ROTATIONAL SPECTRUM OF THE FIRST TORSIONAL EXCITED STATE OF ACETONE, CH_3COCH_3

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The first report on the rotational spectrum (260 to 350 GHz) of the first torsional excited state of acetone (80 cm^{-1} above the ground state) has been presented at an earlier meeting.[a] Since then, measurements in the regions 72-122 and 176-253 GHz (from JPL) have been added to the analysis with the effective rotional Hamiltonian for molecules with two periodic large-amplituded motions.[b] Several hundred frequencies have been assigned and fit to near experimental precision The microwave spectrum of acetone at room temperature has been recorded between 12 and 18 GHz with the Kiel Fourier-transform waveguide instrument. Assignment of the transitions of the first torsional excited state in this region is in progress. In contrast to expectations based on the assignments at higher frequencies, this is not a trivial affair. Many other transitions in the mm/sub-mm region of the spectrum have been assigned, but the least-squares fit deteriorates significantly when they are included.

[a] P. Groner et al., 53rd Ohio State University International Symposium, 1998, presentation TH02
[b] P. Groner, J. Chem. Phys. 107, 4483 (1997)