

Study of Molecular Spectroscopy of 4-n-octyl, 4'-cyanobiphenyl (8CB) and 4'-octyloxy-4-cyanobiphenyl (8OCB) liquid crystal Molecules using Density Functional Theory

Divya Singh^{1*} & R.K. Singh²

¹Department of Chemistry, Bareilly College, Bareilly

²Department of Chemistry, M.L.K. (P.G.) College, Balrampur

*Email: divyasingh1962@gmail.com

ABSTRACT

KEYWORD

DS:

8CB,
8OCB,
liquid
crystal, IR,
Raman,
DFT

In this article, an attempt has been made to obtain the optimized geometry and calculate the IR and Raman vibration frequencies of 8CB and 8OCB liquid crystals using DFT/B3LYP method with basis set 6-31G(d,p). The molecules selected for the present investigation are quite interesting because they show excellent chemical and thermal stability due to the strong, and unique physical properties of the C–N bond, which contributes to the performance and photonic applications.

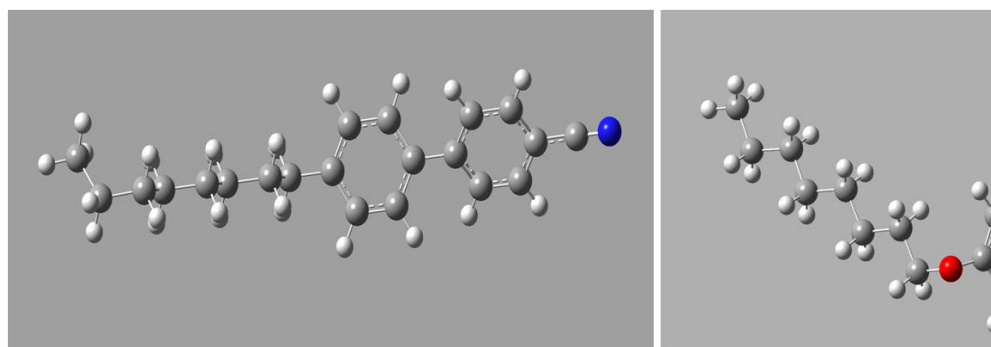


Figure 1. Molecular geometries of 8cb and 8ocb molecules

Copyright © 2021 International Journals of Multidisciplinary Research
Academy. All rights reserved.

1. INTRODUCTION

Liquid crystal materials are typically composed of molecules that have many common characteristics, such as strong dipoles, highly anisotropic structures or easily polarizable components. These materials melt in phases i.e. some intermediate phase between anisotropic ordered crystal to isotropic liquid. The rod-like liquid crystal molecule consists of two or more benzene rings linked by a central linkage group and alkyl or alkoxy chains at the terminals. A small change in molecular geometry largely affects the liquid crystalline properties of molecules. The properties of the liquid crystal molecules used for the demonstration are due to their dipole moment and optical anisotropy [1-3]. The dipole moment of the molecules should allow their orientation to be controlled by an electric field. For electro-optic applications, liquid crystals with nematic twist bend transitions are suitable. But these are only singular in phase and operate within a narrow range of temperatures. These liquid crystals lose their stability on cooling and are found to be workable at very low room temperatures [3-4]. The alkoxy group is more favorable than the alkyl group due to the representation of electrons. To design new liquid crystals, one must know the structure property relationship that leads to the specular properties in the desired liquid crystal. Since the alkoxy group is a polar substituent with a strong dipole moment, it can enhance the mesomorphic behavior. In this article, an attempt has been made to obtain the optimized geometry and calculate the IR and Raman vibration frequencies of 8CB and 8OCB liquid crystals using DFT/B3LYP method with basis set 6-31G(d, p). The molecules selected for the present investigation are quite interesting because they show excellent chemical and thermal stability due to the strong, and unique physical properties of the C–N bond, which contributes to the performance and photonic applications [4-13].

Computational Methodology

Quantum chemical calculations have been performed using gradient corrected density functional theory (DFT) with Li, Yang and cross correlation functional theory as well as hybrid functional B3 parameter for the exchange part. This is supplemented with the standard 6-31G(d,p) basis set in the Gaussian 09 program for the calculation of molecular structure, bond lengths, bond angles, and vibrational frequencies along with IR intensities and Raman scattering activities of 8CB and 8OCB liquid crystal molecule. The 6-31G(d, p) split valence-shell basis set augmented by the 'd' polarization function on heavy atoms and the 'p' polarization function on hydrogen atoms has been used [14-19].

Results and Discussion

A complete vibrational analysis of 8CB and 8OCB liquid crystal molecules has been performed based on DFT/B3LYP/6-311G(d,p) quantum chemical calculations. Optimized structural parameters were used in the calculation of vibrational frequencies to characterize all stationary points as minimums. The IR and Raman spectrum of 8CB and 8OCB liquid crystal molecules are shown by figures 2 and 3 respectively. At the frequency of 2341cm^{-1} , molecule shows the C-N stretching, which is found in IR spectrum of 8CB molecule but this stretching frequency change in 8OCB liquid crystal molecule. The 8CB molecule shows symmetric stretching in the benzene ring in between C-C atom at frequency 1660cm^{-1} which is found in IR and Raman both spectrum and due to alkoxy group this vibration shows at 1535cm^{-1} . At frequency 1256cm^{-1} , molecule shows stretching in between C-O atom which is also found in IR spectrum of 8OCB liquid crystal molecule. The dipole moment moments of 8CB and 8OCB liquid crystal molecules are 6.02 and 5.74 Debye respectively.

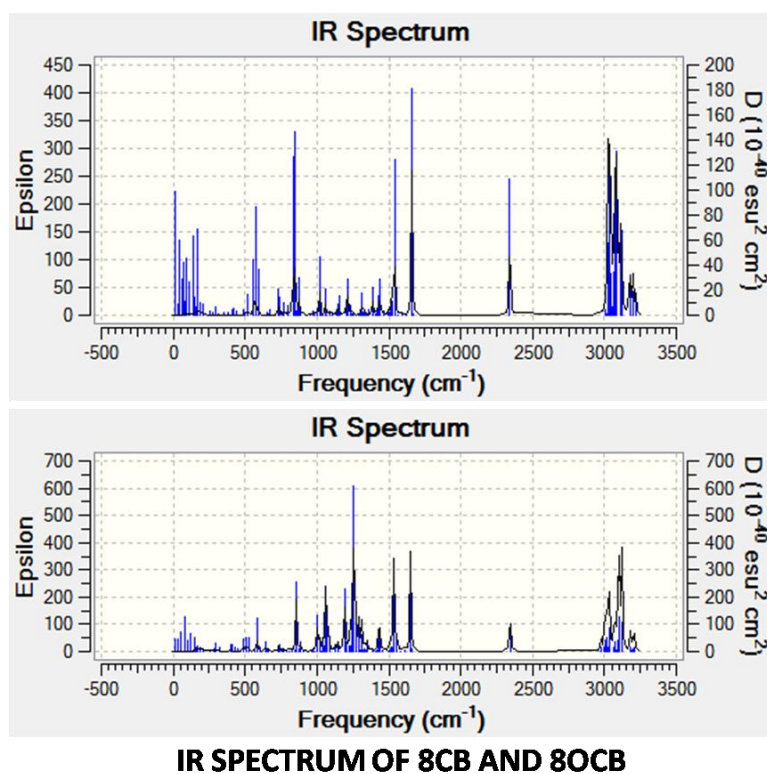
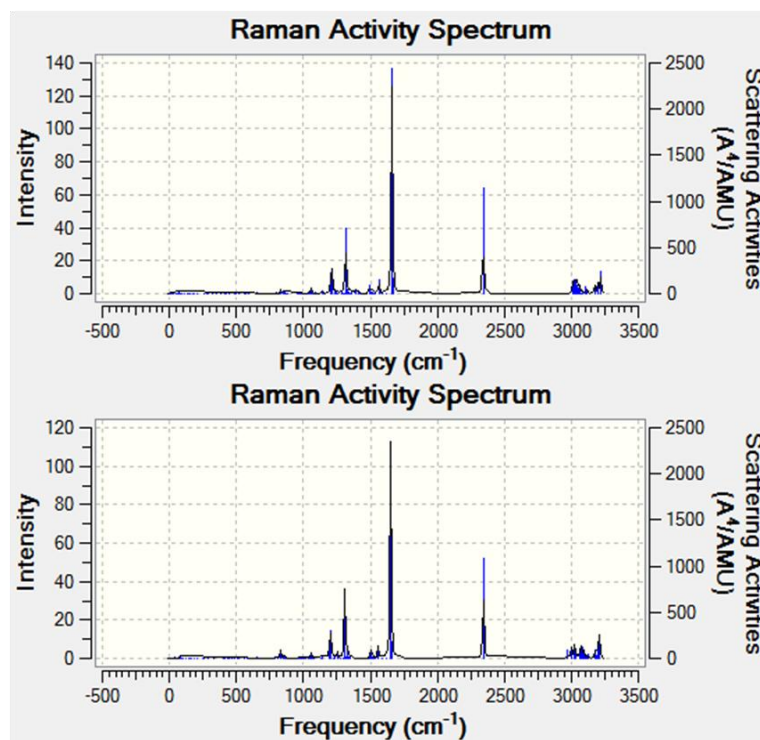


Figure 2: IR activity of of 8CB and 8OCB liquid crystal molecules



RAMAN ACTIVITY SPECTRUM OF 8CB AND 8OCB

Figure 3: Raman activity of 8CB and 8OCB liquid crystal molecules

Conclusion

The dipole moment of 8OCB molecule is less than the 8CB liquid crystal molecule, Due to the presence of oxygen atom in terminal group, IR spectrum of 8OCB liquid crystal molecule also different from 8CB liquid crystal molecule. The vibration frequency of C-N bond also changed.

References

1. G. Zhao, K. Tatani, T. Yoshihara, Y. Ozaki, J. Phys. Chem. B. 107(2003) 4227.
2. M. Kuribayashi, K. Hori, Liq. Cryst. 26 (1999) 809.
3. S. Ekgasit, M. Fulleborn, H.W. Siesler, Vib. Spectrosc.19 (1999) 85.
4. P.J. Collings, J.S. Patel, Handbook of Liquid Crystal Research, Oxford University Press, New York, 1997.
5. K.J. Toyne, G.W. Gray, Thermotropic Liquid Crystals, ed., Wiley, New York 1987.
6. A. Weber, Raman Spectroscopy of Gases and Liquids, Springer-Verlag, New York, 1979.
7. R.M. Blanchard, A.R. Noble-Luginbuhl, R.G. Nuzzo, Anal. Chem.72 (2000) 1365.

8. I. Gnatyuk, T. Gavrilko, G. Puchkovska, I. Chashechnikova, J. Baran, H. Ratajczak, J. Mol. Struct. 614 (2002) 233.
9. G.W. Gray, Molecular Structure and Properties of Liquid Crystals, Academic Press, New York 1962.
10. J. Workman Jr., K.E. Creasy, S. Doherty, L. Bond, M. Koch, A. Ullman, D.J. Veltkamp, Anal. Chem. 73 (2001) 2705.
11. D. Demas, J.W. Goodbye, G.W. Gray, H.W. Spies, V. Vill, Handbook of Liquid Crystals Vol.1, Wiley VCH, New York 1998.
12. A.R. Noble-Luginbuhl, R.M. Blanchard, R.G. Nuzzo, J. Am. Chem. Soc. 122 (2000) 3917.
13. T.I. Shabatina, E.V. Vovk, V.A. Timoshenko, Y.N. Morosov, G.B. Sergeev, Colloid Surf. A 198–200 (2002) 255. P.J. Hay, W.R. Wadt, J. Chem. Phys. 82, 299 (1985).
14. R. Ditchfield, W. J. Hehre, J. A. Pople, J. Chem. Phys. 54, 724 (1971).
15. C. Lee, W. Yang, R.G. Parr, Phys. Rev. B 37, 785 (1988).
16. A.D. Becke, J. Chem. Phys. 98, 5648 (1993).
17. P. C. Hariharan, J. A. Pople, Theo. Chim. Acta. 28, 213 (1973).
18. M. S. Gordon, Chem. Phys. Lett. 76, 163 (1980).
19. W. J. Hehre, R. Ditchfield, J. A. Pople, J. Chem. Phys. 56, 2257 (1972).
21. P. C. Hariharan, J. A. Pople, Mol. Phys. 27, 209 (1974).