

ELECTRONIC SPECTROSCOPY OF PROTONATED AND HYDROGENATED QUINOLINE ISOLATED IN SOLID *PARA*-HYDROGEN

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Cationic, protonated, and hydrogenated polycyclic aromatic hydrocarbons (PAH) and their nitrogen-substituted derivatives (PANH) have been proposed as possible carriers of unidentified infrared (UIR) emission bands. These compounds might also be promising candidates for carriers of the diffuse interstellar bands (DIB), electronic absorption bands of interstellar origin observed in the visible to near-IR region. However, laboratory spectra of such species suitable for comparison with astronomical observations are rarely available.

We present the fluorescence excitation and dispersed fluorescence spectra of N-protonated quinoline ($C_9H_7NH^+$) and isomers of hydrogenated quinoline (HC_9H_7N), derivatives of the smallest PANH, isolated in solid *para*- H_2 (*p*- H_2) at 3 K. These molecules were generated by electron bombardment during the deposition of a mixture of quinoline (C_9H_7N) and *p*- H_2 . We located the 0_0^0 band of the S_1-S_0 transition at 27778 cm^{-1} for $C_9H_7NH^+$, indicating a red-shift induced by the *p*- H_2 environment. This shift was $\sim 90\text{ cm}^{-1}$ relative to gas-phase experiments conducted at room temperature by Hansen et al.^a and $\sim 122\text{ cm}^{-1}$ relative to gas-phase experiments at 40 K by Féraud et al.,^b both using photodissociation spectroscopy. Furthermore, we observed the spectral signature of at least one HC_9H_7N isomer, which exhibited a fluorescence lifetime of $\sim 40\text{ ns}$. We tentatively assign this band system with its 0_0^0 band at 18756 cm^{-1} to 5- HC_9H_7N and provide the first vibronic assignments for the dispersed fluorescence and fluorescence excitation spectra of this molecule according to the Franck-Condon Herzberg-Teller simulations using the (TD-)B3LYP/6-311++G(2d,2p) method.

^aHansen et al. *Phys. Chem. Chem. Phys.* 17, 25882-25890 (2015).

^bFéraud et al. *J. Phys. Chem. A*, 121, 2580-2587 (2017).