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Quantum Mechanical Study of Biphhenyl Ester Liquid Crystal Molecule

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Abstract
The quantum mechanical calcualtion werer carried out on 4-Substituted phenyl-4-substituted biphenyl-4-carboxylates with methoxy groups. These compounds are very much useful for liquid crystal display devices. The IR spectra as well as Raman activities were discussed. The atomic charges with multi pole moments were also presented and discussed.
Keywolds: *Biphenyl Ester, Liquid Crystals, Mesogen, IR Spectra, Raman Activities.*

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I. INTRODUCTION:

A phenyl ring with biphenyl ester is a fundamental core for most of liquid crystalline materials. Its alkyl chain length variations leads to different liquid crystalline properties including Ferromagnetic as well as Anti-Ferromagnetic properites. Murth and Sadashiv [1] synthesized and characterised five homologous series of symmetrical compounds composed of banana-shaped molecules containing a biphenyl moiety. Korley et al. [2] studied liquid crystalline properties of biphenyl-based liquid crystals for elevated temperature processing with different polymers. They concluded that the use of these types liquid crystals can be use in the environment require elevated processing conditions to produce materials with enhanced mechanical or gas barrier properties. Mohammad et al. [3] synthesized mesogenic compounds possessing a biphenyl ester and ether moiety . They found that these compounds exhibited enantiotropic smectic A and nematic mesophases. The liquid crystalline properties were depend on the spacer and terminal alkoxy- chain and alkoxy- ester moiety of the molecules. Smaller the alkyl chain showed a smectic phase, while higher alkyl chain members showed a nematic phase. Yildiz et al. [4] used Dieletric Spectroscopy to studyt he dielectric and impedance characteristics Ethyl 4-(7,7,8,8,9,9,10,10,10-nonafluorodecyloxy)biphenyl-4′-carboxylate liquid crystal and analyzed over the frequency range of 100 Hz to MHz in the temperature region from room temperature to 180 °C. Zhu et al. [5] studied the effect of terminal epoxy modification on the mesomorphic and thermal stability of biphenyl ester liquid crystals.

In the this paper we will discuss about IR and Raman activities of 4-Substituted phenyl-4-substituted biphenyl-4-carboxylates with methoxy groups (BELC). The geometry were taken from article by Hori et al. [6]

COMPUTATIONAL METHOD:

The geometry was optimized using DFT method B3LYP [7,8] using 6-31G** [9, 10] which was found suitable for these type of systems [11] with keeping all atoms free. The analytical frequencies as well as Raman activities were calculated. All calculation were done using Gaussian09 programme suit.[12]

II. RESULTS:

The optimized geometry of BELC molecule is shown in figure 1. The inter ring angle between biphenyl is 35.6^{o} and inter ring seperation is 1.48Å. The angle between biphenyl and ester group is 0.7^{o} and seperation is 1.49Å. The methoxy group is planar to biphenyl ring and seperation is 1.36Å.

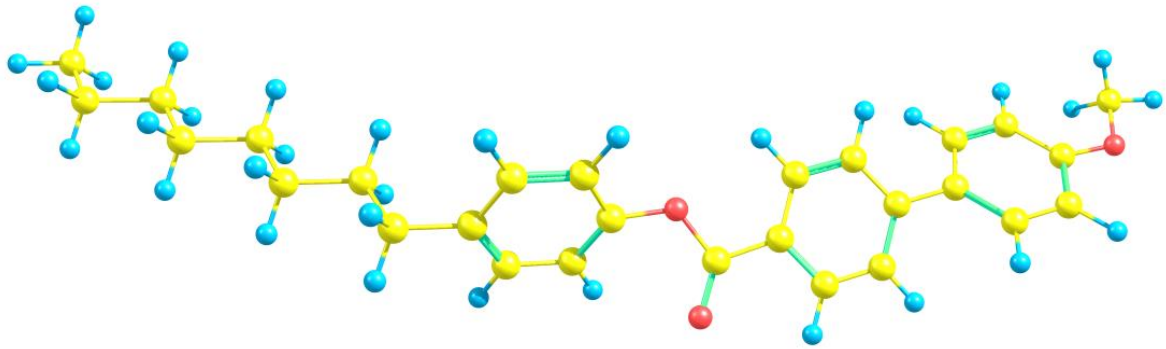

Figure 1: The optimized structure of the BELC molecule.

Table 1 present the charges as well as multipoles corresponding each atoms of BELC molecule. Since multipole depends on the coordinates of each atoms therefore coordinates are aslo tabulated here.

Sr. No.	Atom	Coordinates			Charge	Multipole (au)		
		X	Y	Z				
1	C	-0.09124	0.036575	0.374296	0.341458	-0.33832	-1.12651	0.143012
2	C	1.292582	0.083226	0.603774	-0.51114	-0.26351	0.127925	-0.06018
3	C	1.977878	1.28414	0.498662	-0.10468	-0.79337	-0.45345	-0.05394
4	C	1.315554	2.480642	0.1589	0.125871	0.449279	0.614303	0.000093
5	C	-0.06649	2.412635	-0.06744	-0.23151	-0.03955	-0.29516	0.019936
6	C	-0.77165	1.212835	0.03711	-0.30081	0.847719	0.032767	0.150181
7	C	2.052593	3.761035	0.047024	-0.10968	-0.01514	0.088461	-0.07149
8	C	3.130414	4.055464	0.903882	-0.17006	0.029807	0.341551	-0.26363
9	C	3.822205	5.255308	0.799482	-0.05578	0.064068	0.42478	-0.15674
10	C	3.456318	6.204484	-0.16569	-0.31751	-0.37751	-0.21009	-0.27581
11	C	2.383994	5.925831	-1.02541	-0.13252	-0.17893	-0.19007	-0.06561
12	C	1.697544	4.721327	-0.91889	-0.40979	0.188703	-0.0179	0.247861
13	C	4.235425	7.468186	-0.22492	0.939127	-0.18807	-0.07296	-0.091
14	O	3.776595	8.289702	-1.22114	-0.2787	0.125448	0.347659	-0.0963
15	C	4.369269	9.528731	-1.46826	0.412433	0.19694	0.430157	-0.0933
16	C	4.678921	10.44134	-0.45994	-0.35976	0.051813	0.231309	0.227136
17	C	5.199398	11.68511	-0.81652	-0.23815	-0.00486	-0.10957	0.094566
18	C	5.412263	12.04114	-2.15532	-0.24741	-0.15082	-0.20332	0.280038
19	C	5.085765	11.10298	-3.14357	-0.02873	-0.07849	-0.17798	0.675707
20	C	4.568418	9.852809	-2.80876	-0.45681	-0.15884	-0.41789	-0.34726
21	C	5.93816	13.41185	-2.52296	0.761116	-0.3945	-0.32243	0.079796
22	C	4.822037	14.45973	-2.7076	-0.31813	-0.13583	0.429179	-0.08991
23	C	5.352177	15.84999	-3.07896	0.344927	0.092053	-0.30119	0.10321
24	C	4.244464	16.89532	-3.26187	0.364344	-0.05275	0.123138	-0.0359
25	C	4.769831	18.28796	-3.63362	0.30242	0.132944	-0.07053	0.025558
26	C	3.661576	19.33246	-3.816	0.486234	-0.12885	0.069738	-0.00332
27	C	4.184842	20.72604	-4.18713	0.369608	0.052285	0.110108	-0.02439
28	C	3.070762	21.76192	-4.36856	0.322968	-0.02419	0.175715	-0.05733
29	O	-0.67274	-1.18914	0.503601	-0.94414	-0.02585	-0.29648	0.032746

30	C	-2.06906	-1.29975	0.274457	1.412324	0.045135	1.294667	-0.08222
31	O	5.160558	7.743611	0.507976	-0.49079	0.026539	0.000068	0.010625
32	H	1.807139	-0.83892	0.853296	0.289477	-0.03099	0.0822	-0.01871
33	H	3.052365	1.292711	0.65505	0.371219	-0.13959	0.022646	-0.01768
34	H	-0.61487	3.319854	-0.30325	0.228214	0.042514	-0.05763	0.017302
35	H	-1.84155	1.21024	-0.13434	0.386928	0.182551	0.061408	0.017987
36	H	3.407716	3.344988	1.67639	0.291516	-0.03068	0.079908	-0.0731
37	H	4.647297	5.484211	1.465547	0.104854	0.008915	-0.07173	0.042686
38	H	2.101631	6.649984	-1.78072	0.128321	-0.01045	0.001959	-0.01414
39	H	0.889996	4.506231	-1.61186	0.282557	0.083296	0.032921	0.061887
40	H	4.532961	10.17901	0.579589	0.130095	-0.00603	-0.03646	0.025428
41	H	5.449281	12.39397	-0.03075	0.10135	0.002216	0.006767	0.027325
42	H	5.243316	11.34982	-4.19068	0.31169	-0.02731	-0.05156	0.099171
43	H	4.3182	9.123019	-3.57196	0.034793	-0.0064	-0.01742	-0.06872
44	H	6.629999	13.76056	-1.74568	-0.09667	0.077965	0.053175	0.076242
45	H	6.522215	13.34544	-3.44972	-0.09734	0.069168	0.003047	-0.09786
46	H	4.23426	14.5235	-1.78202	0.001726	-0.03508	-0.0411	0.056447
47	H	4.127436	14.10967	-3.48305	0.011408	-0.03294	-0.05257	-0.02309
48	H	6.050385	16.19233	-2.30166	-0.15002	0.094867	0.068241	0.090698
49	H	5.941842	15.77914	-4.00427	-0.13787	0.077169	0.014309	-0.12309
50	H	3.655407	16.965	-2.3363	-0.16249	-0.08808	-0.00707	0.130685
51	H	3.546365	16.55169	-4.03852	-0.1614	-0.10143	-0.06026	-0.10149
52	H	5.468061	18.6315	-2.85689	-0.17118	0.107228	0.056578	0.10601
53	H	5.358901	18.21832	-4.55937	-0.16261	0.088457	-0.00103	-0.12996
54	H	3.071875	19.40229	-2.89056	-0.21262	-0.09975	-0.00127	0.154859
55	H	2.963199	18.98968	-4.59311	-0.2107	-0.11695	-0.06567	-0.12671
56	H	4.774481	20.65624	-5.11148	-0.17494	0.098947	-0.01864	-0.13657
57	H	4.881239	21.06931	-3.40986	-0.17176	0.111479	0.043775	0.110594
58	H	2.378475	21.46385	-5.16437	-0.11495	-0.09387	-0.04236	-0.09572
59	H	3.475403	22.74489	-4.63138	-0.16224	0.061864	0.153864	-0.0379
60	H	2.48483	21.8785	-3.44961	-0.10942	-0.07862	0.007047	0.114959
61	H	-2.31623	-2.3519	0.423206	0.142399	0.04039	-0.00916	-0.00949
62	H	-2.33573	-1.00776	-0.74938	-0.45381	-0.08813	-0.00153	-0.33185
63	H	-2.64537	-0.69068	0.982686	-0.54327	-0.23029	0.145732	0.293611

Table 1: The charge, coordinates and multipoles corresponding each atoms of BELC molecule.

Various energies components with zero point corrections of BELC molecule is tabulated in Table 2.

Energies Components	**Hartree**
Sum of electronic and zero-point Energies	-1311.445264
Sum of electronic and thermal Energies	-1311.414946
Sum of electronic and thermal Enthalpies	-1311.414002
Sum of electronic and thermal Free Energies	-1311.512597

Table 2: Energies Components such as electronic, thermal and Free energies

Table 3 presents dipole monent, exact polarizability, approx. polarizability and hyperpolarizability of BELC molecules.

Dipole Monent	5.0844 debye
Exact Polarizability	232.406
Approx Polarizability	392.754
Hyperpolarizability	3.77358183D+00

Table 3: Dipole monent, exact polarizability, approx. polarizability and hyperpolarizability of BELC molecules.

The IR spectra of BELC molecule is shown in figure 2. From figure 3 it is visual that there are several peak and the highest peak (IR intensity) is at 389.49 cm^{-1}. This frequency is associated with twisting of ester group and it terminal group with respect to biphenyl plane.

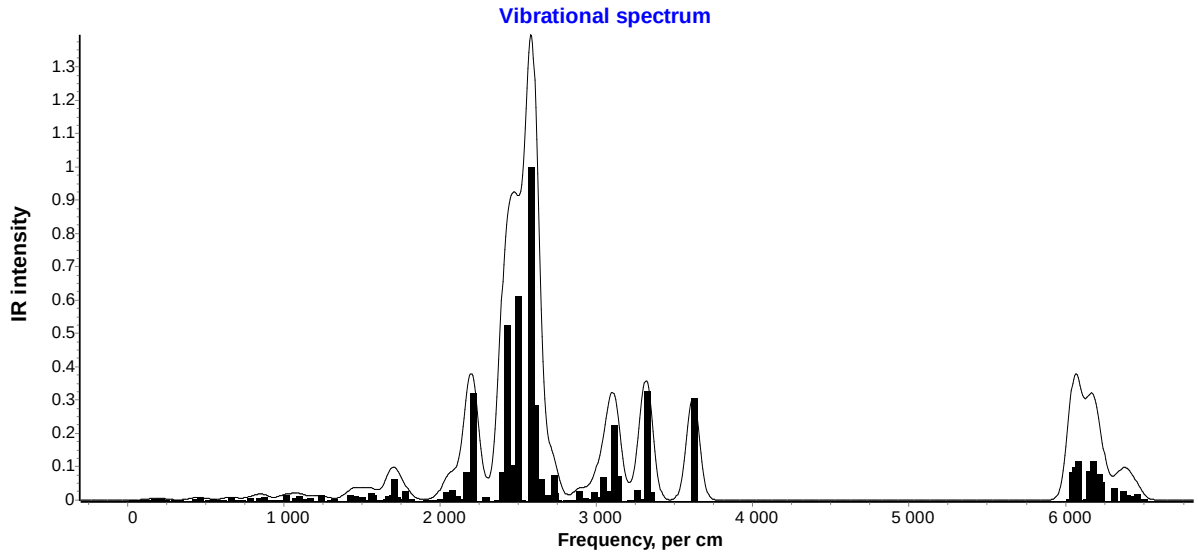

Figure 2: IR Spectra of BELC molecule.

Figure 3 represent Raman activities of BELC molecule. There are various peaks and the highest Raman activity is at 504.9 cm^{-1}. The frequency is associated with twisting of biphenyl ring with respect to ester group.

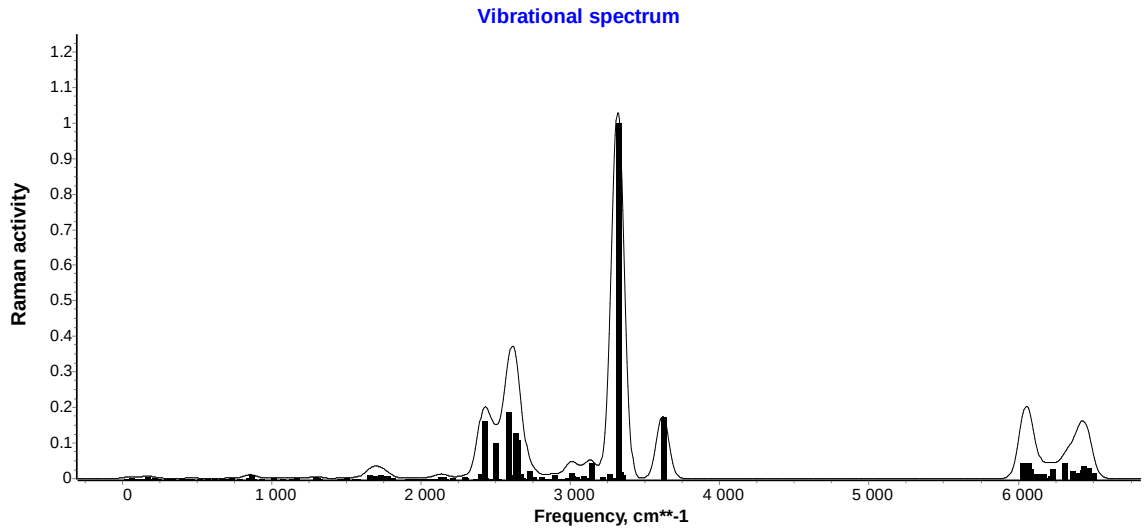

Figure 3: Raman activitty of BELC molecule.

III. CONCLUSION:

Electronic structure analysis of 4-Substituted phenyl-4-substituted biphenyl-4-carboxylates with methoxy groups molecule is carried out using DFT methods. The IR spectra and Raman activities were explained.

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