Astronomical IR Emission Bands and Polycyclic Aromatic Hydrocarbons (Pahs)

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The astrophysical infrared emission features at 3.3, 6.2, 7.7, 8.6, 11.2 and 12.7 micron (3030, 1610, 1300, 1160, 890 and 790 cm^{-1}) are attributed to vibrational transitions in polycyclic aromatic hydrocarbon (PAH) molecules. These aromatic infrared bands (AIBs) are ubiquitously observed in a variety of objects from star-forming regions to late-type stars and even in external galaxies. The AIB profile variations correlate with object type indicating different PAH types and populations in the different regions. Theoretical infrared study of a large set of PAHs points towards the possible presence of large sized PAHs in benign regions around planetary nebulae and small- to medium-sized PAHs in harsh UV-dominated star-forming regions. But neither specific PAH has been identified nor has simultaneous match with all observed AIBs been possible. Using quantum chemical calculations a study of PAH derivatives and PAHs with side groups is being reported to obtain constraints on possible mixture of molecules that can explain all AIBs simultaneously. In particular attempt is made to match the A, B and C type profiles of the 6.2 and 7.7 micron AIBs that are related to ring vibrations. The information of the size, shape and charge states of such molecules in the interstellar medium will lead to an understanding of physical conditions in the region and of the molecular evolution therein.