FOURIER TRANSFORM MICROWAVE AND INFRARED SPECTROSCOPIC INVESTIGATION OF PROPIOLACTONE

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The pure rotational spectrum of the four-membered ester ring propiolactone ($C_3H_4O_2$) has been measured in a supersonic jet between 7 and 22 GHz using Fourier transform microwave (FTMW) spectroscopy. For the normal isotopologue, a total of 19 *a*- and *b*-type transitions have been recorded. Fifteen transitions due to three different ^{13}C isotopologues have also been observed. The microwave spectrum was analyzed to obtain an improved set of ground state rotational constants in comparison to earlier microwave experiments[a]. The new set of rotational parameters was used to predict the rovibrational band structure of the lowest frequency modes of propiolactone. A total of 12 vibrational band origins have been observed between 400 and 1500 cm^{-1} using the far infrared beamline of the Canadian Light Source coupled to a Bruker IFS125HR spectrometer. The spectra were recorded with a resolution of 0.000969 cm^{-1} and although the intensities of the bands vary, 9 bands are of sufficient quality for complete rovibrational assignment. The progress of the assignment of this rich spectrum will be discussed.

[a] D. W. Boone, C O. Britt and J. E. Boggs *J. Chem. Phys.* **43** (1190), 1965.