UV-FTMW DOUBLE RESONANCE SPECTROSCOPY AND CONFORMATIONAL STRUCTURAL DETERMINATION OF BIOLOGICALLY RELEVANT MOLECULES

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Our Chirped-Pulse FTMW spectrometer has been used to obtain the pure rotational spectrum of various biomolecules with high signal-to-noise. The spectrometer operates from 7.5 to 18.5 GHz and records spectra with 80 kHz resolution for each individual valve pulse, where signal averaging is used to reach the desired signal-to-noise level. This allows for rapid acquisition of the pure rotational spectrum. We also demonstrate the ability to obtain conformer selective electronic spectra using UV-FTMW double resonance spectroscopy following the work of Endo.[a] For biomolecules where many conformers are populated in the supersonic expansion, assigning UV bands to the correct conformer can be difficult. Upon assignment of the pure rotational spectrum, the rotational transition from a specific conformer can be monitored as a function of the laser frequency. When resonant, the laser modulates the amplitude of the pure rotational transition indicating UV absorbance and providing instant conformer assignment with rotational resolution. UV excitation is performed using a YAG pumped dye laser with 0.025 cm^{-1} bandwidth. Results will be presented for para-methoxyphenethylamine, a neurotransmitter, which has seven conformers populated in the supersonic expansion.[b]

[a] M. Nakajima, Y. Sumiyoshi, and Y. Endo, *Rev. Sci. Inst.* **73** (2002), 165.
[b] J.T. Yi, E.G. Robertson, and D.W. Pratt, *Phys. Chem. Chem. Phys.* **4** (2002), 5244.