

# On the aliphatic versus aromatic content of the carriers of the ‘unidentified’ infrared emission features

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Although it is generally accepted that the unidentified infrared emission (UIE) features at 3.3, 6.2, 7.7, 8.6, and 11.3 micron are characteristic of the stretching and bending vibrations of aromatic hydrocarbon materials, the exact nature of their carriers remains unknown: whether they are free-flying, predominantly aromatic gas-phase molecules, or amorphous solids with a mixed aromatic/aliphatic composition are being debated. Recently, the 3.3 and 3.4 micron features which are commonly respectively attributed to aromatic and aliphatic C—H stretches have been used to place an upper limit of ~2% on the aliphatic fraction of the UIE carriers (i.e., the number of C atoms in aliphatic chains to that in aromatic rings). Here we further explore the aliphatic versus aromatic content of the UIE carriers by examining the ratio of the observed intensity of the 6.2 micron aromatic C—C feature ( $I_{6.2}$ ) to that of the 6.85 micron aliphatic C—H deformation feature ( $I_{6.85}$ ). To derive the intrinsic oscillator strengths of the 6.2 micron stretch ( $A_{6.2}$ ) and the 6.85 micron deformation ( $A_{6.85}$ ), we employ density functional theory to compute the vibrational spectra of seven methylated polycyclic aromatic hydrocarbon molecules and their cations. By comparing  $I_{6.85}/I_{6.2}$  with  $A_{6.85}/A_{6.2}$ , we derive the fraction of C atoms in aliphatic form to be at most ~000%, confirming the earlier finding that the UIE emitters are predominantly aromatic. We have also computed the intrinsic strength of the 7.25 micron feature ( $A_{7.25}$ ), another aliphatic C—H deformation band. With  $A_{6.85}$  appreciably exceeding  $A_{7.25}$ , this explains why the 6.85 micron feature is more frequently detected than the 7.25 micron feature.