REDUCTION OF SPIN TORSION ROTATION HAMILTONIAN

J. H. WESTERFIELD, , , , ; S E WORTHINGTON-KIRSCH, *Department of Chemistry, York University, Toronto, ON, Canada*.

When considering a C_s molecule with a single spin source and single internal rotor, the group theoretically complete Hamiltonian up to 4th order has 168 allowed operators. To remove the redundancies and interdependencies between these operators, Watson's famous contact transformation procedure has been followed. However, only 43 operators can be removed thus resulting in a great many possibilities for the reduction. The second order Hamiltonian can be reduced to form either the Principal Axis Method or the Rho Axis Method. Reductions of the 4th order Hamiltonian will be carried out to resemble the Watson-A and the Watson-S as best as possible for the more complicated case of spin-torsion-rotation with lower symmetry. Alternative possibilities of the reduction as well as modifications to the westerfit package to accommodate these reductions will also be discussed.