THE QUANTUM SOLVATION OF CYANOACETYLENE WITH HELIUM ATOMS: MICROWAVE SPECTROSCOPIC STUDIES

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The rotational spectra of He_N-cyanoacetylene clusters (N = 1, 2,3, 4, 5..) have been measured in the 3-27 GHz range using a high-resolution Fourier transform microwave spectrometer. The weakly bound clusters were generated in a pulsed free jet expansion. Manipulating the sample and nozzle conditions allowed some degree of control over the successive solvation of the molecule with He-atoms. Both the HCCCN and DCCCN isotopomers have been studied, allowing information about cluster geometry and dynamics to be determined. The presence of ^{14}N and D nuclei in the clusters causes nuclear quadrupole hyperfine splitting of the He_N-HCCCN and He_N-DCCCN rotational transitions. This hyperfine structure was resolved, assigned, and analysed for low-J transitions. The value of the rotational constants decreases towards the helium nanodroplet value with increasing cluster size for small clusters. A "turn-around" in rotational constant value is expected for N >6. Hyperfine fitting parameters and rotational constants will be interpreted in terms of the structure and dynamics of He_N-HCCCN clusters.