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Conformational stability, vibrational spectral assignments, UV-Vis, NMR, NBO, HOMO-LUMO and NLO properties of a series of trimethyl-pentane based on DFT calculations

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The structure of a hydrocarbon fuel has a profound impact on its ignition and other combustion properties. Based on experimental studies, the roles of fundamental kinetic properties of these hydrocarbon fuels on ignition rates have become clearer. Trimethyls pentane (TMP) compounds are of particular industrial interest as they are used in commercial gasoline to increase the octane number because their ability to withstand compression and reducing contribution to pollution. Then, it is necessary to identify the right computational method for modeling them, especially their conformational isomerism and their rich infrared and Raman vibrational spectra. In the present work, the theoretical study was carried out by DFT quantum methods for a series of trimethylpentane molecular (2,2,4-, 2,2,3-, 2,3,3- and 2,3,4-TMP), in order to have insight into electronic properties of each studied molecule and to differentiate between its conformers. After the conformational optimization, the rotational barriers between the most stable conformers have been calculated. The Natural bond orbital (NBO) analysis have also been carried out to analyze the effects of intramolecular charge transfer. HOMO and LUMO frontier orbitals, molecular electrostatic potential (MEP), the polarizability (α) and first order hyperpolarizability (β) and related properties were calculated. In addition to NMR and UV simulations, the normal mode calculations of the most stable conformers using a scaled force field in terms of non-redundant local symmetry coordinates have been made to approach the vibrational spectra temperature dependency.

Speaker Biography

Aziz Aboulmouhajir has completed his PhD in Molecular Modeling and spectroscopy, at the age of 25 years from Instelling Antwerpen University in Belgium with High Distinction. He is holder of the STAS Prize of the Royal Academy of Sciences, Letters and Arts of Brussels, in Belgium. For the last ten years, he was head of the Molecular Modeling and Spectroscopy E2MS Team at Chouaib Doukkali University. He is currently professor and director of several thesis projects in Molecular Recognition and spectroscopy in Hassan II University (Morocco).

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