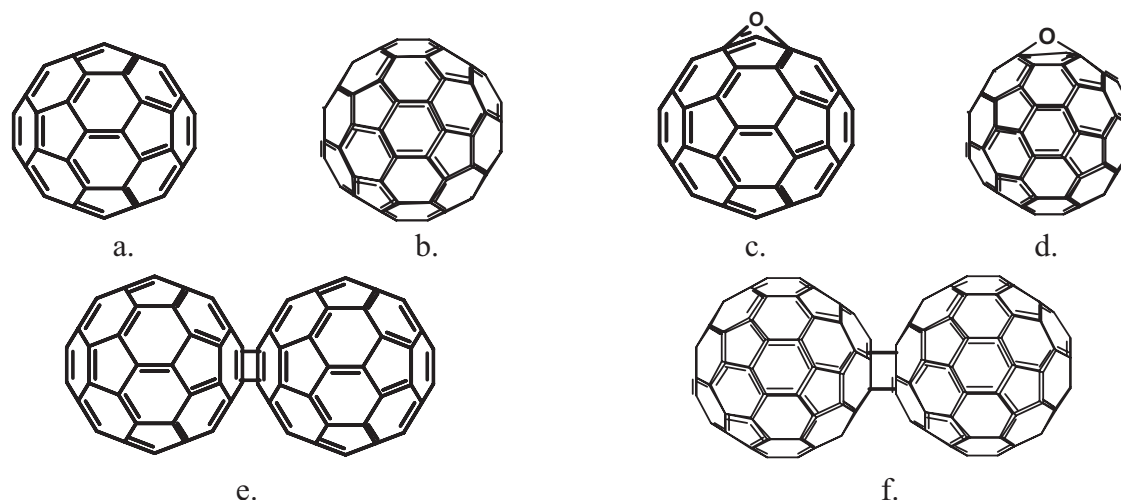


Figure 1. Optimized structure of a.: C₆₀, b.: C₈₀, c.: C₆₀-O, d.: C₈₀-O, e.: C₆₀ dimer, and finally f.: C₈₀ dimer which are calculated at Mopac PM3 semiempirical level.

effects on the mouse skin epidermis.²³ Genotoxicity of fullerene C₆₀ has been determined in a prokaryotic in vitro test and in an eukaryotic in vivo system. Only at the highest possible fullerene concentration of 2.24 micrograms per 1 mL medium, a slight genotoxic effect was observed in wing cells. Fullerol demonstrates no mutagenic effect at a concentration of 2.46 mg/mL.²⁴

In the present work both the structure and vibrational spectra were evaluated for two fullerenes C₆₀, C₈₀ with their dimers as well as their epoxide isomers.

Calculation details

Calculations were carried out on a personal computer, using semiempirical quantum mechanics package, MOPAC 2002 which implemented with the version 1.33 CAChe Program (by Fujitsu), at the Spectroscopy Department, National Research Center, Egypt. The initial geometry optimization of both C₆₀ and C₈₀ was performed with the molecular mechanics (MM+) force field. The lowest energy conformations obtained by MM+, the method were further optimized at semiempirical methods PM3.²⁵

Results and discussion

MOPAC is used directly to predict numerous chemical and physical properties, such as geometry and infrared spectra. All the studied molecules were first subjected to geometry optimization at semiempirical PM3 level then the vibrational spectra were calculated at the same level.

Optimized geometry parameters: The geometry of both C₆₀, C₈₀ and their dimers as well as their epoxides are optimized. The optimized geometries of which are shown in Figure 1. It is found from the optimized structure that, the molecular point group of C₆₀ is corresponding to I_h symmetry. For C₈₀ the symmetry number for point group Ci is equal to 1. On the other hand, the symmetry number for point group C_s is also 1, for both of C₆₀-O and C₈₀-O. In addition, both molecules are in ground state and are not linear. For each of the studied fullerenes all carbon atoms are equivalent.

Table 1. Calculated bond lengths in angstrom for both C₆₀, C₈₀ and their epoxides as well as their dimers which are optimized at MOPAC, PM3 semiempirical level.

Bond distance, Å	C ₆₀		C ₈₀			
	monomer	epoxide	dimer	monomer	epoxide	dimer
C-C	1.4045	1.3839	1.3927	1.4322	1.4322	1.4324
C-O		2.3934			2.9536	
COC angle		152.7			111.5	

The distances between the carbon atoms are calculated as in Table 1. For both C₆₀ and C₈₀, the C-C distance increased from 1.4045 Å to 1.4322 Å respectively. Oxygen is bonded to the two six rings, 6-6 bond, potentially forming a three COC ring. The isomer under investigation is the epoxide 6-6 bonded. The distance C-C was nearly quite similar in case of C₆₀ and its epoxide. Furthermore, C-C shows identical bonds for C₈₀ and its epoxide. Again, the distance C-O is longer for C₈₀ epoxide than C₆₀ epoxide in contrast to the angle COC. This means that C₈₀ epoxide is characterized by

a very long bridging carbon distance as compared with C_{60} . Studying the structure of carbon dimer is the first step towards understating the structure of carbon crystal. Regarding Table 1 and comparing C–C distances of both dimer as well as monomer, it is clear that the C–C distance was not affected as a result of dimerization.

Infrared spectra: The calculated spectra are tabulated in both Table 2 and Table 3, and the spectra are illustrated in Figure 2. According to the calculated vibrational spectra the number of genuine vibrations is 174 and 177 for C_{60} and its epoxide. The similar vibrations for C_{80} and its epoxide were 234 and 237 respectively. All the vibrational modes are mentioned and tabulated.

Although C_{60} possesses 174 ($3 \times 60 - 6$) normal vibrations, it exhibits only 4 characteristic vibrational modes according to their higher IR intensity, and hence there are only 4 active bands. A C_{60} line at 591.94 cm^{-1} is observed, and assigned as lowest frequency H_g “squashing” mode of Buckminsterfullerene. Accordingly the $A_g(1)$ mode was obtained at around 781.83 cm^{-1} . The two strong C_{60} lines, found at 1444.65 cm^{-1} and 1797.99 cm^{-1} , can accordingly be assigned to the two totally symmetric $A_g(2)$ modes. As compared to C_{60} , $C_{60}\text{-O}$ showed a shift in the four characteristic bands towards the lower frequencies, in addition two bands appear at 393.61 cm^{-1} and 1138.96 cm^{-1} due to the existing of oxygen. It is worth to mention that, C_{80} has 8 intense vibrational modes. The spectra of C_{80} showed the same vibrational feature of C_{60} with a noticeable shift towards a lower frequency. $C_{80}\text{-O}$ showed 10 intense vibrational bands, the four characteristic bands are considerably shifted towards lower frequencies. Finally, the striking reduction in the number of active bands as compared with the total calculated bands is evidently due to the molecule’s extremely high symmetry (I_h point group).

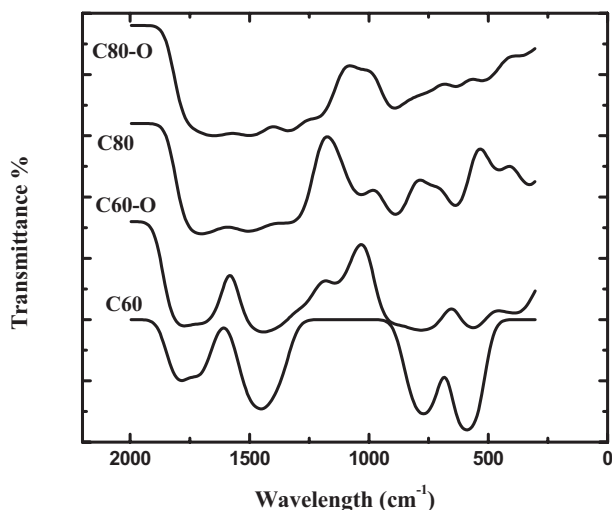


Figure 2. Active vibrational modes for C_{60} as well as its epoxide $C_{60}\text{-O}$ and C_{80} and its epoxide $C_{80}\text{-O}$.

Comparison with Experimental results: Figure 3 presents the experimental FTIR spectrum.²⁶ of 1.4 mm thick film of C_{60} . The figure shows the four characteristic bands of C_{60} . The comparison between calculated and experimental frequencies revealed that, the calculated bands are shifted to higher frequencies. The reason is that, the harmonic vibrational frequencies are typically higher than the fundamental ones which are observed experimentally. A major source of this disagreement is the neglect of anharmonicity effects in the theoretical treatment. In addition, an error also arises because of incorporation of electron correlation.

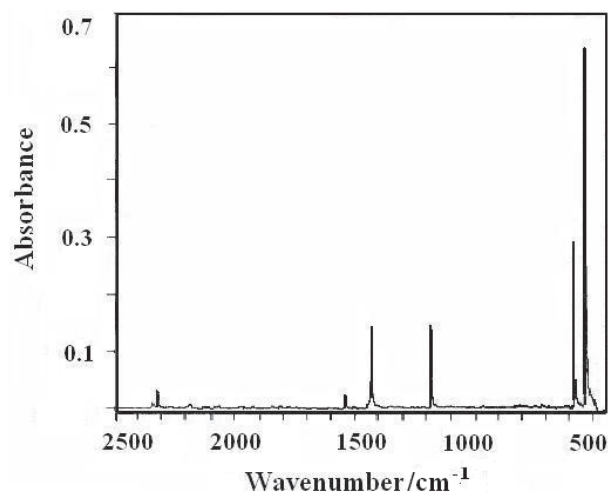


Figure 3. FTIR spectra of 1.44 mm thick film of C_{60} .

Final heat of formation: Other important physical parameter which is calculated for the studied fullerene is the final heat of formation. It is relates to the elements in their standard state at 298 K. The final heat of formation is calculated as $-811.087 \text{ kcal/mol}$ at 298 K.

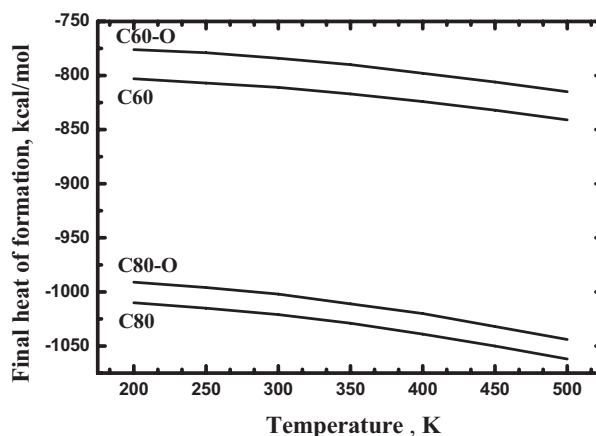


Figure 4. The change in final heat of formation in kcal/mol, as a function of temperature in K for C_{60} , C_{80} , $C_{60}\text{-O}$ and finally $C_{80}\text{-O}$ respectively.

Table 2. Calculated vibrational spectra for C_{60} and its epoxide.

C_{60}					$C_{60}\text{-O}$				
266.38	266.38	266.38	266.38	266.38	241.44	250.58	261.79	266.82	269.05
354.94	354.94	354.94	356.00	356.00	329.71	331.13	346.10	349.03	351.29
356.00	356.00	406.43	406.43	406.43	355.91	356.99	363.33	380.59	393.61
406.43	406.43	440.18	440.18	440.18	398.08	404.95	423.36	423.36	432.36
440.18	440.18	488.09	488.09	488.09	434.59	437.21	440.85	449.40	474.99
488.09	546.77	546.77	546.77	546.77	480.59	483.24	489.76	522.55	527.77
546.77	557.93	557.93	557.93	584.80	531.22	537.88	542.43	543.93	546.87
584.80	584.80	591.94	591.94	591.94	550.70	558.42	575.09	576.89	585.78
591.94	612.71	612.71	612.71	622.75	590.11	591.71	601.75	606.97	607.38
699.58	699.58	699.58	699.58	699.58	611.96	613.35	659.47	684.26	685.76
732.98	732.98	732.98	757.57	757.57	697.05	701.96	703.81	711.92	725.17
757.57	757.57	757.57	762.34	762.34	732.42	732.72	746.89	752.93	757.03
762.34	781.83	781.83	781.83	781.83	759.29	759.42	760.59	779.11	779.79
815.28	815.28	815.28	815.28	815.28	788.41	795.80	798.64	803.26	804.94
816.34	816.34	816.34	850.21	850.21	809.60	813.97	816.61	817.44	835.91
850.21	850.21	865.28	865.28	865.28	837.64	840.34	850.11	850.30	865.07
908.84	908.84	908.84	908.84	912.56	865.31	872.54	890.38	907.52	908.46
912.56	912.56	940.96	940.96	940.96	910.16	910.94	912.00	916.57	920.23
940.96	940.96	977.11	1124.37	1124.37	921.93	932.77	942.11	946.06	970.61
1124.37	1124.37	1158.55	1158.55	1158.55	1073.59	1104.78	1124.38	1124.86	1138.96
1245.80	1245.80	1245.80	1245.80	1290.04	1146.69	1162.08	1198.88	1235.83	1241.89
1290.04	1290.04	1290.04	1290.04	1337.55	1245.46	1253.70	1272.89	1273.20	1288.00
1337.55	1337.55	1376.21	1376.21	1376.21	1296.40	1304.00	1324.00	1325.82	1338.95
1377.86	1377.86	1377.86	1377.86	1377.86	1354.59	1365.69	1373.57	1375.11	1375.90
1435.53	1435.53	1435.53	1435.53	1435.53	1382.61	1386.82	1387.01	1412.85	1420.75
1438.83	1438.83	1438.83	1444.65	1444.65	1429.96	1433.49	1437.02	1438.85	1442.75
1444.65	1444.65	1474.87	1474.87	1474.87	1443.29	1445.84	1450.14	1453.70	1456.24
1474.87	1499.72	1499.72	1499.72	1499.72	1470.24	1476.24	1481.25	1493.21	1494.31
1499.72	1516.50	1516.50	1516.50	1654.03	1500.35	1502.79	1502.99	1512.01	1517.43
1654.03	1654.03	1654.03	1668.52	1668.52	1525.34	1528.33	1624.27	1635.48	1641.74
1668.52	1668.52	1668.52	1707.18	1707.18	1660.41	1661.75	1665.84	1666.60	1676.52
1707.18	1728.13	1728.13	1728.13	1728.13	1680.59	1691.87	1708.36	1709.11	1720.95
1750.29	1775.45	1775.45	1775.45	1797.99	1724.51	1731.07	1740.58	1749.50	1767.44
1797.99	1797.99	1797.99	1812.47	1812.47	1774.10	1785.32	1791.56	1793.53	800.26
1812.47	1812.47	1812.47	1812.47		1800.97	1801.30	1808.97	1809.27	1810.24
					1815.76	1819.36			

Figure 4 shows the final heat of formation, studied as a function of temperature from 200 K up to 500 K. The calculated heat of formation was -803.142 kcal/mol at 200 K then changed gradually to reach -841.127 kcal/mol at 500 K. Regarding C_{80} , the calculated heat of formation was -1021.204 kcal/mol at 298 K. As seen in Figure 4 the calculated heat of formation has changed from -1010.100 kcal/mol, up to -1062.175 kcal/mol over a temperature range from 200 up to 500 K. Finally it is clear that, the final heat of formation changes as a function of temperature for both C_{60} and C_{80} . Comparing between both types of carbons, the final heat of formation of C_{80} is lower than that of C_{60} by 210.0 kcal/mol. The calculated final heat of formation has slightly increased by 30 kcal/mol, in case of C_{60} epoxide

and 20 kcal/mol, for the case of C_{80} epoxide. The change in the values of final heat of formation for the studied fullerenes indicates that, this property can be considered as a function of fullerenes molecular structure.

Conclusions

In this work both structure and vibrational properties of both C_{60} and C_{80} were studied using semiempirical PM3 calculations. The obtained results of vibrational frequencies are shifted to higher frequencies as a result of anharmonicity effects in theoretical treatment as well as the incorporation of electron correlation. On the other hand, PM3 results are considered to be fast and satisfactory as compared to other methods.

Table 3. Calculated vibrational spectra for C₈₀ and its epoxide.

C ₈₀					C ₈₀ -O				
162.92	207.92	224.91	225.06	225.85	199.63	210.81	220.93	222.21	222.57
227.54	274.64	286.40	288.26	294.21	271.47	279.95	286.09	287.57	292.23
306.89	326.27	331.29	341.45	342.28	294.93	296.73	309.05	327.11	332.99
353.04	354.71	356.09	363.54	368.35	339.02	347.11	356.15	359.21	363.12
376.13	380.87	395.70	401.48	422.39	363.46	364.60	366.99	376.23	381.54
442.04	449.40	451.01	458.31	464.02	385.93	397.06	439.42	443.25	445.80
470.59	476.64	478.32	483.88	489.29	452.15	454.31	454.66	460.10	465.15
492.65	498.25	502.52	507.08	509.44	473.74	478.01	481.41	485.93	494.65
513.87	521.40	527.98	531.93	538.28	501.56	502.73	505.27	508.39	509.55
540.74	544.34	549.38	555.17	563.38	521.05	526.76	531.39	535.11	538.49
607.34	623.59	625.75	631.06	633.27	542.28	545.62	557.76	595.14	599.00
638.44	640.73	642.57	644.86	650.98	613.31	620.15	622.55	625.60	626.93
655.08	668.59	673.77	676.48	681.55	635.52	640.12	641.82	644.40	650.00
684.37	690.00	694.22	697.37	701.15	655.01	666.55	672.13	677.46	682.53
704.19	720.31	724.53	726.72	732.53	685.82	687.70	689.93	692.05	698.64
733.64	738.90	742.88	764.03	766.39	700.81	722.98	725.38	726.93	731.47
768.40	773.27	775.60	777.12	778.83	735.01	736.43	747.70	756.37	761.55
787.92	791.39	792.41	793.75	830.27	769.12	771.03	772.69	781.09	785.87
833.73	836.03	840.80	843.00	846.98	787.41	790.17	791.20	793.84	795.09
857.28	858.60	859.91	862.10	867.85	799.06	810.27	820.32	821.41	829.35
868.71	870.30	873.79	879.21	881.40	831.51	833.68	834.50	836.59	840.41
901.56	903.82	908.59	910.15	911.04	849.00	854.17	859.09	860.03	864.39
912.58	913.62	914.88	920.66	921.05	866.96	870.37	872.51	876.54	879.48
957.21	1004.95	1007.89	1022.45	1050.01	897.25	900.89	902.32	906.82	909.12
1066.85	1079.50	1082.54	1124.02	1161.26	911.19	912.10	912.17	916.27	917.11
1183.11	1194.77	1201.47	1208.48	1214.49	969.49	991.04	1001.19	1009.14	1031.56
1214.91	1222.54	1236.50	1267.39	1269.37	1048.32	1065.16	1090.39	1133.05	1150.54
1271.06	1294.61	1298.92	1305.58	1308.78	1165.79	1181.53	1191.24	1199.96	1203.58
1310.77	1319.49	1326.98	1329.14	1342.06	1205.06	1209.72	1230.05	1238.69	1258.93
1343.83	1352.29	1360.76	1369.86	1372.70	1266.00	1280.06	1282.92	1285.92	1297.53
1379.20	1382.42	1390.80	1399.99	1403.12	1300.17	1311.12	1324.15	1330.71	1332.59
1416.69	1421.10	1423.97	1442.72	1447.79	1338.21	1339.60	1350.48	1354.55	1362.07
1450.31	1457.36	1471.52	1472.41	1483.62	1365.25	1377.51	1387.85	1392.99	1405.65
1483.70	1494.73	1499.72	1501.94	1509.47	1414.29	1421.21	1425.40	1436.96	1443.86
1514.37	1516.96	1520.72	1526.46	1532.75	1448.59	1448.59	1451.00	1460.04	1462.86
1541.70	1541.74	1557.56	1564.24	1565.15	1462.86	1473.88	1475.71	1479.98	1491.75
1572.68	1573.13	1580.62	1583.96	1589.00	1492.87	1505.47	1508.49	1515.06	1519.75
1590.98	1604.74	1607.72	1610.83	1618.36	1521.05	1522.51	1532.66	1537.35	1540.64
1621.21	1629.69	1632.11	1633.04	1644.69	1543.64	1555.37	1566.59	1572.58	1573.90
1646.25	1654.82	1655.53	1662.30	1668.01	1577.54	1581.38	1582.95	1595.36	1602.07
1683.17	1672.83	1675.26	1693.58	1694.39	1604.57	1610.58	1618.27	1627.35	1635.30
1701.25	1706.57	1708.21	1718.32	1721.78	1638.34	1694.91	1700.55	1705.63	1710.17
1723.64	1724.96	1733.78	1735.94	1743.35	1719.42	1724.13	1726.19	1737.30	1738.10
1745.36	1748.41	1752.33	1757.14	1757.69	1739.74	1742.75	1747.70	1752.42	1755.24
1760.24	1760.39	1763.80	1767.63	1769.43	1758.85	1761.48	1762.09	1763.40	1763.97
1776.44					1767.22	1769.12	1773.03	1777.39	

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Povzetek

Derivati fullerenov so se pokazali za zelo uporabne v različne namene in so zato predmet številnih raziskav. S kvantnomehansko semiempirično metodo PM3 smo raziskali strukturne in vibracijske lastnosti fullerenov C_{60} in C_{80} ter njihovih epoksidov. Rezultati kažejo na podobnosti med strukturami fullerenov in epoksidov ter med njihovimi dimerami. Tvorben entalpija tako C_{80} kot tudi njegovega epoksida je višja od tvorben entalpije ustreznih struktur s C_{60} . Če upoštevamo anharmoničnost in elektronsko korelacijo, so vrednosti frekvenc v izračunanih spektrih za C_{60} višje od eksperimentalnih.