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Theoretical-experimental study of asphaltene properties

Lyzette G.M. de Moura, Jaldyr J. G. Varela Jr, Auro A. Tanaka

Laboratório de Química Quântica Computacional, Universidade Federal do Maranhão, Cidade Universitária Dom Delgado, Avenida dos Portugueses, 1966, Vila Bacanga, São Luís, Maranhão, CEP 65065-545

Asphaltenes are structures mainly constituted by polycondensed aromatic rings, also presenting aliphatic lateral chains, some functional groups containing oxygen, nitrogen, and sulfur, in addition to trace quantities of metals as vanadium and nickel. The heteroatoms (N, O, and S) are strongly involved in the interactions (hydrogen bond, charge transfer, etc.) responsible for the asphaltene self-association [1-3]. This work aim to investigate a serie of properties (thermodynamics, structurals, and electronics) of asphaltenes and the intermolecular interactions of this fraction in the crude oil medium, such as, energy bonding, charge distribution, HOMO-LUMO gap, π-π interaction, vibration frequency, heat of formation, enthalpy, and free energy, focusing on the determination of characteristics such as molar mass and volume, based on the density functional theory, DFT. This will make possible to propose stable structural conformations that will be validate comparing data from literature and experimental results of characterization of asphaltenes from Brazilian crude oils. Preliminary experimental data obtained from LDI-MS provided a molar mass value of approximately 760 Da (n-heptane insoluble asphaltenes) and results from RMN indicated the presence of nitro group (-NO_2) and aromatic rings, information that conducted to the minima molecular formula $C_{51}H_{100}NO_2$. These data were used to propose two kinds of structures (an island and an archipelago) that are being evaluated and optimized employing the functional B3LYP; the basis set 6-311++G(d,p), LANL2TZ(f) and aug-cc-pVDZ will be applied to the determination of thermodynamics, structurals, and electronics parameters.

Key-words: asphaltenes, DFT, thermodynamic properties
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