Infrared spectra of isomers of hydrogenated acenaphthylene isolated in solid *para*-hydrogen

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Polycyclic aromatic hydrocarbons (PAHs) and their derivatives have been proposed to be potential carriers responsible for the unidentified infrared (UIR) emission bands observed in the interstellar medium.[1] Also, spectral characterization of mono-hydrogenated PAH provides an opportunity to investigate the formation of super-hydrogenated PAH or to study the catalytic H_2-formation in ISM.

In this work, we report the infrared (IR) spectra of four isomers of mono-hydrogenated acenaphthylene (2–, 3–, 4– and 5–$HC_{12}H_8$). The H atoms are produced from the $C_{12}H_8/Cl_2/p\text{-}H_2$ matrices at 3.2 K upon irradiation at 365 nm to generate Cl atoms, followed by IR irradiation that initiates the reaction $Cl + H_2 (v = 1) \rightarrow HCl + H$. The hydrogenation of $C_{12}H_8$ at 3.2 K in darkness can be initiated via quantum tunneling.

Spectral groupings were achieved according to the behaviors of lines upon secondary photolysis at various wavelengths, selected according to the vertical electronic transitions of these isomers of $HC_{12}H_8$ predicted with the TD-B3LYP/6-311++G(d,p) method. The spectral assignments were achieved on comparison of the experimental results with the vibrational wavenumbers and IR intensities of possible isomers predicted with the B3LYP/6-311++G(d,p) method. All spectra of $HC_{12}H_8$ are new.

For $HC_{12}H_8$, major lines were observed at 13.08, 12.43, 13.34, and 14.05 µm for 2–$HC_{12}H_8$, 3–$HC_{12}H_8$, 4–$HC_{12}H_8$, and 5–$HC_{12}H_8$, respectively. Based on the overall spectral pattern, these hydrogenated species are unlikely to be the carriers of the UIR bands, characterized by emission bands near 3.3, 6.2, 7.7, 8.6, 11.2, and 12.0 µm.

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[1] Leger, A.; Puget, J. L. Identification of the 'unidentified' IR emission features of interstellar dust? *Astron. Astrophys.* **1984**, *137*, L5-L8.