A FITTING PROGRAM FOR MOLECULES WITH TWO EQUIVALENT TOPS AND C_{2V} POINT-GROUP SYMMETRY AT EQUILIBRIUM: APPLICATION TO EXISTING MICROWAVE, MILLIMETER, AND SUB-MILLIMETER WAVE MEASUREMENTS OF ACETONE

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We will present a new theoretical tool, a program called PAM-C2v-2tops, for analysis of the high-resolution torsion-rotation spectra of molecules with two equivalent methyl rotors and C_{2V} symmetry at equilibrium. The new tool belongs to the broad class of effective Hamiltonians, is based on Longuet-Higgins' group theoretical ideas and uses G_{36} permutation-inversion group-theoretical considerations, the principal axis method and a two-step diagonalization procedure. The program was used to carry out a weighted least-squares fit of 1720 microwave, millimeter-wave, and sub-millimeter-wave line frequencies of acetone [$(CH_3)_2CO$] that are available in the literature. The weighted root-mean-square deviation of 0.93 obtained for a joint fit of the microwave lines belonging to the ground, the lower torsional fundamental, and the higher torsional fundamental states of acetone represents significant progress in comparison with previous fitting attempts, especially for the excited torsional states.