

First infrared spectra of the acrylonitrile-water hydrogen-bonded complexes isolated in solid neon

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The nitrile molecules have been detected in a variety of interstellar environments and these molecules are interest in astrochismity. The experimental study of the complexation of acrylonitrile molecule (AN) with water has been undertaken from a vibrational point of view in solid neon at 3 K from 80 to 6000 cm^{-1} using Fourier transform infrared spectroscopy. From concentration effects and with the help of theoretical results we have identified several vibrational transitions for AN-H₂O and AN-(H₂O)₂ complexes. For the AN-H₂O complex, in which the two submolecules interacting through hydrogen bonding, the infrared spectral changes (frequencies as well as intensities) indicate that the water plays the role of the proton donor. We highlight the presence of three isomers for the AN-H₂O complex and two isomers for the AN-(H₂O)₂ complex. Theoretical calculations at the MP2/AVTZ level have been performed to obtain their equilibrium geometries and vibrational spectra at the harmonic level and comparison with experimental data allows us to give structures of these complexes.