IDENTIFICATION OF PROTONATED PYRENE (1-$C_{16}H_{11+}$) AND ITS NEUTRAL COUNTERPART ISOLATED IN SOLID PARA-HYDROGEN

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Protonated polycyclic aromatic hydrocarbons (H^+PAH) have been reported to have infrared (IR) bands at wavenumbers near those of unidentified infrared (UIR) emission bands from interstellar objects. We report the IR spectra of protonated pyrene (1-$C_{16}H_{11}{}^+$) and hydropyrenyl radical (1-$C_{16}H_{11}$) trapped in solid para-hydrogen (p-H_2). These species were produced on electron bombardment of a mixture of p-H_2 and pyrene during deposition. The IR features of 1-$C_{16}H_{11}{}^+$ were identified on observing the decay of IR lines, whereas those of 1-$C_{16}H_{11}$ were identified with increased intensity, after the matrix sample was maintained in darkness for an extended period or upon irradiation of the matrix sample with UV light at 365 nm. Observed relative intensities and wavenumbers agree satisfactorily with the IR intensities and scaled vibrational wavenumbers predicted for these species with the B3PW91/6-311++G(2d, 2p) method. Compared with literature spectra of protonated polycyclic aromatic hydrocarbons recorded previously with IR photodissociation of Ar-tagged compounds[a] or IR multiphoton dissociation, [b] our method has the advantages of producing IR spectra with high resolution, true intensity and wide spectral coverage for both protonated polycyclic aromatic hydrocarbons and their neutral counterparts. This method is relatively clean with little interference from fragmentation and can be readily applied to larger H^+PAH.

[a] A. M. Ricks, G. E. Douberly and M. A. Duncan, *Astrophys. J.* **702**, 301 (2009).
[b] O. Dopfer, *PAHs and the Universe,* **46**, 103 (2011).