ANALYSIS AND FIT OF THE FTMW SPECTRUM OF THE TWO-TOP MOLECULE N-METHYLACETAMIDE

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About 837 hyperfine components of torsion-rotation transitions in N-methylacetamide (CH_3-NH-C(=O)-CH_3) have been measured between 9.9 and 26.5 GHz using the jet-cooled Fourier transform microwave spectrometer at NIST. The molecule is assumed to have a plane of symmetry at equilibrium, so that a permutation-inversion group G_{18} with the six symmetry classes A_1, A_2, E_1, E_2, E_3, E_4 is appropriate. Assignments were carried out primarily with the help of combination differences and computer-calculation guidance. A number of global least-squares fits of the transitions for all these symmetry species were carried out using a recently written two-top internal rotation program, which also includes nuclear quadrupole hyperfine interaction terms. At the time of writing the abstract, our best fit of the total data set, which involves 152 torsion-rotation levels with $J \leq 8$ and $K \leq 2$, required 3 hyperfine parameters and 42 torsion, rotation, and torsion-rotation parameters to obtain a root-mean-square residual of 5.7 kHz. This residual is essentially equal to the experimental measurement uncertainty because of the numerous occurrences of partially or completely blended hyperfine components. Aspects of the programming algorithm, which uses a pseudo principal-axis-method, and of the qualitative behavior of the low-barrier two-top energy levels will be discussed.