Chemical Structures of Interstellar Polycyclic Aromatic Hydrocarbons

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The so-called "unidentified" infrared emission (UIE) features at 3.3, 6.2, 7.7, 8.6, 11.3 and 12.7 μm, commonly attributed to the stretching and bending vibrations of polycyclic aromatic hydrocarbon (PAH) molecules, are ubiquitously seen in a wide variety of astrophysical regions in the Milky Way and nearby galaxies as well as distant galaxies at redshifts $z \geq 4$. While PAH is a precisely defined *chemical* term (i.e., PAHs are fused benzene rings made up of C and H atoms), astronomical PAHs are not necessarily *pure* aromatic compounds as strictly defined by chemists. Instead, PAH molecules in astronomical environments may include ring defects, substituents, partial deuteration, partial dehydrogenation, and sometimes super-hydrogenation. Astro−nomical PAHs often also include an aliphatic component (e.g., aliphatic side-groups like methyl $–CH_3$ may be attached as functional groups to PAHs). In this talk, I will review our current understanding of the chemical structures of PAHs, with special attention paid to methylation, deuteration, super-hydrogenation, and N-, S- and O-substitution. The high sensitivity and high spatial resolution capabilities of *JWST* will open up an infrared window unexplored by *Spitzer* and unmatched by *ISO* observations for gaining insight into the chemical structures of PAHs.