COMBINED ANALYSIS OF THE $\tilde{A}^2 E'' - \tilde{X}^2 E'$ GAS-PHASE EXCITATION AND EMISSION SPECTRA OF Ag₃

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Metal clusters are of considerable interest as they bridge the atomic and solid states. Among the heavier homonuclear coinage metals is silver trimer Ag₃, a particularly interesting molecule in that although the orbitally degenerate $\tilde{X}^2 E'$ and $\tilde{A}^2 E'' D_{3h}$ states can undergo Jahn-Teller (JT) distortion to C_{2v} states, spin-orbit splitting may partially quench this distortion. Both laser-induced fluorescence (LIF) and dispersed fluorescence (DF) spectra have been reported for Ag₃. Preliminary JT analyses for the $\tilde{A}^2 E''$ and $\tilde{X}^2 E'$ states have been based, respectively, on the LIF and DF data. However the interpretation has been subject to some ambiguity. High level *ab-initio* calculations have been performed with the express purpose of estimating the Jahn-Teller constants and spin-orbit effects in both states. These theoretically predicted molecular parameters initiated the Jahn-Teller simulations of the LIF and DF spectra, leading to an overall understanding of the spin-vibronic structure in each case.