

A NEW PROGRAM FOR RADICALS WITH INTERNAL ROTATION

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

The presently available tools of rotational spectroscopy do not provide a meaningful way to treat small organic radicals with methyl groups. This in turn prevents astrochemical detection of these species as it is not possible to accurately predict rotational spectra complicated by both spin-rotation coupling and methyl torsions. This work presents a new program capable of treating these interactions in C_s molecules as well as a new operator to account for spin-torsion interactions. The program, written in Julia, utilizes BELGI's two stage diagonalization process to address the torsions in the first stage with the spin-rotation and spin-torsion terms being added into the second diagonalization stage. SPCAT and PGOPHER were used to test just the spin-rotation implementation while BELGI was used to test the torsional-rotation implementation. This preliminary testing of the new program has shown initial agreement with the existing programs. The current status of the program and the next stages in its implementation will be discussed.