# COMPARATIVE ANALYSIS OF THE RENNER EFFECT IN THE $\tilde{A}\ ^3\Pi$ STATE OF CCO, CSiO, SiCO, AND SiSiO WITH EQUATION OF MOTION COUPLED CLUSTER THEORY (EOM-CCSD)

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Equation of motion coupled cluster theory (EOM-CCSD) has been employed to systematically study the Renner effect in the first triplet excited state ($\tilde{A}\ ^3\Pi$) in a series of CCO radical analogues (14 valence electrons). The total energies and physical properties including equilibrium geometries, dipole moments, and harmonic vibrational frequencies of CCO, CSiO, SiCO, and SiSiO were predicted using SCF, CISD, CCSD, CCSD(T) and EOM-CCSD with a wide range of basis sets. The $\tilde{A}\ ^3\Pi$ state of all of these molecules are linear at equilibrium. The potential energy surface of the $\tilde{A}\ ^3\Pi$ state of the CCO analogues splits into $^3A''$ and $^3A'$ states on bending and each surface has its own minimum at the linear configuration. The two distinct bending frequencies were determined and used to predict the Renner parameter, $\epsilon$, and the average harmonic bending frequency, $\omega_2$, neglecting anharmonicity and spin-orbit coupling effects. Theoretically predicted harmonic stretching vibrational frequencies of $\tilde{A}\ ^3\Pi$ CCO were in close agreement with experimental fundamental frequencies, indicating relatively small anharmonicities. The relative ordering of the Renner splitting at the EOM-CCSD level of theory with a TZ3P(2f) basis for this series of radicals was determined to be CSiO $>$ CCO $>$ SiCO $>$ SiSiO. The computation of $\epsilon$ resulted in negative values for all of these radicals due to the energy ordering of the split potential energy surfaces. The $\epsilon$ predicted for $\tilde{A}\ ^3\Pi$ CCO (-0.153 at TZ3P(2f) EOM-CCSD) is good agreement with the $\epsilon$ value of -0.172 from Devillers and Ramsay's[a] experimental analysis.

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[a] Devillers, M. C. and Ramsay, D. A., *Can. J. Phys.*, **1971**, *49*, 2839.