IDENTIFICATION OF α- AND β-PROTONATED NAPHTHALENE ($C_{10}H_9{}^+$) AND THEIR NEUTRAL COUNTERPARTS ISOLATED IN SOLID PARA-HYDROGEN

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We report the infrared (IR) spectra of protonated naphthalene ($C_{10}H_9{}^+$) and hydronaphthyl radical ($C_{10}H_9$) in both α- and β-forms trapped in solid para-hydrogen (p-H_2). These species were produced on electron bombardment of a mixture of p-H_2 and naphthalene during deposition. The IR features of α-$C_{10}H_9{}^+$ were identified on observing the decay of IR lines, whereas those of α-$C_{10}H_9$ and β-$C_{10}H_9$ were identified with the increased intensity after the matrix sample was maintained in darkness for an extended period. IR features of α-$C_{10}H_9$ and β-$C_{10}H_9$ were further characterized on irradiation of a matrix sample with UV or visible light. Irradiation of the matrix sample with visible light (495-700 nm) generated neutral $C_{10}H_9$ in both forms, whereas irradiation with light at 365 nm generated only α-$C_{10}H_9$. Lines due to β-$C_{10}H_9{}^+$ were observed only during the initial period of acquisition of an IR spectrum after secondary photolysis of the matrix sample. Observed wavenumbers and relative intensities agree satisfactorily with the anharmonic vibrational wavenumbers and IR intensities predicted for these species with the B3LYP/6-311++G(2d,2p) method. Compared with literature spectra 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 with little interference from other fragments. With these advantages, the IR spectra of α-$C_{10}H_9{}^+$ and β-$C_{10}H_9{}^+$ were clearly distinguished.

[a] A. M. Ricks, G. E. Douberly and M. A. Duncan, *Astrophys. J.* **702**, 301 (2009).
[b] U. J. Lorenz, N. Solcá, J. Lemaire, P. Maître and O. Dopfer, *Angew. Chem. Int. Ed,* **46**, 6714 (2007).