ROTATIONAL SPECTRA OF DIMETHYL ETHER AND ACETONE IN GROUND AND TORSIONAL EXCITED STATES UP TO 600 GHz

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The spectra of both dimethyl ether and acetone are complicated by splittings of the rotational transitions into four components due to the interactions with the internal rotations. An effective rotational Hamiltonian for molecules with two internal rotors ^{*a*} has been used to analyze the spectra. For dimethyl ether in the vibrational ground state, over 1600 lines (J < 50, 8 to 560 GHz) have been fit to experimental precision with only 22 parameters and more than 6000 line frequencies have been predicted ^{*b*}. For each of the two lowest torsional excited states, about 400 frequencies (360 to 450 GHz) have been fit to almost experimental precision. The results are not quite satisfactory for acetone for which the splittings are two to three orders of magnitude larger. Although about 700 frequencies (J < 60, 4 to 600 GHz) could be fit to experimental precision, many frequencies had to be deleted from the fit. Transitions in the lowest torsional excited state of acetone have been identified and assigned. Work is still in progress on acetone and the excited states of dimethyl ether.

^aP. Groner J. Chem. Phys. 107, 4483 (1997).

^bP. Groner, S. Albert, E. Herbst and F. C. De Lucia Astrophys. J. <u>500</u>, 1059 (1998).