WHAT MAKES WATER WET? TERAHERTZ AND IR CAVITY RINGDOWN SPECTROSCOPY RESULTS FOR WATER CLUSTERS

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Vibration-Rotation-Tunneling (VRT) spectra have been measured and analyzed for water clusters as large as hexamer, using cw terahertz laser technology.[a] Force fields, structures, and hydrogen bond rearrangement tunneling dynamics are characterized from these data, wherein the intermolecular vibrations are directly excited. Covalent bond vibrations of water clusters are studied in the mid-IR with newly-emerging cavity ringdown technology.[b] These spectra characterize the significant monomer distortion that accompanies sequential hydrogen bond formation. Progress in deducing a more complete description of liquid water from these data will be described.[c]

[a] K. Liu, J.D. Cruzan, and R.J. Saykally, Science 271, 929 (1996); K. Liu, M.G. Brown, and R.J. Saykally, J. Phys. Chem. A 101, 8995 (1997); K. Liu, M.G. Brown, J.D. Cruzan, and R.J. Saykally, J. Phys. Chem. A 101, 9011 (1997); J.D. Cruzan, M.R. Viant, and R.J. Saykally, J. Phys. Chem. A 101, 9022 (1997); M.R. Viant, J.D. Cruzan, D.D. Lucas, M.G. Brown, K. Liu, and R.J. Saykally, J. Phys. Chem. A 101, 9032 (1997).

[b] J.B. Paul, R.A. Provencal, and R.J. Saykally, J. Phys. Chem. A 102, 3279 (1998); J.B. Paul, R.A. Provencal, C. Chapo, A. Pettersson, and R.J. Saykally, J. Chem. Phys. (in press 1998); J.B. Paul, R.A. Provencal, C. Chapo, K. Roth, R. Casaes, and R.J. Saykally, J. Phys. Chem. A (in press 1999).

[c] R.S. Fellers, L.B. Braly, C. Leforestier, and R.J. Saykally, J. Chem.Phys. (in press 1999); C. Leforestier, L.B. Braly, K. Liu, M.J. Elrod, and R.J. Saykally, J. Chem. Phys. 106, 8527 (1997).