Quantum Mechanical Study of 4-Alkyl 4'-Cyano Biphenyls: Part I: C₉H₁₉-C₆H₅-C₆H₅-CN

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Abstract

The quantum mechanical calcualtion werer carried out on 4-Alkyl 4'-Cyano Biphenyls (C_9H_{19} - C_6H_5 - C_6H_5 -CN). 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. Wu et al. [5] were studied the infra red applications of Perdeuterated cyanobiphenyl liquid crystals and found that it exhibits a much cleaner and reduced infrared absorption. Bernard et al. [6] studied the vibrational spectra of 4-octyloxy, 4'-cyanobiphenyl CN stretching in smectic, nematic, isotropic, and solution phases. 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.

In the this paper we will discuss about IR as well as Raman activities of 4-Alkyl 4'-Cyano Biphenyls ($C_9H_{19}-C_6H_5-C_6H_5-CN$; **9CB**). The geometry were taken from article by Murty et al. [10]

COMPUTATIONAL METHOD:

The geometry was optimized using DFT method B3LYP [11,12] using 6-31G** [13, 14] which was found suitable for these type of systems [15] with keeping all atoms free. The analytical frequencies as well as Raman activities were calculated. All calculation were done using Gaussian09 programme suit.[16]

RESULTS:

The optimized geometry of 9CB molecule is shown in figure 1. The inter ring angle between biphenyl is 37.1° and inter ring seperation is 1.48Å. The angle between biphenyl and alkyl chain

is 88.3° and seperation is 1.52Å. The cyano group is planar to biphenyl ring and seperation is 1.43Å.

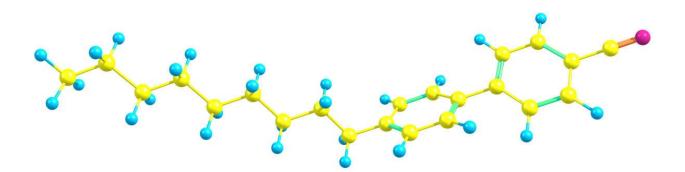


Figure 1: The optimized structure of the 9CB molecule.

Table 1 present the charges as well as multipoles corresponding each atoms of 9CB molecule. Since multipole depends on the coordinates of each atoms therefore coordinates are aslo tabulated here.

Sr.		Coordinates						
No.	Atom	Х	Y	Z	Charge		Multipole (a	au)
1	С	-7.28584	-0.80234	0.15476	-0.41472	2.163058	0.691982	-0.11544
2	С	-6.38667	-1.44759	-0.71108	-0.50104	-0.21483	-0.37504	-0.23279
3	С	-5.0635	-1.02852	-0.77703	-0.11962	-0.38434	-0.08979	0.014535
4	С	-4.5959	0.04076	0.00895	0.219482	0.220105	-0.00987	-0.08415
5	С	-5.50887	0.67735	0.86973	-0.08879	-0.11159	-0.08467	-0.02069
6	С	-6.83393	0.26636	0.9474	-0.38713	-0.31934	0.335216	0.399678
7	С	-3.18298	0.48371	-0.06798	0.047686	-0.04294	-0.02514	0.052863
8	С	-2.49574	0.91927	1.07741	-0.22512	0.208283	0.123707	0.030561
9	С	-1.17016	1.3391	1.00067	-0.08564	0.100522	-0.14033	-0.81293
10	С	-0.47823	1.34461	-0.21811	-0.21578	0.214147	-0.00997	-0.56291
11	С	-1.16484	0.91069	-1.36052	-0.3303	0.004584	0.010291	-0.08672
12	С	-2.48937	0.48682	-1.28998	-0.1582	0.310566	0.104008	0.154252
13	С	0.97097	1.7706	-0.29216	0.34409	0.056441	-0.21283	0.092493
14	С	1.95936	0.60076	-0.10623	0.072314	-0.02917	-0.35917	-0.10706
15	С	3.42703	1.03913	-0.17753	0.576164	-0.03395	0.129852	0.065898
16	С	4.4207	-0.11506	0.00653	0.367397	0.016558	-0.22406	-0.07934
17	С	5.88816	0.32684	-0.06053	0.448017	0.067063	0.159798	0.025659

Table 1: The charge, coordinates and multipoles corresponding each atoms of 9CB molecule.

18C6.88614.0.82330.124710.4415480.044586.0.172360.0.0360619C8.35254.0.378210.060750.3687860.1529410.1946390.01157420C9.35283.0.120310.2420230.4023720.4031280.0432160.00431221C8.6515.1.230120.228720.432682.397010.767060.1240822C8.6515.1.230120.228720.436282.397010.017020.0124823N-9.76053.1.577360.228720.436282.397010.017220.0124824H-6.7302.2.2791.317620.901060.01444-0.07220.0129825H-5.779680.727791.61010.013330.05990.0247390.00465126H-7.577680.72791.61010.137330.05990.247390.04265127H-7.657860.72791.61010.107330.05790.047430.0043428H-7.657860.72791.61010.107330.05790.014150.0434329H-0.658290.91855-2.322750.914790.014160.494840.00475930H1.065810.146940.202810.016110.037030.045750.0141531H1.16330.249960.022810.016110.014930.014510.1280133H1.6253									
20 C 9.35283 -1.52603 0.24802 0.422943 0.040173 -0.09896 0.000419 21 C 10.8145 -1.0715 0.18519 0.203792 0.15885 0.043216 0.132542 22 C -8.6515 -1.23012 0.22872 0.43628 2.397011 0.76076 -0.12408 23 N -9.76053 -1.57736 0.28886 0.427409 0.721226 0.218077 -0.03794 24 H -6.7302 -2.279 -1.31762 0.090106 -0.01444 -0.01722 -0.01298 25 H -4.37292 -1.55349 -1.42977 0.18411 -0.00791 0.01136 0.020826 26 H -5.17968 1.5221 1.46631 0.13712 -0.0099 0.04245 0.007679 27 H -7.52786 0.77279 1.6101 0.1733 -0.06415 0.04373 28 H -0.6615 1.66654 1.90434 0.320654 -0.10471	18	С	6.88614	-0.8233	0.12471	0.441548	0.044586	-0.17236	-0.03606
21 C 10.8145 -1.0715 0.18519 0.203792 0.15885 0.043216 0.132542 22 C -8.6515 -1.23012 0.22872 0.43628 2.397011 0.76076 -0.12408 23 N -9.76053 -1.57736 0.28886 0.427409 0.721226 0.218077 -0.03794 24 H -6.7302 -2.279 -1.31762 0.090106 -0.01444 -0.01722 -0.01298 25 H -4.37292 -1.55349 -1.42927 0.184311 -0.00991 0.013136 0.020826 26 H -5.17968 1.5221 1.46631 0.13712 -0.0099 0.004245 0.007679 27 H -7.52786 0.77279 1.6101 0.17335 -0.05996 0.02473 0.042648 30 H -0.6615 1.6654 1.90434 0.32054 -0.01741 -0.04343 31 H -0.6512 0.18698 -0.21831 0.014616 0.049073	19	С	8.35254	-0.37821	0.06075	0.368786	0.152941	0.194639	0.011574
22 C -8.6515 -1.23012 0.22872 0.43628 2.397011 0.76076 -0.12408 23 N -9.76053 -1.57736 0.28886 0.427409 0.721226 0.218077 -0.03794 24 H -6.7302 -2.279 -1.31762 0.090106 -0.01444 -0.01228 25 H -4.37292 -1.55349 -1.42927 0.184311 -0.00999 0.004245 0.000769 26 H -5.17968 1.5221 1.46631 0.137122 -0.0099 0.004245 0.007679 27 H -7.52786 0.77279 1.6101 0.017335 -0.0599 0.042051 28 H -0.6615 1.66654 1.90434 0.320654 -0.00749 -0.01415 -0.02434 30 H -0.66152 0.18698 -2.32275 0.91479 -0.01415 0.04343 31 H -3.02275 0.18698 -2.19895 0.21811 0.014616 0.049773	20	С	9.35283	-1.52603	0.24802	0.422943	0.040173	-0.09896	0.000419
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26H-5.179681.52211.466310.137122-0.00090.0042450.00767927H-7.527860.772791.61010.017335-0.059960.0247390.04205128H-2.996660.906592.041070.1905060.0483590.00917-0.035129H-0.66151.666541.904340.320654-0.10671-0.04374-0.0624830H-0.658290.91855-2.322750.91479-0.0749-0.01415-0.0434331H-3.002750.18698-2.198950.2189110.016160.049808-0.0497332H1.163382.24901-1.26089-0.074810.0146160.049808-0.1014133H1.169452.530280.47439-0.02283-0.012170.0372030.04575934H1.76235-0.16085-0.87262-0.18355-0.02121-0.1146-0.1175435H1.764090.116170.85976-0.1151-0.0193-0.046760.12800136H3.614171.804970.58888-0.22310.031610.1290280.1311938H4.23276-0.605390.97235-0.1749-0.0251-0.074810.15082139H4.23578-0.8797-0.76141-0.23067-0.3566-0.1404-0.1558741H6.071011.092630.70695-0.21480.028160.1280990.128165 <t< td=""><td>24</td><td>Н</td><td>-6.7302</td><td>-2.279</td><td>-1.31762</td><td>0.090106</td><td>-0.01444</td><td>-0.01722</td><td>-0.01298</td></t<>	24	Н	-6.7302	-2.279	-1.31762	0.090106	-0.01444	-0.01722	-0.01298
27H-7.527860.772791.61010.017335-0.059960.0247390.04205128H-2.996660.906592.041070.1905060.0483590.00917-0.035129H-0.66151.666541.904340.320654-0.10671-0.04374-0.0624830H-0.658290.91855-2.322750.091479-0.00749-0.01415-0.0434331H-3.002750.18698-2.198950.2189110.0216140.0126450.04977332H1.163382.24901-1.26089-0.074810.014160.049808-0.1001433H1.169452.530280.47439-0.02283-0.012170.0372030.04575934H1.76235-0.16085-0.87262-0.18355-0.03212-0.1146-0.1175435H1.764090.116170.85976-0.11151-0.01993-0.046760.12800136H3.61311.52824-1.14444-0.205310.032670.081659-0.1649137H3.614171.804970.58888-0.222310.0316610.1290280.1311938H4.23578-0.8797-0.76141-0.23067-0.03566-0.1404-0.1350840H6.075230.81748-1.02649-0.21480.028140.1280910.12816541H6.071011.092630.70695-0.21480.02826-0.78170.155572<	25	Н	-4.37292	-1.55349	-1.42927	0.184311	-0.00971	0.013136	0.020826
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29H-0.66151.666541.904340.320654-0.10671-0.04374-0.0624830H-0.658290.91855-2.322750.091479-0.00749-0.01415-0.0434331H-3.002750.18698-2.198950.2189110.0216140.0126450.04977332H1.163382.24901-1.26089-0.074810.0146160.049808-0.1001433H1.169452.530280.47439-0.02283-0.012170.0372030.04575934H1.76235-0.16055-0.87262-0.18355-0.03212-0.11466-0.1175435H1.764090.116170.85976-0.11151-0.01993-0.046760.12800136H3.613311.52824-1.14444-0.205310.032670.081659-0.1649137H3.614171.804970.58888-0.222310.031610.1290280.1311938H4.23276-0.605390.97235-0.17949-0.0251-0.074810.15082139H4.23578-0.8797-0.76141-0.23067-0.03566-0.1404-0.1550840H6.075250.81748-1.02649-0.208190.0314730.83667-0.12816541H6.071011.092630.70695-0.21480.028160.128446-0.12806142H6.6981-1.314981.08999-0.18458-0.02826-0.78170.155572	27	Н	-7.52786	0.77279	1.6101	0.017335	-0.05996	0.024739	0.042051
30 H -0.65829 0.91855 -2.32275 0.091479 -0.0749 -0.01415 -0.04343 31 H -3.00275 0.18698 -2.19895 0.218911 0.021614 0.012645 0.049773 32 H 1.16338 2.24901 -1.26089 -0.07481 0.014616 0.049808 -0.10014 33 H 1.16945 2.53028 0.47439 -0.02283 -0.01217 0.037203 0.045759 34 H 1.76235 -0.16085 -0.87262 -0.18355 -0.03212 -0.1146 -0.11754 35 H 1.76409 0.11617 0.85976 -0.11151 -0.0193 -0.04676 0.128001 36 H 3.6131 1.52824 -1.14444 -0.20531 0.03267 0.081659 -0.16491 37 H 3.61417 1.80497 0.58888 -0.2231 0.031661 0.129028 0.13191 38 H 4.23578 -0.60539 0.97235 -0.17949 <td>28</td> <td>Н</td> <td>-2.99666</td> <td>0.90659</td> <td>2.04107</td> <td>0.190506</td> <td>0.048359</td> <td>0.000917</td> <td>-0.0351</td>	28	Н	-2.99666	0.90659	2.04107	0.190506	0.048359	0.000917	-0.0351
31H3.002750.18698-2.198950.2189110.0216140.0126450.04977332H1.163382.24901-1.26089-0.074810.0146160.049808-0.1001433H1.169452.530280.47439-0.02283-0.012170.0372030.04575934H1.76235-0.16085-0.87262-0.18355-0.03212-0.1146-0.1175435H1.764090.116170.85976-0.11151-0.01993-0.046760.12800136H3.613311.52824-1.14444-0.205310.032670.081659-0.1649137H3.614171.804970.58888-0.222310.0316610.1290280.1311938H4.23276-0.605390.97235-0.17949-0.0251-0.074810.15082139H4.23578-0.8797-0.76141-0.23067-0.03566-0.1404-0.1350840H6.075250.81748-1.02649-0.218160.028160.02816-0.12800941H6.6781-1.314981.08999-0.19458-0.02826-0.078170.15557243H6.6981-1.314981.08999-0.21480.0249670.079249-0.1290644H8.541710.11272-0.90485-0.201360.0249670.079249-0.1653745H8.533370.387870.82863-0.205970.0223610.124460.124902<	29	Н	-0.6615	1.66654	1.90434	0.320654	-0.10671	-0.04374	-0.06248
32H1.163382.24901-1.26089-0.074810.0146160.049808-0.1001433H1.169452.530280.47439-0.02283-0.012170.0372030.04575934H1.76235-0.16085-0.87262-0.18355-0.03212-0.1146-0.1175435H1.764090.116170.85976-0.1151-0.01993-0.046760.12800136H3.613311.52824-1.14444-0.205310.032670.081659-0.1649137H3.614171.804970.58888-0.22310.0316610.1290280.1311938H4.23276-0.605390.97235-0.17949-0.0251-0.074810.15082139H4.23578-0.8797-0.76141-0.23067-0.03566-0.1404-0.1350840H6.075250.81748-1.02649-0.208190.0314730.083667-0.1655641H6.071011.092630.70695-0.21480.02810.1280990.12816542H6.6981-1.314981.08999-0.19458-0.02826-0.078170.15557243H6.70523-1.58848-0.64385-0.21816-0.02982-0.13244-0.1290644H8.541710.11272-0.90485-0.201360.0249670.079249-0.1653745H8.533370.387870.82863-0.205970.0223610.1244460.124902 <td>30</td> <td>Н</td> <td>-0.65829</td> <td>0.91855</td> <td>-2.32275</td> <td>0.091479</td> <td>-0.00749</td> <td>-0.01415</td> <td>-0.04343</td>	30	Н	-0.65829	0.91855	-2.32275	0.091479	-0.00749	-0.01415	-0.04343
33H1.169452.530280.47439-0.02283-0.012170.0372030.04575934H1.76235-0.16085-0.87262-0.18355-0.03212-0.1146-0.1175435H1.764090.116170.85976-0.11151-0.01993-0.046760.12800136H3.613311.52824-1.14444-0.205310.032670.081659-0.1649137H3.614171.804970.58888-0.222310.0316610.1290280.1311938H4.23276-0.605390.97235-0.17949-0.0251-0.074810.15082139H4.23578-0.8797-0.76141-0.23067-0.03566-0.1404-0.1350840H6.075250.81748-1.02649-0.208190.0314730.083667-0.1655641H6.071011.092630.70695-0.21480.02810.1289090.12816542H6.6981-1.314981.08999-0.21480.0282-0.078170.15557243H6.70523-1.58848-0.64385-0.21816-0.02982-0.13244-0.1290244H8.541710.11272-0.90485-0.201360.0249670.079249-0.1653745H8.533370.387870.82863-0.20570.0223610.1244660.12490246H9.16328-2.016821.21251-0.18056-0.02925-0.078510.148268<	31	Н	-3.00275	0.18698	-2.19895	0.218911	0.021614	0.012645	0.049773
34H1.76235-0.16085-0.87262-0.18355-0.03212-0.1146-0.1175435H1.764090.116170.85976-0.11151-0.01993-0.046760.12800136H3.613311.52824-1.14444-0.205310.032670.081659-0.1649137H3.614171.804970.58888-0.222310.0316610.1290280.1311938H4.23276-0.605390.97235-0.17949-0.0251-0.074810.15082139H4.23578-0.8797-0.76141-0.23067-0.03566-0.1404-0.1350840H6.075250.81748-1.02649-0.208190.0314730.083667-0.1655641H6.071011.092630.70695-0.21480.02810.1289090.12816542H6.6981-1.314981.08999-0.19458-0.02826-0.078170.15557243H6.70523-1.58848-0.64385-0.21816-0.02982-0.13244-0.129644H8.541710.11272-0.90485-0.201360.0249670.079249-0.1653745H8.533370.387870.82863-0.205970.0223610.1244460.12490246H9.16328-2.016821.21251-0.18056-0.02925-0.078510.14826847H9.17382-2.29076-0.52023-0.16411-0.01312-0.10628-0.10999<	32	Н	1.16338	2.24901	-1.26089	-0.07481	0.014616	0.049808	-0.10014
35H1.764090.116170.85976-0.11151-0.01993-0.046760.12800136H3.613311.52824-1.14444-0.205310.032670.081659-0.1649137H3.614171.804970.58888-0.222310.0316610.1290280.1311938H4.23276-0.605390.97235-0.17949-0.0251-0.074810.15082139H4.23578-0.8797-0.76141-0.23067-0.03566-0.1404-0.1350840H6.075250.81748-1.02649-0.208190.0314730.083667-0.1655641H6.071011.092630.70695-0.21480.02810.1289090.12816542H6.6981-1.314981.08999-0.19458-0.02826-0.078170.15557243H6.70523-1.58848-0.64385-0.21816-0.02982-0.13244-0.129644H8.541710.11272-0.90485-0.201360.0249670.079249-0.1653745H8.533370.387870.82863-0.20570.0223610.1244460.12490246H9.16328-2.20076-0.52023-0.16411-0.01312-0.10628-0.1090948H11.5022-1.91230.32345-0.100870.087198-0.115820.00458749H11.04495-0.60941-0.78163-0.052680.0194510.036257-0.09783<	33	Н	1.16945	2.53028	0.47439	-0.02283	-0.01217	0.037203	0.045759
36H3.613311.52824-1.14444-0.205310.032670.081659-0.1649137H3.614171.804970.58888-0.222310.0316610.1290280.1311938H4.23276-0.605390.97235-0.17949-0.0251-0.074810.15082139H4.23578-0.8797-0.76141-0.23067-0.03566-0.1404-0.1350840H6.075250.81748-1.02649-0.208190.0314730.083667-0.1655641H6.071011.092630.70695-0.21480.02810.1289090.12816542H6.6981-1.314981.08999-0.19458-0.02826-0.078170.15557243H6.70523-1.58848-0.64385-0.21816-0.02982-0.13244-0.129644H8.541710.11272-0.90485-0.205970.0223610.1244660.12490246H9.16328-2.016821.21251-0.18056-0.02925-0.078510.14826847H9.17382-2.29076-0.52023-0.16411-0.01312-0.10628-0.1090948H11.5022-1.91230.32345-0.100870.087198-0.115820.00458749H11.04495-0.60941-0.78163-0.052680.0194510.036257-0.09783	34	Н	1.76235	-0.16085	-0.87262	-0.18355	-0.03212	-0.1146	-0.11754
37H3.614171.804970.58888-0.222310.0316610.1290280.1311938H4.23276-0.605390.97235-0.17949-0.0251-0.074810.15082139H4.23578-0.8797-0.76141-0.23067-0.03566-0.1404-0.1350840H6.075250.81748-1.02649-0.208190.0314730.083667-0.1655641H6.071011.092630.70695-0.21480.02810.1289090.12816542H6.6981-1.314981.08999-0.19458-0.02826-0.078170.15557243H6.70523-1.58848-0.64385-0.2136-0.02982-0.13244-0.129644H8.541710.11272-0.90485-0.201360.0249670.079249-0.1653745H8.533370.387870.82863-0.205970.0223610.1244460.12490246H9.16328-2.016821.21251-0.18056-0.02925-0.078510.14826847H9.17382-2.29076-0.52023-0.16411-0.01312-0.10628-0.1090948H11.04495-0.60941-0.78163-0.052680.0194510.036257-0.09783	35	Н	1.76409	0.11617	0.85976	-0.11151	-0.01993	-0.04676	0.128001
38H4.23276-0.605390.97235-0.17949-0.0251-0.074810.15082139H4.23578-0.8797-0.76141-0.23067-0.03566-0.1404-0.1350840H6.075250.81748-1.02649-0.208190.0314730.083667-0.1655641H6.071011.092630.70695-0.21480.02810.1289090.12816542H6.6981-1.314981.08999-0.19458-0.02826-0.078170.15557243H6.70523-1.58848-0.64385-0.21186-0.02982-0.13244-0.129644H8.541710.11272-0.90485-0.201360.0249670.079249-0.1653745H8.533370.387870.82863-0.205970.0223610.1244460.12490246H9.16328-2.016821.21251-0.18056-0.02925-0.078510.14826847H9.17382-2.29076-0.52023-0.16411-0.01312-0.10628-0.1090948H11.5022-1.91230.32345-0.100870.087198-0.115820.00458749H11.04495-0.60941-0.78163-0.052680.0194510.036257-0.09783	36	Н	3.61331	1.52824	-1.14444	-0.20531	0.03267	0.081659	-0.16491
39H4.23578-0.8797-0.76141-0.23067-0.03566-0.1404-0.1350840H6.075250.81748-1.02649-0.208190.0314730.083667-0.1655641H6.071011.092630.70695-0.21480.02810.1289090.12816542H6.6981-1.314981.08999-0.19458-0.02826-0.078170.15557243H6.70523-1.58848-0.64385-0.21816-0.02982-0.13244-0.129644H8.541710.11272-0.90485-0.201360.0249670.079249-0.1653745H8.533370.387870.82863-0.205970.0223610.1244460.12490246H9.16328-2.016821.21251-0.18056-0.02925-0.078510.14826847H9.17382-2.29076-0.52023-0.16411-0.01312-0.10628-0.1090948H11.5022-1.91230.32345-0.100870.087198-0.115820.00458749H11.04495-0.60941-0.78163-0.052680.0194510.036257-0.09783	37	Н	3.61417	1.80497	0.58888	-0.22231	0.031661	0.129028	0.13119
40H6.075250.81748-1.02649-0.208190.0314730.083667-0.1655641H6.071011.092630.70695-0.21480.02810.1289090.12816542H6.6981-1.314981.08999-0.19458-0.02826-0.078170.15557243H6.70523-1.58848-0.64385-0.21816-0.02982-0.13244-0.129644H8.541710.11272-0.90485-0.201360.0249670.079249-0.1653745H8.533370.387870.82863-0.205970.0223610.1244460.12490246H9.16328-2.016821.21251-0.18056-0.02925-0.078510.14826847H9.17382-2.29076-0.52023-0.16411-0.01312-0.10628-0.1090948H11.5022-1.91230.32345-0.100870.087198-0.115820.00458749H11.04495-0.60941-0.78163-0.052680.0194510.036257-0.09783	38	Н	4.23276	-0.60539	0.97235	-0.17949	-0.0251	-0.07481	0.150821
41H6.071011.092630.70695-0.21480.02810.1289090.12816542H6.6981-1.314981.08999-0.19458-0.02826-0.078170.15557243H6.70523-1.58848-0.64385-0.21816-0.02982-0.13244-0.129644H8.541710.11272-0.90485-0.201360.0249670.079249-0.1653745H8.533370.387870.82863-0.205970.0223610.1244460.12490246H9.16328-2.016821.21251-0.18056-0.02925-0.078510.14826847H9.17382-2.29076-0.52023-0.16411-0.01312-0.10628-0.1090948H11.5022-1.91230.32345-0.100870.087198-0.115820.00458749H11.04495-0.60941-0.78163-0.052680.0194510.036257-0.09783	39	Н	4.23578	-0.8797	-0.76141	-0.23067	-0.03566	-0.1404	-0.13508
42H6.6981-1.314981.08999-0.19458-0.02826-0.078170.15557243H6.70523-1.58848-0.64385-0.21816-0.02982-0.13244-0.129644H8.541710.11272-0.90485-0.201360.0249670.079249-0.1653745H8.533370.387870.82863-0.205970.0223610.1244460.12490246H9.16328-2.016821.21251-0.18056-0.02925-0.078510.14826847H9.17382-2.29076-0.52023-0.16411-0.01312-0.10628-0.1090948H11.5022-1.91230.32345-0.100870.087198-0.115820.00458749H11.04495-0.60941-0.78163-0.052680.0194510.036257-0.09783	40	Н	6.07525	0.81748	-1.02649	-0.20819	0.031473	0.083667	-0.16556
43H6.70523-1.58848-0.64385-0.21816-0.02982-0.13244-0.129644H8.541710.11272-0.90485-0.201360.0249670.079249-0.1653745H8.533370.387870.82863-0.205970.0223610.1244460.12490246H9.16328-2.016821.21251-0.18056-0.02925-0.078510.14826847H9.17382-2.29076-0.52023-0.16411-0.01312-0.10628-0.1090948H11.5022-1.91230.32345-0.100870.087198-0.115820.00458749H11.04495-0.60941-0.78163-0.052680.0194510.036257-0.09783	41	Н	6.07101	1.09263	0.70695	-0.2148	0.0281	0.128909	0.128165
44H8.541710.11272-0.90485-0.201360.0249670.079249-0.1653745H8.533370.387870.82863-0.205970.0223610.1244460.12490246H9.16328-2.016821.21251-0.18056-0.02925-0.078510.14826847H9.17382-2.29076-0.52023-0.16411-0.01312-0.10628-0.1090948H11.5022-1.91230.32345-0.100870.087198-0.115820.00458749H11.04495-0.60941-0.78163-0.052680.0194510.036257-0.09783	42	Н	6.6981	-1.31498	1.08999	-0.19458	-0.02826	-0.07817	0.155572
45H8.533370.387870.82863-0.205970.0223610.1244460.12490246H9.16328-2.016821.21251-0.18056-0.02925-0.078510.14826847H9.17382-2.29076-0.52023-0.16411-0.01312-0.10628-0.1090948H11.5022-1.91230.32345-0.100870.087198-0.115820.00458749H11.04495-0.60941-0.78163-0.052680.0194510.036257-0.09783	43	Н	6.70523	-1.58848	-0.64385	-0.21816	-0.02982	-0.13244	-0.1296
46H9.16328-2.016821.21251-0.18056-0.02925-0.078510.14826847H9.17382-2.29076-0.52023-0.16411-0.01312-0.10628-0.1090948H11.5022-1.91230.32345-0.100870.087198-0.115820.00458749H11.04495-0.60941-0.78163-0.052680.0194510.036257-0.09783	44	Н	8.54171	0.11272	-0.90485	-0.20136	0.024967	0.079249	-0.16537
47H9.17382-2.29076-0.52023-0.16411-0.01312-0.10628-0.1090948H11.5022-1.91230.32345-0.100870.087198-0.115820.00458749H11.04495-0.60941-0.78163-0.052680.0194510.036257-0.09783	45	Н	8.53337	0.38787	0.82863	-0.20597	0.022361	0.124446	0.124902
48 H 11.5022 -1.9123 0.32345 -0.10087 0.087198 -0.11582 0.004587 49 H 11.04495 -0.60941 -0.78163 -0.05268 0.019451 0.036257 -0.09783	46	Н	9.16328	-2.01682	1.21251	-0.18056	-0.02925	-0.07851	0.148268
49 H 11.04495 -0.60941 -0.78163 -0.05268 0.019451 0.036257 -0.09783	47	Н	9.17382	-2.29076	-0.52023	-0.16411	-0.01312	-0.10628	-0.10909
	48	Н	11.5022	-1.9123	0.32345	-0.10087	0.087198	-0.11582	0.004587
50 H 11.03326 -0.33169 0.96382 -0.12823 0.030914 0.106031 0.102167	49	Н	11.04495	-0.60941	-0.78163	-0.05268	0.019451	0.036257	-0.09783
	50	Н	11.03326	-0.33169	0.96382	-0.12823	0.030914	0.106031	0.102167

Various energies components with zero point corrections of 9CB molecule is tabulated in Table 2.

Table 2: Energies Components such as electronic, thermal and Free energies of 9CB molecules.

Energies Components	Hartree
Sum of electronic and zero-point Energies	-908.962125
Sum of electronic and thermal Energies	-908.938789
Sum of electronic and thermal Enthalpies	-908.937845
Sum of electronic and thermal Free Energies	-909.01957

Table 3 presents dipole monent, exact polarizability, approx. polarizability and hyperpolarizability of 9CB molecules.

Table 3: Dipole monent, exact polarizability, approx. polarizability and hyperpolarizability of9CB molecules.

Dipole Monent	5.9993 debye		
Exact Polarizability	186.209		
Approx Polarizability	325.194		
Hyperpolarizability	-1.80352607D+01		

The IR spectra of 9CB 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 3074.8659 cm⁻¹. Second peak is at 3086.036 cm⁻¹. The next peak is at 3106.3828 cm⁻¹. All these frequencies are associated with twisting of alkyl chain with respect to biphenyl plane. Another peak hieght is at 2341.886 cm⁻¹. This is associated with bond streching of CN group. Next peak is at 1659.8402 cm⁻¹. This is associated with twisting of phenyl group attached with CN group. Next peak is at 1539.8855 cm⁻¹. This frequency is associated with streching of inter bond separation of phenyl ring.

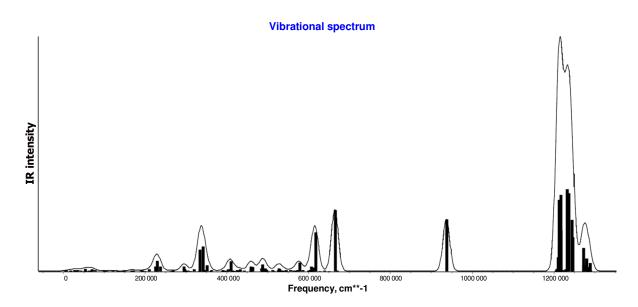


Figure 2: IR Spectra of 9CB molecule.

Figure 3 represent Raman activities of 9CB molecule. There are various peaks and the highest Raman activity is at 1659.8402 cm⁻¹. The frequency is associated twisting of phenyl ring as well as streching of phenyl and CN bond.

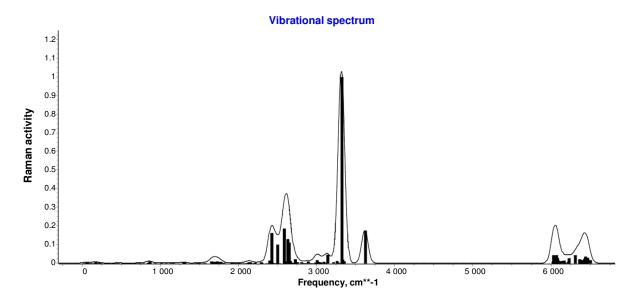


Figure 3: Raman activitty of 9CB molecule.

CONCLUSION:

Electronic structure analysis of on 4-Alkyl 4'-Cyano Biphenyls ($C_9H_{19}-C_6H_5-C_6H_5-CN$) molecule is carried out using DFT methods. The IR spectra and Raman activities were explained.

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