

Investigation of Interstellar Polycyclic Aromatic Hydrocarbon molecules as carriers for mid-infrared emission bands: combined approach

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Interstellar Polycyclic Aromatic Hydrocarbon (PAH) molecules exist in diverse forms depending on the local physical environment of the Interstellar Medium (ISM). Formation of ionized PAHs (anions and cations) is favorable in the extreme condition of the ISM. Besides its pure form, PAHs are likely to exist in substituted forms, for example, PAHs with functional groups, dehydrogenated PAHs, protonated and deuterated PAHs, etc (Buragohain et al., 2015, 2016). These PAHs may convert into alternate forms as a result of ongoing chemical processes in the ISM. Fullerene (C_{60}^+) has recently been detected as a crucial component of the ISM (Campbell et al., 2015; Ehrenfreund and Foing, 2015). Dehydrogenated PAHs might be an intermediary between PAHs and Fullerenes (Berné and Tielens, 2012).

The spectral evidence of PAH molecules and its variants in the ISM is observed via the mid-infrared bands, particularly at 3.3, 6.2, 7.7, 8.6, 11.2 and 12.7 μm (Tielens, 2008). These bands, also known as ‘Aromatic Infrared Bands (AIBs)’ are widely present in the ISM and arise from the vibrational relaxation of PAH molecules on absorption of background UV photons. However, the exact form of PAH molecules that are responsible for the AIBs is still ambiguous. Here, we discuss the possible form of interstellar PAH molecules as carriers for AIBs. Density Functional Theory (DFT) calculation on several classes of PAHs is employed to study its spectral characteristics in infrared. We compare our results with *SUBARU* observations in quest of any correlation that establishes its presence in the ISM.

References

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