INFRARED SPECTROSCOPY OF BENZENE-HCN IN HELIUM-DROPLETS

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Infrared spectra are reported for several $(C_6H_6)_m$-$(HCN)_n$ and $(C_6D_6)_m$-$(HCN)_n$ clusters in liquid helium nanodroplets. A large electric field can be used to collapse the rotational structure in these spectra, which aids in the initial searching. In the 1:1 clusters the HCN ν_{CH} stretching vibration at 3253.2 cm^{-1} (C_6H_6-HCN) and 3252.9 cm^{-1} (C_6D_6-HCN) are red-shifted by approximately 60 cm^{-1} compared to the monomer, indicative of strong intermolecular hydrogen bonds between the CH-group and the aromatic π-clouds of the benzenes. Zero field spectra show considerable rotational structure consistent with a symmetric rotor structure as determined in the gas-phase by microwave spectroscopy.[a]

Moreover several trimers and tetramers of HCN and Benzene have been observed, all of which are further red-shifted than the 1:1 complexes. Pressure-dependency studies allow the size assignments of these clusters. The frequency shifts and rotational contours of the bands allows one to infer the structures of these clusters in liquid helium.

[a] H.S. Gutowski, E. Arunan, T. Emilson, S.L. Tschopp, and C.E. Dykstra, *J. Chem. Phys.* **103**(1995), 3917.