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The Quantum Mechanical Study of UV-Visible Spectra of some Ferroelectric Liquid Crystal

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Abstract: Ferroelectric liquid crystalline materials are of great interest due to their important industrial applications. In recent years, a field of research that is growing steadily is the photo-induced phenomenon in which the wavelengths of incident light impinge on the material stability. Photo stability of liquid crystal (LC) materials play a crucial role in affecting the lifetime of liquid crystal display (LCD), and memory devices. In direct-view displays, ultraviolet (UV) light is often used to seal the LC panels. Here we will discuss the photo responsive behavior of ferroelectric liquid crystal based on the quantum mechanical calculations. The electronic transitions, UV-Visible absorption wavelength, HOMO (highest occupied molecular orbital) and LUMO (lowest unoccupied molecular orbital) energies will also be presented. Further, ultraviolet (UV) stability of the molecules will be discussed in the light of absorption wavelength and electronic transition oscillator strength (f).

Keywords: Ferroelectric liquid crystal, DFT, UV-VIS, Raman.

I. INTRODUCTION

Liquid crystals (LCs) are advance material because of its physical properties. They possess large birefringence and extremely sensitive towards external field. Ferroelectric liquid crystals are enhanced phase of LCs owing to its chemical and physical view point. The most attractive aspects of this new class of liquid crystals are in their polarity and hilarity.[1, 2, 3,4,5]

Despite being formed from achiral molecules, the absorption in the ordinary axis is higher as compared to the extraordinary axis because of the rod-like shape of the ferroelectric LCs. The rod like molecules can move around their long axis while the oscillations around the short axis are slow. Electro-optical response of Ferroelectric liquid crystal is much faster than other liquid crystal. We have observed the properties like polar switching and electro-convection pattern in the entire nematic range. Ferroelectric phases are not only be of fundamental scientific interest for soft matter physics, but also these phases are considered as possible next generation LC displays with enhanced switching performance. [6].

In this paper molecular structure along with physical and Spectroscopic properties of non racemic liquid crystal materials of general structure **A** of figure 1**,** possessing a phenyl benzoate core and chiral nonracemic 2-alkoxy-1-propoxy tail unit derived from ethyl acetate, are described. These interesting compounds, and a number of other FLC molecule have a long chain hydrocarbon head and ending with a straight terminus. The simulation of UV–Vis spectra by computational chemistry tools is particularly appealing since contemporary approaches are proficient to provide the results with good accuracy. Of particular importance in this sense, methods based on density function theory (DFT) and time-dependent density functional theory (TD-DFT) both of the method provide very accurate results. [7,8]

II. METHODOLOGY

Optimization of molecular geometry and total-energy calculations were performed utilizing density-functional theory (DFT) which has a proven track record for characterization/ correlation/ explanation of properties of vivid variety of molecules.[9,10]The structures were created using Gauss View 5.0. The molecular structures were fully optimized without any constrain and frequency were calculated with B3LYP [11, 12, 13] hybrid functional for Gaussian type orbital's (GTOs) and 6-31G**[14] basis set using Gaussian 09[15]. Same software has also been used for determining UV-VIS spectroscopy through time-dependent density functional theory (TD-DFT).

III. RESULT

Optimized geometry of these compounds have shown in figure 2. Physical and spectral properties of these compounds are listed in Table 1 and Table 2 respectively. Spectroscopic results namely UV-VIS absorption spectra, Raman Activity and IR spectra have been presented in figure 3 and figure 4.

Figure 4 shows the UV absorption spectra of DOBA (curve 1), DOBAMBC (curve c), and HOBACPC (curve 4), suspension in the range of 440-300 nm, which is due to the π–π^* transitions. In case of DOBA_8 (curve 2) and MORA_6 (curve 6) the transition peak 180 nm, a small shoulder near to 250 nm.

Compound (4) is most stable as it has the lowest total energy -1711.378621 a.u. and (5) has the highest energy

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1218.293876 a.u. HOMO-LUMO gap of compound (2) is greatest while that of (4) is least amongst all at 0.157476 a.u. and 0.136483 a.u respectively. Dipole Moment of these compounds varies from 3.4024 a.u. for compound (3) which is lowest to 5.479 a.u. for compound (5) which is highest. Zero field polarizability of compound (5) is lowest at 336.6193333 a.u. and that of compound (2) is highest at 459.46 a.u.

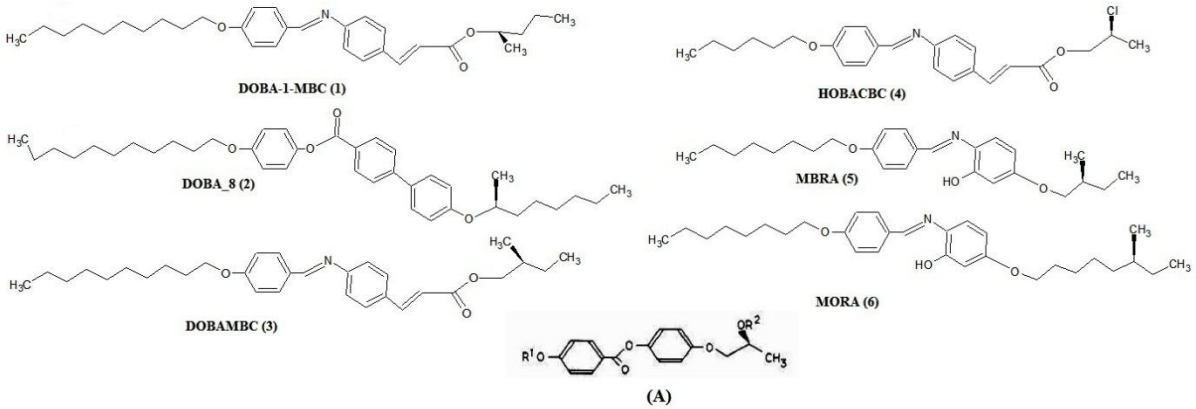

Fig.1. Chemical structures of the compounds.

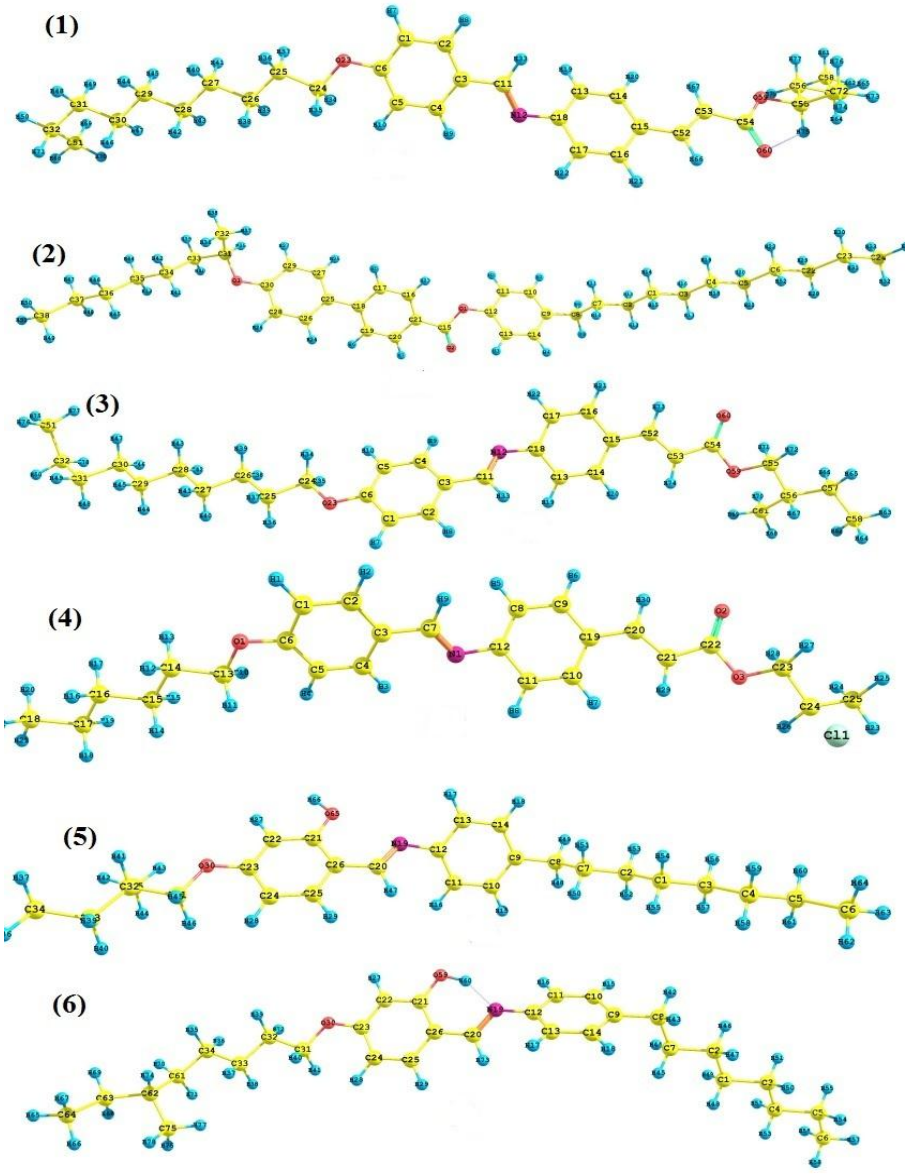

Fig.2. Optimized geometry of compounds.

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TABLE 1. PHYSICAL PROPERTIES

MOLECULE NAME	TOTAL ENERGY (a.u.)	HOMO-LUMO GAP (a.u.)	DIPOLE MOMENT (a.u.)	POLARIZABILITY (a.u.)
DOBA	-1487.684411	0.137109	5.2929	435.1103333
DOBA_8	-1705.146717	0.157476	3.8988	459.46
DOBAMBC	-1487.680203	0.137022	5.479	434.283
HOBACPC	-1711.378621	0.136483	5.4307	375.9716667
MBRA	-1218.293876	0.155362	3.8773	336.6193333
MORA	-1375.573387	0.1495	3.4024	387.9413333

TABLE2. SPECTRAL PROPERTIES

MOLECULE NAME	UV-VIS (nm) peak	INFRA RED (cm^{-1}) peak	RAMAN (cm^{-1}) peak
DOBA	360	1200	1650
DOBA_8	180	1250	1700
DOBAMBC	360	1200	1600
HOBACPC	360	1200	1600
MBRA	170	1350	1650
MORA	180	1700	1650

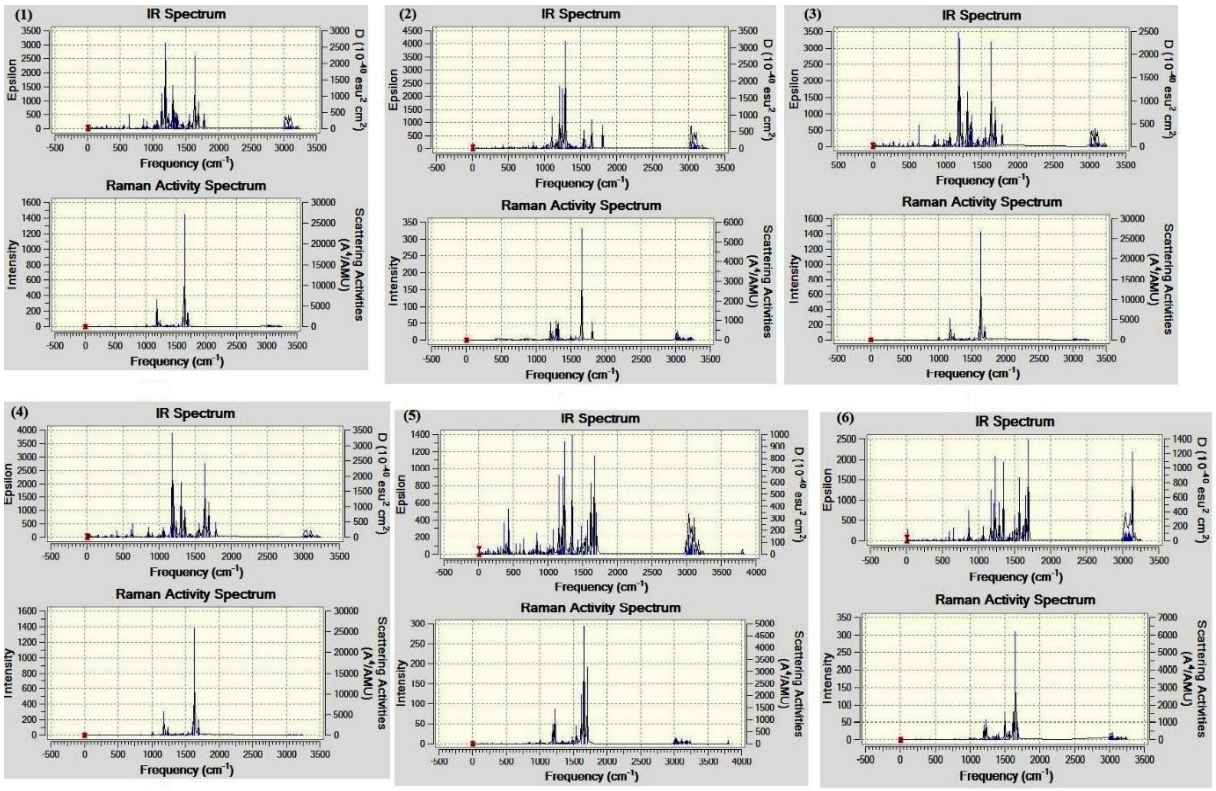

FIG.3. IR Spectra and Raman Activity spectra of compounds

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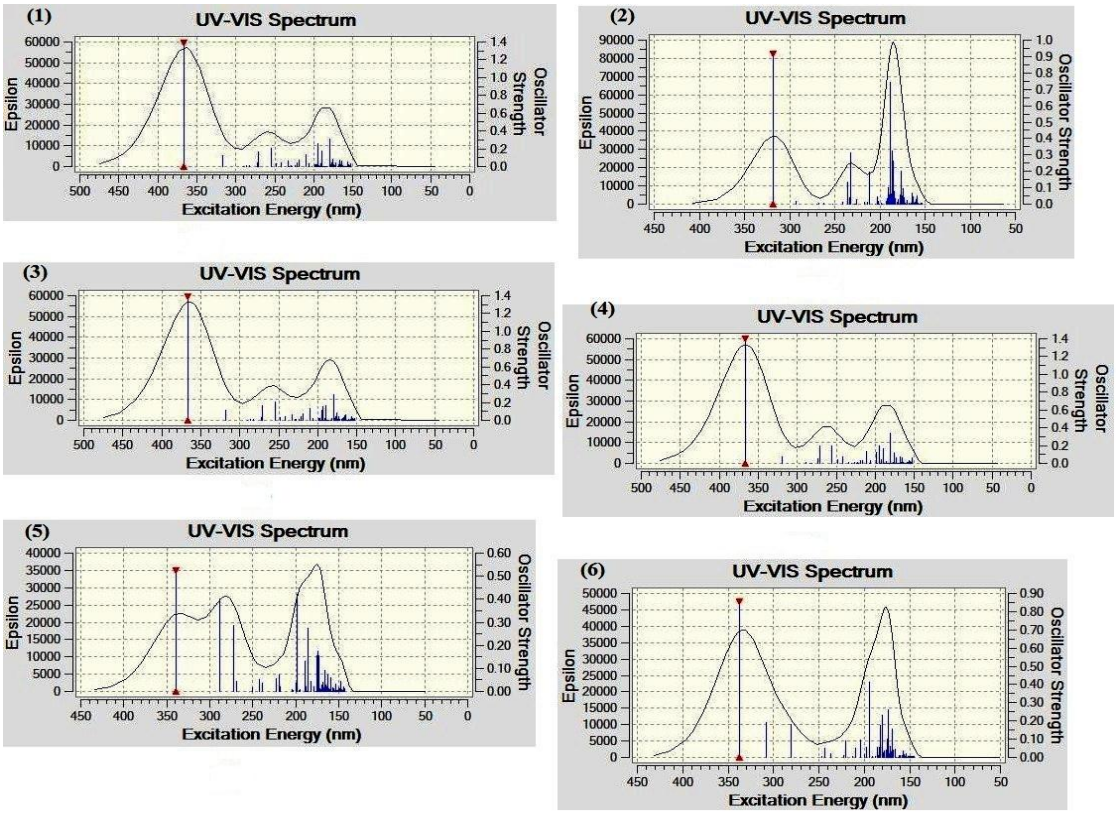

FIG.4. UV-VIS Spectrum of compounds.

IV. DISCUSSION AND CONCLUSION

Total energy of MBRA has the highest while HOBACPC is having lowest energy among these. HOMO-LUMO GAP of DOBAMBC is least. HOBACPC possesses highest dipole moment. DOBA_8 has the greatest value of molecular polarizability. Although all these compounds are very similar in their basic structures, still these variations are arising due to difference in substituent groups and end alkyl chains. There is also presence of hydrogen bond in compound (6).

In recent years many unusual property of the ferroelectric Liquid crystal have been reported, The B3LYP/6-31G** method is good for the structural and electronic properties of analysis. The molecular orbital analysis of (HOMO and LUMO) of molecules 1-6 provides a reasonable qualitative indication of the excitation properties and the electron transport because of the relative order of the orbitals.

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