A NEW HAMILTONIAN FOR RADICALS WITH INTERNAL ROTATION

J. H. WESTERFIELD, KYLE N. CRABTREE, *Department of Chemistry, The University of California, Davis, CA, USA*.

Rotational spectroscopy has proved itself to be an invaluable tool for detecting small radicals and organic molecules in the interstellar medium. Unpaired electrons complicate rotational spectra from spin-rotation coupling and the torsions of methyl groups which couple to the molecular rotations. Presently, there exist methods for studying either of these complications but not both simultaneously. Thus preventing the laboratory analysis and the detection of small organic radicals with methyl rotors in space. This work presents a new Hamiltonian for accounting for spin-torsion interactions as well as the established spin-rotation and torsion-rotation terms for C_s molecules. The program utilizes BELGI's two stage diagonalization process to address the torsions with the spin-rotation and spin-torsion terms being added into the second diagonalization stage. Preliminary testing of the program has shown initial agreement with existing programs. This work will provide the means for laboratory analysis of previously unstudied molecules as well as their detection in space.