DFT study of Interstellar PAH molecules with aliphatic side groups

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Polycyclic Aromatic Hydrocarbon (PAH) molecules have emerged as a potential constituent of the Interstellar Medium (ISM) that emit strong features at 3.3, 6.2, 7.7, 8.6, 11.2 and 12.7 μm with weaker and blended features distributed in the 3-20 μm region. These features are proposed to arise from the vibrational relaxation of PAH molecules on absorption of background UV photons. These IR features also known as Aromatic Infrared Bands (AIBs) have been observed towards almost all types of astronomical objects; say HII regions, photodissociation regions, reflection nebulae, planetary nebulae, young star forming regions, external galaxies, etc. Astrophysical PAHs are proposed to exist in various forms, viz, ionized, both substituted and unsubstituted. Some interstellar PAHs are also identified to carry an aliphatic component that gives rise to 3.4 μm feature near the aromatic 3.3 μm feature. The 3.3 and 3.4 μm features are characteristics of stretching of an aromatic and aliphatic C-H bond in a PAH molecule. Despite the extensive research and wide acknowledgement of PAH molecules as carriers for AIBs, the identification of exact form of carriers still faces major challenges. In this work, we consider PAH molecules with aliphatic side groups to see any spectral similarities with the observed UIR features. This work reports a Density Functional Theory calculation of PAHs with -H, -CH_3, -CH_2-CH_3, -CH=CH_2 to determine the expected region of emission features and to find an aliphatic/aromatic ratio from moderate to large PAHs. We also include a deuterium (D) component in the aliphatic side group to see any possible consequences. We present a detailed analysis of the IR spectra of these molecules and discuss the possible astrophysical implications.