OVERTONE AND COMBINATION BAND SPECTROSCOPY OF JET COOLED METHANOL

DAVID RUEDA, O.V. BOYARKIN, AND T.R. RIZZO, *INSTITUT DE CHIMIE PHYSIQUE MOLECULAIRE, EPFL, CH - 1015 LAUSANNE*; ANDREI CHIROKOLAVA, INDRANATH MUKHOPADHYAY, AND DAVID S PERRY, *DEPARTMENT OF CHEMISTRY, UNIVERSITY OF AKRON, AKRON, OHIO 44325*.

Overtone spectra of jet-cooled methanol have been recorded from 5,000 to 14,000 cm^{-1} using Infrared Laser Assisted Photofragment Spectroscopy (IRLAPS) for the detection of the vibrationally excited molecules.
In addition to the OH stretch overtones (nν_1), the major components of the spectra are the overtones of the CH stretch (up to $5\nu_{CH}$) as well as combinations of the OH stretch with the CO stretch (nν_1+ν_8), the COH bend (nν_1+ν_6), and both (nν_1+ν_6+ν_8). These data, together with photoacoustic data [1] up to 18,250 cm^{-1} and previously reported IRLAPS data [2] up to 22,166 cm^{-1}, have been fit to an anharmonic Hamiltonian. In this Hamiltonian, the CH stretch vibrations are treated as a pair of local modes, ν_a and ν_b, for v_{CH} = 3 and higher. The other modes are treated as the usual normal vibrations.

[1] H.L. Fang, D.M. Meister, R.L. Swofford, J. Phys. Chem. 88, 405-409 (1984).
[2] O.V. Boyarkin, L. Lubich, R.D.F. Settle, D.S. Perry, T.R. Rizzo, J. Chem. Phys. 107, 8409-8422 (1997).