TERAHERTZ VIBRATION-ROTATION- TUNNELING SPECTROSCOPY OF WATER CLUSTERS IN THE TRANSLATIONAL BAND REGION

F. N. KEUTSCH, *Department of Chemistry, Harvard University, Cambridge, MA 02138*; M. G. BROWN, *Department of Chemistry, University of Oregon, Eugene, OR 97403*; P. B. PETERSEN, and R. J. SAYKALLY, *Department of Chemistry, University of California, Berkeley, CA 94720*; M. GELEIJNS, and A. VAN DER AVOIRD, *Institute of Theoretical Chemistry, NSR-Center, University of Nijmegen, Toernooiveld, 6525 ED Nijmegen, The Netherlands*.

We report the first direct observation of the hydrogen-bond stretching vibration for a water cluster. A perpendicular band of $(D_2O)_3$ was measured by terahertz laser vibration- rotation-tunneling spectroscopy at 142.8 cm^{-1} in the "translational band" region of the liquid corresponding to the hindered translational motions of water molecules. We have tentatively assigned the spectrum to transitions from the vibrational ground state to the degenerate hydrogen-bond stretch or a combination or mixed state of the degenerate stretch and a torsional vibration.[a] Comparison with theoretical results shows that calculated frequencies are much too high, presumably because they do not include coupling between the torsional and stretching vibrations.

[a] F. N. Keutsch, M. G. Brown, P. B. Petersen, and R. J. Saykally, M. Geleijns, and A. van der Avoird *J. Chem. Phys.* **114** (9), 3994 February (2001).