LIGHT ON THE 3 μm EMISSION BAND FROM SPACE WITH MOLECULAR BEAM SPECTROSCOPY

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The majority of interstellar objects shows IR emission features also known as unidentified infrared (UIR) emission bands. These UIR bands are attributed to IR emission of highly-excited gaseous polycyclic aromatic hydrocarbons (PAHs). To understand the physical conditions and chemical evolution of the interstellar environment a precise identification of the emission carriers is desired. The 3 μm UIR feature is represented by a strong band at 3040 cm^{-1}, a plateau from 3150 to 2700 cm^{-1} and a number of weak features within this plateau. The 3040 cm^{-1} component is assigned to fundamental CH-stretch vibrations of PAHs, but there still remain many questions on the origin of the other features. In this work we have studied experimentally the 3 μm region of regular, hydrogenated and methylated PAHs (up to 5 rings), combining molecular beam techniques with IR-UV ion dip spectroscopy, and theoretically by density functional theory (DFT) calculations within the harmonic and anharmonic approximation. We find that (a) the 3 μm region of PAHs is dominated by Fermi resonances and thereby cannot be treated within the harmonic approximation; (b) the periphery structure of the molecules strongly affects the shape of the 3 μm band. In particular, the two-component emission interpretation can be explained by the presence of molecules with and without bay-hydrogens; (c) due to strong Fermi resonances of fundamental modes with combination bands regular PAHs can significantly contribute to the 3 μm plateau in the 3150-2950 cm^{-1}, while hydrogenated and methylated species are primarily responsible for features in the 2950-2750 cm^{-1} region.