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Quantum Mechanical Study of 4-Alkyl 4'-Cyano Biphenyls: Part II: $C_{10}H_{21}$-C_6H_5-C_6H_5-CN

Devesh Kumar

Department of Physics, Siddharth University, Kapilvastu, Siddharthnagar (U. P.) INDIA 272 202

Abstract: The quantum mechanical calcualtion were carried out on 4-Alkyl 4'-Cyano Biphenyls ($C_{10}H_{21}$-C_6H_5-C_6H_5-CN) using DFT. The IR spectra and Raman activities and its vibration association were discussed. The atomic charges with multipole moments were also computed and discussed.

Keywolds: Cyano Biphenyl, Liquid Crystals, Mesogen, IR Spectra, Raman Activities.

INTRODUCTION:

Alkyl and alkoxy cyano biphenyls are higly studied liquid crystals which are suitable for application in electro-optic devices and their properties as liquid crystal devices were well established [1,2]. Dunmur et al. [3] were measured the electric permittivities, refractive indices and densities of the homologous series of alkyl-cyano-biphenyls as a function of temperature in the various phases. Merkel et al. [4] has calculated and analyzed the vibration spectra for cyanobiphenyl liquid crystals using DFT methods. Grey et al. studied that when the nCB liquid crystals having a exclusive property for the alkyl chain length is changed, then the molecular properties of the mesophase change [5, 6]. Delabre et al. [7] studied the specificities of wetting behaviour of the series of cyanobiphenyl liquid crystals (LCs) on usual substrates, i.e. oxidized silicon wafers, water and glycerol, at both the macroscopic and microscopic scale, in the nematic range of temperature. Paterson et al. [8] synthesized and studied the role of a terminal chain in promoting the twist-bend nematic phase. Wang et al. [9] synthesised and studied the properties of hydroxy tail-terminated cyanobiphenyl liquid crystals. Chaudhary et al. computed the electro-optical parameters with adverse order of 10CB liquid crystal molecules studied under the influence of an external high electric field.[10] Kumar et al. [11] Odd−Even effect observed in the electro−optical properties of the homologous Series of H_nCBP liquid crystal studied under the impact of the electric field.

In the this paper we will discuss about IR as well as Raman activities of 4-Alkyl 4'-Cyano Biphenyls (C10H21-C6H5-C6H5-CN; **10CB**). The geometry were taken from article by Murty et al. [12]

COMPUTATIONAL METHOD:

The geometry was optimized using DFT method B3LYP [13,14] using 6-31G** [15, 16] which was found suitable for these type of systems [17] with keeping all atoms free. The analytical frequencies as well as Raman activities were calculated. All calculation were done using Gaussian09 programme suit.[18]

RESULTS:

The optimized geometry of 10CB molecule is shown in figure 1. The inter ring angle between biphenyl is 36.8° and inter ring seperation is 1.48Å. The angle between biphenyl and alkyl chain is 88.4° and seperation is 1.51Å. The cyano group is planar to biphenyl ring and seperation is 1.43Å.

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Figure 1: The optimized structure of the 10CB molecule.

Table 1 present the charges as well as multipoles corresponding each atoms of 10CB molecule. Since multipole depends on the coordinates of each atoms therefore coordinates are aslo tabulated here.

Table 1: The charge, coordinates and multipoles corresponding each atoms of 10CB molecule.

Sr. No.	Atom	Coordinates			Charge	Multipole (au)		
		X	Y	Z				
1	C	0.07166	-0.114	-0.51427	-0.56934	0.916419	1.423507	0.290105
2	C	1.47102	-0.06255	-0.39474	-0.32492	-0.11699	0.04625	-4.8E-05
3	C	2.10481	1.15063	-0.15744	-0.2845	0.224475	-0.21099	-0.01784
4	C	1.37294	2.346	-0.025	0.202797	0.192022	0.057904	0.057782
5	C	-0.02804	2.27647	-0.14545	-0.04312	0.126034	-0.77423	-0.14539
6	C	-0.67374	1.07068	-0.38858	-0.36449	-0.85566	-0.38124	-0.11081
7	C	2.05421	3.63532	0.23294	-0.16491	-0.31362	-0.06168	-0.18442
8	C	3.201	3.70521	1.03688	-0.0943	-0.27625	0.10409	-0.26118
9	C	3.84997	4.91394	1.28995	-0.22365	0.053486	-0.11453	0.096072
10	C	3.35413	6.09862	0.73001	0.386162	-0.26999	0.060826	-0.20957
11	C	2.2081	6.04801	-0.08	-0.4892	-0.16319	-0.24963	-0.10857
12	C	1.57312	4.8391	-0.31947	-0.34715	0.404935	0.03636	0.321531
13	O	3.90086	7.33105	0.90784	-0.74872	-0.44309	-0.30449	-0.24979
14	C	5.07343	7.4588	1.71415	1.227314	-0.64811	-1.181	-0.25918
15	C	5.46022	8.93076	1.74252	0.875957	-0.53712	-0.14444	-0.33276
16	C	6.71545	9.19224	2.58444	0.772344	-0.03457	-0.49368	-0.05244
17	C	7.11093	10.67391	2.63013	0.503007	-0.13694	0.000242	-0.06266
18	C	8.36508	10.94575	3.47017	0.411069	0.107434	-0.2136	-0.05225
19	C	8.75876	12.42752	3.51959	0.341761	-0.09162	0.007785	-0.05856
20	C	10.01193	12.70143	4.36065	0.186849	0.02201	-0.18865	-0.13002
21	C	10.40685	14.18249	4.40283	-0.0776	-0.30688	-0.2343	0.047248
22	C	11.65747	14.45197	5.24838	0.392008	0.084803	-0.33356	-0.44925
23	C	12.08536	15.91503	5.25417	0.884893	-0.16607	-0.21442	-0.49903
24	O	12.44106	16.2811	3.92445	-1.1334	0.086961	-0.02476	-0.3392
25	C	-0.588	-1.3614	-0.76202	0.299509	1.048047	2.044915	0.401735
26	N	-1.12363	-2.37491	-0.96277	0.426467	0.347617	0.643175	0.128535
27	H	2.05138	-0.9731	-0.50131	0.224794	-0.03079	0.043189	0.004482

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28	H	3.18821	1.17891	-0.0994	0.118307	-0.01611	-0.00228	0.000754
29	H	-0.62006	3.17749	-0.02058	0.360849	0.088039	-0.12534	-0.01719
30	H	-1.75501	1.03441	-0.47104	-0.07374	-0.13121	0.025545	-0.00791
31	H	3.58396	2.80215	1.50302	0.217551	0.003847	0.072497	-0.01264
32	H	4.72568	4.92203	1.92755	0.067744	0.0156	-0.081	0.022142
33	H	1.84272	6.97167	-0.51666	0.244261	0.02323	-0.04974	0.037759
34	H	0.70429	4.82115	-0.97065	0.3588	0.131045	0.015083	0.098637
35	H	5.88581	6.84962	1.29177	-0.38393	0.24279	-0.10765	-0.1005
36	H	4.87074	7.0903	2.7303	-0.38758	-0.01941	-0.03454	0.284996
37	H	4.61444	9.507	2.13711	-0.34912	-0.21758	0.165649	0.105112
38	H	5.61883	9.27124	0.71202	-0.34092	0.036142	0.092144	-0.26957
39	H	7.55494	8.60586	2.18473	-0.36825	0.237409	-0.14167	-0.09457
40	H	6.55241	8.83019	3.60957	-0.31537	-0.02073	-0.06411	0.245687
41	H	6.27116	11.25985	3.02952	-0.21652	-0.14378	0.106834	0.062873
42	H	7.27318	11.03684	1.60547	-0.22203	0.016712	0.071062	-0.18775
43	H	9.20478	10.3604	3.06895	-0.25045	0.165859	-0.11304	-0.06949
44	H	8.20282	10.57899	4.49395	-0.17662	-0.02122	-0.04454	0.157207
45	H	7.91815	13.01267	3.91929	-0.14765	-0.10721	0.074113	0.051001
46	H	8.92231	12.79416	2.49629	-0.17485	0.017412	0.060473	-0.15874
47	H	10.85145	12.11423	3.96177	-0.15302	0.121848	-0.07344	-0.046
48	H	9.84803	12.33639	5.38517	-0.08676	-0.01415	-0.02115	0.104662
49	H	9.56802	14.77191	4.80135	-0.07028	-0.06803	0.0509	0.026471
50	H	10.58425	14.54933	3.3853	0.035336	0.026784	0.026626	-0.04068
51	H	12.49587	13.85049	4.8735	-0.2878	0.182438	-0.13501	-0.07599
52	H	11.48468	14.13981	6.28731	-0.03596	-0.01246	0.001149	0.078252
53	H	11.25854	16.54111	5.63014	-0.13745	-0.06335	0.061142	0.047239
54	H	12.93606	16.04867	5.942	-0.05483	0.049226	0.026212	0.036662
55	H	12.65607	17.22157	3.91783	0.560649	-0.02765	-0.10022	0.031358

Various energies components with zero point corrections of 10CB molecule is tabulated in Table 2.

Table 2: Energies Components such as electronic, thermal and Free energies of 10CB molecules.

Energies Components	**Hartree**
Sum of electronic and zero-point Energies	-948.249306
Sum of electronic and thermal Energies	-948.224670
Sum of electronic and thermal Enthalpies	-948.223726
Sum of electronic and thermal Free Energies	-948.308243

Table 3 presents dipole monent, exact polarizability, approx. polarizability and hyperpolarizability of 10CB molecules.

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Table 3: Dipole monent, exact polarizability, approx. polarizability and hyperpolarizability of 10CB molecules.

Dipole Monent	6.1892 debye
Exact Polarizability	197.522
Approx Polarizability	344.868
Hyperpolarizability	8.60457617D+00

The IR spectra of 10CB molecule is shown in figure 2. From figure 2 it is visual that there are several peak and the highest peak (IR intensity) is at 3028.5004 cm^{-1}. This frequency is associated with twisting of alkyl chain with respect to biphenyl plane. Second peak is at 1659.8414 cm^{-1}. The next peak is at 1539.7347 cm^{-1}. These frequencies is associated with twisting of phenyl ring. Another peak hieght is at 796.6465 cm^{-1}. This is associated with bond streching of CN group. Next peak is at 651.6584 cm^{-1}. This is associated with twisting of phenyl group attached with CN group.

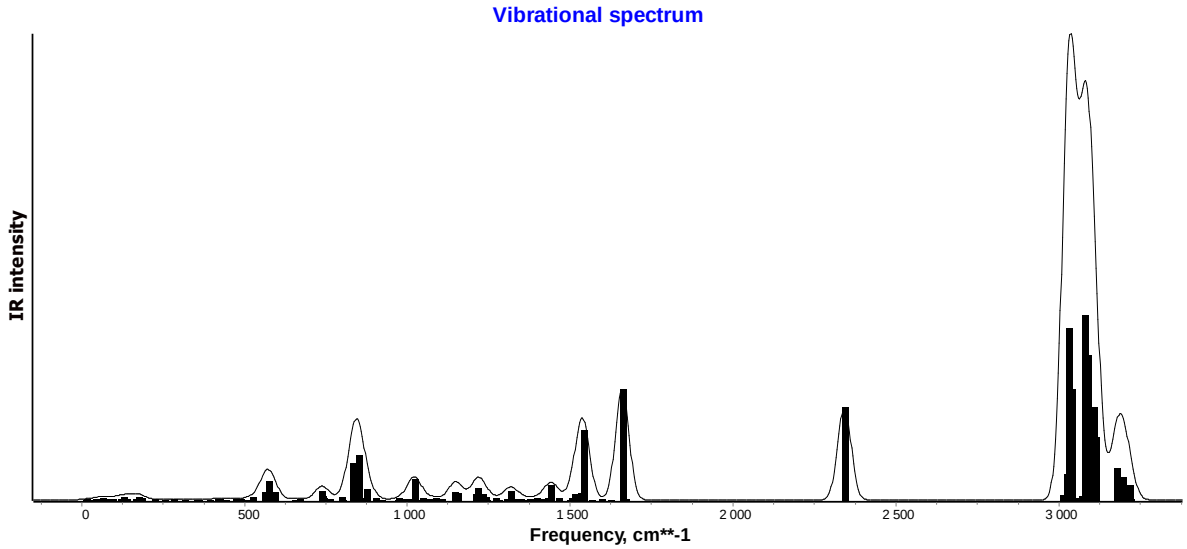

Figure 2: IR Spectra of 10CB molecule.

Figure 3 represent Raman activities of 10CB molecule. There are various peaks and the highest Raman activity is at 1659.8414 cm^{-1}. The frequency is associated twisting of phenyl ring as well as streching of phenyl and CN bond. Next peak is at 2341.8487 cm^{-1} which associated with CN bond strechingh.

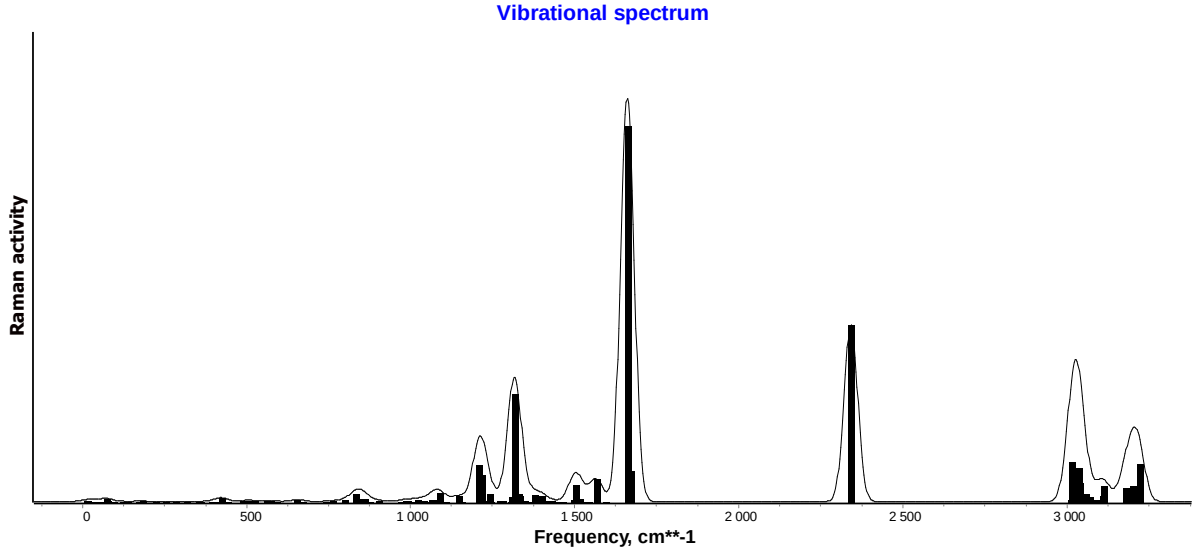

Figure 3: Raman activitty of 10CB molecule.

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CONCLUSION:

Electronic structure analysis of on 4-Alkyl 4'-Cyano Biphenyls ($C_{10}H_{21}$-C_6H_5-C_6H_5-CN) molecule is carried out using DFT methods. The IR spectra and Raman activities were explained.

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