MICROWAVE SPECTROSCOPIC INVESTIGATION OF THE XE-H_2O AND XE-$(H_2O)_2$ VAN DER WAALS COMPLEXES

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The intermolecular interactions of xenon with one and two water molecules were investigated using spectroscopic and *ab initio* methods. Rotational spectra of the Xe-H_2O and Xe-$(H_2O)_2$ complexes were recorded using a pulsed-nozzle Fourier transform microwave spectrometer. Transitions within two internal rotor states, namely the $\Sigma 0_{00}$ and $\Sigma 1_{01}$ states, were measured and assigned for the Xe-H_2O dimer. Nine a- type and twelve b- type transitions were measured for the Xe-$(H_2O)_2$ complex. The ^{131}Xe (I = 3/2), D (I = 1), and ^{17}O (I = 5/2) nuclear quadrupole hyperfine structures were resolved and analyzed in case of Xe-H_2O. For Xe-$(H_2O)_2$, only the ^{131}Xe nuclear quadrupole hyperfine structure could be detected. The determined spectroscopic constants, including nuclear quadrupole coupling constants, were used to obtain information about the structure and dynamics of these two complexes. The experimental data of Xe-H_2O were complemented by the construction of an *ab initio* potential energy surface at the CCSD(T) level of theory. An overall goal of this work is to determine how the successive solvation of xenon with water molecules affects the xenon electron distribution and its intermolecular interactions. The results may aid in the molecular level interpretation of ^{129}Xe and ^{131}Xe NMR data from imaging experiments.