INFRARED LASER SPCTROSCOPY OF ORGANIC MOLECULES AND MOLECULAR COMPLEXES

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We have recently coupled a room temperature external cavity quantum cascade laser at the 6 µm region into an infrared spectrometer equipped with an astigmatic multipass cell aligned for 366 passes. We have used this instrument to study high resolution infrared spectra of organic molecules, such as methyl acetate (MA), and of water and ammonia containing complexes. MA has two inequivalent methyl tops, i.e., the acetate CH₃ and methoxy CH₃ groups, which have significantly different internal rotation barriers. Using the ground state combination differences calculated from the rotational constants of the vibrational ground state recently determined by a global fit of the microwave and millimeterwave lines, the spectral assignment of the C=O stretching band has been made. The spectroscopic constants of the vibrationally excited state have been determined. NH₃-HCCH, a prototypical C-H⁻⁻N weak hydrogen bonded complex, has been studied at the vicinity of the v4 band of NH₃. The study of the related NH₃-OCS complex has also been carried out. The structural and dynamical information obtained will be presented.

^a J. Sheridan, W. Bossert, and A. Bauder, J. Mol. Spectrosc. **80** (1), 1980.

^b M. Tudorie and I. Kleiner, private communication.