A State of the Art Infrared Spectral Analysis of the Chemical Evolution of Carbonaceous Molecules During Star Formation

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Strong infrared (IR) emission features between 3.3 and 12.7 μm are ubiquitous and are the most luminous mid-infrared spectral features originating from the ambient interstellar medium (ISM). They are valuable diagnostics of its chemical composition, thermal excitation and evolution of carbonaceous dust. IR emission features at 3.3, 6.2, 7.7, 8.6, 11.2 μm and 12.7 μm are observed in many astronomical sources at various stages of evolution, from young HII regions, to older post asymptotic giant branch stars, planetary nebulae, transition objects, novae, the Galactic disk and even extragalactic sources like irregular, starburst and ultraluminous galaxies. These mysterious features are generally attributed to polycyclic aromatic hydrocarbon (PAH) molecules, although the exact identification of the carriers of these infrared features with specific molecules has remained elusive, leading to their being termed the "unidentified infrared (UIR) emission features." Our primary focus is the interaction between laboratory work by Hudgins and Allamandola and theoretical studies by the authors to determine the origins and evolution of the carriers of the "UIR" bands and the critical role these molecules play in the thermodynamics, physics and chemistry of star and planet forming regions. We analyse and interpret observational data using our state of the art theoretical models of IR emission. These are based upon a comprehensive and unique quantum chemical and laboratory database of the spectral characteristics of neutral, negative and positively charged (up to charge +3) PAHs. The models simultaneously take into account the IR characteristics of specific PAH species, photoelectric charging and electron recombination, ultraviolet (UV) photon excitation (single and multiple) followed by IR relaxation and PAH photochemistry, which are driven by the illuminating stellar radiation field and the (ion-molecule) chemistry with the gas. In this way, we derive a unified model of macromolecular species in different astrophysical environments, built on a firm foundation of experimental measurements, extended to the innovative realms of theoretical astrophysics and quantum chemistry.