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High-temperature infrared spectroscopy of large aromatic molecules

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Large aromatic molecules are ubiquitous in astrophysical environments such as star forming regions, galaxies and planetary nebulae in which they emit the Aromatic Infrared Bands (AIBs). These molecules include polycyclic aromatic hydrocarbons (PAHs) but also fullerenes, C₆₀ being the only molecule of this class identified so far. Emission in the AIBs is triggered by the absorption of a UV photon via an electronic transition and a sequence of radiationless transitions converting most of the absorbed energy to a vibrational excitation in the electronic ground state. The hot molecule then relaxes by emitting IR photons, the resulting spectrum being dominated by a large number of hot bands, all slightly shifted with respect to the corresponding 1-0 fundamentals due to anharmonicity. The resulting bands are very broad and their interpretation complex. In order to progress on the analysis of the IR spectra of these hot large molecules, we are developing an experimental approach to quantify the temperature dependent infrared (IR) spectrum of PAHs. We recorded the IR spectrum of solid pyrene (C₁₆H₁₀) in KBr pellets from 14K to 723K. With increasing temperature a gradual red shift of the band positions and increase of the bandwidth were observed. For the higher temperatures, we compared these data with the few available data recorded in gas-phase [1]. That allows us to gain confidence into the relevance of these measurements in solid phase to derive anharmonic constants for isolated molecules. We therefore used the same experimental approach to study the temperature-dependent IR spectra of larger species such as coronene (C₂₄H₁₂) and fullerene C₆₀. In this presentation we will discuss and summarize these results.

References

[1] Joblin, C.; Boissel, P.; Léger, A.; d'Hendecourt, L. & Défourneau, D. *Astron. Astrophys.* 835, 299 (1995)

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