JAHN-TELLER AND SPIN-ORBIT COUPLING IN THE ^{2}E GROUND STATE OF CF_3O AND CF_3S

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The electronic spectra of the $\tilde{A}\ ^2\mathrm{A} \leftrightarrow \tilde{X}\ ^2\mathrm{E}$ transition of the CF_3O and CF_3S radicals are complex because of Jahn-Teller activity in the ^{2}E ground states. Proper analyses of the spectra require the inclusion of both Jahn-Teller coupling and spin-orbit coupling. For CF_3O, the couplings are similar in magnitude whereas in CF_3S the spin-orbit coupling clearly dominates, although Jahn-Teller coupling cannot be ignored. The analysis of the emission spectra have included first-order and second-order Jahn-Teller coupling constants in each of the three Jahn-Teller active e modes, as well as spin-orbit coupling. Results of our analyses will be presented along with improvements to the computational program.