A NEW PROGRAM FOR NON-EQUIVALENT TWO-TOP INTERNAL ROTORS WITH A C\textsubscript{4} FRAME

I. KLEINER, Laboratoire Interuniversitaire des Systèmes Atmosphériques, CNRS et Universités Paris 7 et Paris 12, 61 av. Général de Gaulle, 94010, Créteil, France; J. T. HOUGEN, Optical Technology Division, National Institute for Standards and Technology, Gaithersburg, MD 20899-8441, USA.

We have written a new program to calculate and fit torsion-rotation transitions in molecules containing two inequivalent methyl tops (C\textsubscript{3v}) and having the rest of the atoms lying in a plane of symmetry. We based our work on the theoretical model and Hamiltonian described by Ohashi et al for the N-methylacetamide molecule\textsuperscript{a}. In the absence of top-top interactions, each asymmetric top energy levels splits into AA, AE, EA and EE components where the individual letters A and E indicate the symmetry species of the wave function with respect to internal rotation of one of the methyl tops. The pair of letters taken together indicates the species in the G\textsubscript{18} permutation-inversion group appropriate for the molecule, so AA, AE, EA, and EE correspond to A\textsubscript{1} (or A\textsubscript{2}), E\textsubscript{2}, E\textsubscript{1} and E\textsubscript{3} \oplus E\textsubscript{4}, respectively. In the previous study, the torsion-rotation Hamiltonian was diagonalized directly in a one-step process using torsion-rotation functions $|J, K > |m\textsubscript{1} > |m\textsubscript{2} >$ where $m\textsubscript{1}$ and $m\textsubscript{2}$ represent the free-rotor basis functions for top 1 and top 2. The one-step diagonalization made however the least-squares fitting of moderate $J$ values very slow, even for rather small values of $m\textsubscript{1}$ and $m\textsubscript{2}$. Our goal is to write a code which will be faster and which allows us to reach higher $J$ values. We follow a two-step procedure to diagonalize the Hamiltonian and implemented a banded-matrix diagonalization routine in order to speed up the code. We tested the code with the published N-methylacetamide Fourier-transform microwave data. The principles of the method, as well as the limitations will be discussed\textsuperscript{b}.


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