THE EFFECTS OF SPIN-ORBIT COUPLING ON THE SPECTROSCOPY OF JAHN-TELLER ACTIVE MOLECULES

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We have developed a program that incorporates spin-orbit coupling directly into the normal Jahn-Teller Hamiltonian. The effects of spin-orbit coupling on the electronic spectroscopy of Jahn-Teller active molecules will be presented. The inclusion of spin-orbit coupling in the Hamiltonian is a necessity when both Jahn-Teller coupling and spin-orbit coupling are significant. Furthermore, the program handles an arbitrary number of Jahn-Teller active modes. We will show that for molecules that have more than one Jahn-Teller active mode, it is necessary to perform one multi-mode Jahn-Teller calculation rather than several one-mode calculations. This combined theory has been applied to the electronic spectroscopy of the methoxy family of radicals and to the group IIA and IIB metalmonomethyl radicals. The relationship of *ab initio* calculations to the spin-orbit Jahn-Teller Hamiltonian will be discussed.