Ab-initio Calculation of IR, UV-Vis and CD Spectra of Boron-nitrogen Azulenes

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INTRODUCTION

Azulene is an isomer of naphthalene. The isomerization of azulene to Naphthalene occurs at high temperature and is exothermic, nearly 40 Kcal/mol[1]. Boron-nitrogen azulene, the equivalent boron-nitrogen compound of azulene, can exist in two isomers. BN-azulene is the one that has a boron-boron linkage and NB-azulene, the one that has a nitrogen-nitrogen linkage. These compounds have not been synthetized yet, so little information is available. The aim of this study is characterize the isomers of boron-nitrogen azulene providing information about the absorption spectra and stability of the isomers.

METHODS

All calculations were performed using *TURBOMOLE* software[2]. The geometries of molecules were optimized in gas-phase at CC2 (Second-Order Approximate Coupled-Cluster) level using TZVPPD basis set. The spectra were also calculated at this level of theory. UV-Vis and CD spectra were obtained using 24 excitations and the Random Phase Approximation.

RESULTS AND DISCUSSION

Figure 1 shows the general structures of the two isomers discussed here. We note that both isomers are planar, which is usually a requirement for aromaticity.

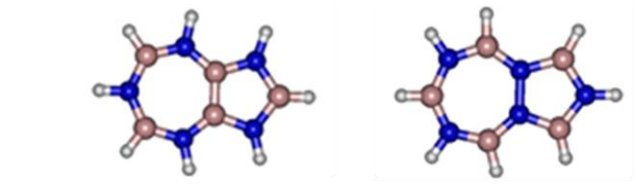

Figure 1. General structures of (a) BN-Azulene and (b) NB-azulene.

The values of total energy were: -402.592 eV (BN-Azulene) and -402.535 eV (NB-Azulene). BN-azulene appears to be more stable since it has the most negative value of total energy.

Figure 2 presents infrared, UV-Vis, CD absorption spectra for both isomers.

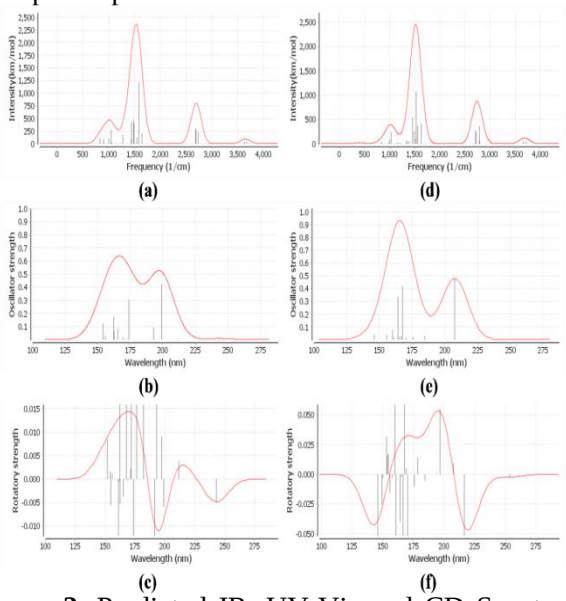

Figure 2. Predicted IR, UV-Vis and CD Spectra of BN-Azulene (a, b, c) and NB-azulene (d, e, f), respectively.

CONCLUSIONS

The calculation performed in this work enable the characterization of boron-nitrogen models to the azulene molecule. Both molecules are planar. However, BN-azulene presents higher stability.

ACKNOWLEDGMENTS

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