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Study of intermolecular and intramolecular vibrations in heterocyclic aromatic hydrocarbons

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The chemical complexity of asphaltenes, which represent the most heavy fraction of oil, make their analyzing and modelling very challenging, because the detailed molecular composition remains unknown. However studies have reported that they consist of a heterogeneous mixture of polycondensed molecules, with heteroatoms such as sulfur, oxygen, and nitrogen. Vibrational spectroscopy has shown to be a tool for the identification and characterization of molecules in ill-defined mixtures, in combination with preditive modelling. In this work, the far- and mid-infrared spectra of a series of heteroaromatic (N, O and S) hydrocarbons and their dimers have been calculated using the ωB97X-D/6-311++G** level of Density Functional Theory (DFT), available in Gaussian09 platform. A perturbational-variational method coupled with potential truncation was incorporated to provide anharmonic corrections. Identification and quantification of peaks from inter and intra molecular vibrations in experimental spectra have been performed. Also experimental IR bands in the far-IR region were identified, it allow differentiating intermolecular and intramolecular vibrations. In addition, interaction energies were studied using DFT-SAPT (The symmetry-adapted perturbation theory based on density functional theory), and PBE0 aug-cc-pVTZ level employing MOLPRO2010. These methods reproduce energies in the same order of magnitude and identify π-π stacking as the dominant electronic interaction. Understanding the interaction between these primary units help to enrich the knowledge of the inter- and intramolecular interactions in asphaltenes and why they tend to aggregate and then to flocculate from the oil condensed phase. This outcome illustrates that the spectral signatures of heteroaromatic compounds can be used to probe the molecular and sub molecular composition, and the intermolecular interactions present in asphaltenes, by spectral decomposition.

Biography

Patricia Guevara Level is a member from Université de Pau et des Pays de l'Adour, France.

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