

CHARACTERIZATION OF AMMONIA-WATER CLUSTERS BY BROADBAND ROTATIONAL SPECTROSCOPY

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Neon carrier gas at 0.3 MPa of backing pressure is flowed over a room-temperature ammonia hydroxide solution before being expanded into a chirped-pulse Fourier transform microwave (CP-FTMW) spectrometer operating between 2 and 8 GHz. A dense spectrum was observed and the investigation allowed unambiguous assignment of the $(\text{NH}_3)_2(\text{H}_2\text{O})_n$ with $n=1,2$ and $\text{NH}_3(\text{H}_2\text{O})_n$ with $n=2,3,4,5,6,8$ with a signal to noise of at least 3:1. The structures show a cyclic arrangement for clusters with up four monomer and then move to a 3D arrangement. These clusters are of interest because of the different possibilities for hydrogen bond network related to the isolated water clusters. Calculations indicate that there are several possible low-energy isomers, with different levels of theory identifying different isomers as the global minimum. The evidence for the assignment and a discussion of the derived properties for the species are presented.