Deciphering the aromatic infrared bands: the LAIBrary project

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The aromatic infrared bands (AIBs) are major emission features resulting from large carbonaceous molecules that are excited by the absorption of individual UV photons from stars. These bands are therefore used to trace the UV radiation field in star-forming regions, from the small scale of protoplanetary disks to the large scale of galaxies [1,2]. They also carry information on the chemical complexity of their carriers and their evolution as a function of physical conditions. Polycyclic aromatic hydrocarbons (PAHs) and related species are good candidates to explain these bands, but other species such as fullerenes also contribute (so far, the C_{60} and C_{60}^+ emission bands could be assigned [3,4]).

A detailed analysis of AIB spectra requires taking into account molecular diversity as well as excitation conditions. In heated molecules, vibrational coupling (anharmonicity) plays a major role, affecting the position and width of bands [5] and leading to a number of new bands such as combination/difference bands and overtones. To disentangle the effects of temperature from chemical complexity, a detailed comparison of observed spectra with synthetic spectra that model the emission of a given PAH molecule in a given UV-visible astrophysical radiation field is required. This is the objective of the LAIBrary project supported by CNES and in relation with the Early Release Science programme, PDR4all, of the James Webb Space Telescope [6].

The objectives and current achievements of the LAIBrary project will be presented, including –(i)- obtaining empirical anharmonic parameters that describe the evolution with temperature of the position and width of the bands, from both experiments and quantum chemistry calculations. The case of pyrene has been studied in detail [7,8] followed more recently by larger species and species containing methyl sidegroups. –(ii)- Development of an emission code to be used by a simulator for a fast calculation of the emission of a given PAH in a given radiation field, and –(iii)- Dissemination of molecular data and tools via publicly available databases and the Cosmic PAH portal (http://cosmic-pah.irap.omp.eu).

Références

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