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Laboratory and Computational Spectroscopy of Jet-Cooled Neutral and Ionized PAHs

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Abstract. We present the gas-phase spectra of neutral and ionized polycyclic aromatic hydrocarbons (PAHs) measured in the near UV to near IR range in an astrophysically relevant environment. The physical conditions of the interstellar medium are simulated in the laboratory by associating a molecular beam with an ionizing discharge to generate a cold plasma expansion. PAH ions are formed from the neutral precursors by DC discharge in the plasma. The spectra of cold ($\leqslant$ 100 K), neutral and ionized PAHs are measured using the high sensitivity methods of cavity ring-down spectroscopy (CRDS) and multiplex integrated cavity output spectroscopy (MICOS). The measured vibronic bands of ionized PAH are found homogenously broadened ($\geqslant$ 25 cm^{-1}) while the bands associated with the neutral precursors are narrower (2-15 cm^{-1}). The measured spectra are interpreted and assigned with the help of quantum chemical calculations [e.g. (time-dependent) density functional theory calculations and ab initio calculations] followed by vibronic and Franck-Condon calculations. The dynamics that is responsible for the different band profiles observed in neutral and ionized PAHs is discussed. These laboratory measurements provide data on PAHs that can now be directly compared to astronomical observations. In particular, the comparison of the interpreted spectra with diffuse interstellar band (DIB) spectra and with the spectra of circumstellar environments of selected carbon stars leads to important implications for the population of interstellar PAHs (see parallel contribution of Cami et al.). This study holds great potential for understanding the chemistry and chemical dynamics in the circumstellar and interstellar environments where chemical evolution takes place.

Keywords. Astrochemistry, molecular data, line: profiles, ISM: molecules

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