FIRST MICROWAVE TRANSITIONS IN THE ROTATIONAL SPECTRUM OF ν_{17} OF ACETONE ASSIGNED BY MW-MW DOUBLE RESONANCE

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The first assignments of rotational transitions of acetone in the ν_{17} state, based on a study of the mm/sub-mm wave spectrum, were published two years ago. [a] Over 700 frequencies of transitions from all four torsional substates (AA, EE, AE, and EA) have been assigned; over 600 have been fit to an effective rotational Hamiltonian for molecules with two internal rotors. [b] However, the fit was not very good (standard deviation 0.48 MHz) and required a large number of ill-determined parameters, some of which were clearly outside the expected range. A search for transitions at lower frequencies by microwave-microwave double resonance has been moderately successful. So far, 12 double resonances involving 6 pump and 8 signal transitions have been found that connect 15 energy levels ($1 < J < 6$) in the EE torsional substate. These frequencies were found within a range of up to seven times the predicted standard errors. The newly assigned transitions were used in least-squares fits together with all previously assigned transitions (or subsets thereof) in an effort to determine more sensible parameters and to achieve more stable fits. We are hoping to assign more transitions, specifically transitions in the AA torsional substate.

[a] P. Groner, I. R. Medvedev, F. C. De Lucia, B. J. Drouin, J. Mol. Spectrosc. 251, 180 (2008).
[b] P. Groner, J. Chem. Phys. 107, 4483 (1997).