ROTATIONALLY-RESOLVED SPECTROSCOPY OF THE BENDING MODES OF DEUTERATED WATER DIMER

JACOB T. STEWART, Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana, IL 61801; BENJAMIN J. McCALL, Departments of Chemistry and Astronomy, University of Illinois at Urbana-Champaign, Urbana, IL 61801.

High-resolution spectroscopy of small gas-phase water clusters has provided a wealth of information regarding the intermolecular interactions between water molecules. Water dimer is of particular interest because high-resolution spectroscopy can yield detailed information about the water pair potential. While there have been extensive studies of water dimer throughout the microwave and infrared regions of the spectrum, to date there has been no reported high-resolution spectrum of the intramolecular bending modes of water dimer. We have obtained rotationally-resolved spectra of the bending modes of deuterated water dimer $(D_2O)_2$, which are, to our knowledge, the first reported spectra of the bending modes of water dimer with rotational resolution. Dimers were produced in a supersonic expansion by bubbling Ar or He through D_2O and expanding the mixture through a 150 μ m × 12 mm slit. The expansion was then probed using continuous wave cavity ringdown spectroscopy with light generated by a quantum cascade laser (QCL) operating near 8.5 μ m. We have assigned the $K_a = 1 \leftarrow 0$ and $K_a = 2 \leftarrow 1$ sub-bands of the bending mode belonging to the hydrogen bond donor and have observed additional transitions which we attribute to the bending mode associated with the hydrogen bond acceptor.