

An atlas of synthetic absorption and emission bands of interstellar PAHs

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Abstract. In the framework of the interstellar PAHs hypothesis, absorption bands in the vis/UV and far-IR skeletal emission bands are expected to be a fingerprint of *specific* species in this class. We developed a detailed Monte-Carlo model of the photophysics of isolated interstellar PAHs which provides a powerful tool for single-molecule identification. We present synthetic spectra predicted by the above general approach for 25 PAHs and their respective cations, ranging in size from naphthalene (C₁₀H₈) to circumcoronene (C₅₄H₁₈), excited by a range of different radiation fields. Synthetic rotational profiles of electronic absorption bands in the vis/UV should be compared to high resolution spectra of diffuse interstellar bands. Infrared emission spectra aim at a direct, quantitative comparison with present (ISO) and forthcoming (Herschel) observations. Since the spectrometers onboard Herschel will be able to observe far-IR emission bands from interstellar PAHs, possibly resolving their rotational envelopes, we also calculated synthetic rotational profiles of their low-energy vibrational modes. The accuracy of these spectra is essentially the same as that of the quantum-chemical calculations used, but can be refined using laboratory data, when the latter are available.

Keywords. Astrochemistry, line: identification, line: profiles, ISM: abundances, ISM: molecules, molecular data, molecular processes, methods: numerical, astronomical data bases: miscellaneous

Acknowledgements

Giuliano Mallocci acknowledges the financial support by INAF-OAC (Istituto Nazionale di Astrofisica, Osservatorio Astronomico di Cagliari).

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