The Carriers of the Unidentified Infrared Emission Features: Clues from Polycyclic Aromatic Hydrocarbons with Aliphatic Sidegroups

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The unidentified infrared emission (UIE) features at 3.3, 6.2, 7.7, 8.6, 11.3 and 12.7 μm are ubiquitously seen in a wide variety of astrophysical regions in the Milky Way and nearby galaxies as well as distant galaxies at redshifts $z \geq 4$. The UIE features are characteristic of the stretching and bending vibrations of aromatic hydrocarbon materials. The 3.3 μm feature which results from the C--H stretching vibration in aromatic species is often accompanied by a weaker feature at 3.4 μm. The 3.4 μm feature is often thought to result from the C--H stretch of aliphatic groups attached to the aromatic systems. The ratio of the observed intensity of the 3.3 μm aromatic C--H feature ($I_{3.3}$) to that of the 3.4 μm aliphatic C--H feature ($I_{3.4}$) allows one to estimate the aliphatic fraction (e.g., $N_{C,aliph}/N_{C,arom}$, the number of C atoms in aliphatic units to that in aromatic rings) of the carriers of the UIE features, provided that the intrinsic oscillator strengths (per chemical bond) of the 3.3 μm aromatic C--H stretch ($A_{3.3}$) and the 3.4μm aliphatic C--H stretch ($A_{3.4}$) are known.

In this work we employ density functional theory and second-order perturbation theory to compute the infrared vibrational spectra of seven polycyclic aromatic hydrocarbon (PAH) molecules with various aliphatic substituents (e.g., methyl-, dimethyl-, ethyl-, propyl-, butyl-PAHs, and PAHs with unsaturated alkyl chains). The mean band strengths of the aromatic ($A_{3.3}$) and aliphatic ($A_{3.4}$) C--H stretches are derived and then employed to estimate the aliphatic fraction of the carriers of the UIE features by comparing the ratio of the intrinsic band strength of the two stretches ($A_{3.4}/A_{3.3}$) with the ratio of the observed intensities ($I_{3.4}/I_{3.3}$).

We conclude that the UIE emitters are predominantly aromatic, as revealed by the observationally-derived ratio $I_{3.4}/I_{3.3} \approx 0.12$ and the computationally-derived ratio $A_{3.4}/A_{3.3} \approx 1.76$ which suggest an upper limit of $N_{C,aliph}/N_{C,arom} \approx 0.02$ for the aliphatic fraction of the UIE carriers.