

Abstract Submitted
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Silver Trimer: An Interesting Coinage-Metal System with Jahn-Teller Activity ILIAS SIOUTIS, RUSSELL PITZER, TERRY MILLER, The Ohio State University — Silver trimer Ag_3 is believed to exhibit large amplitude motions away from the D_{3h} configuration attributable to the single e' mode that shows linear and quadratic Jahn-Teller (JT) activity. Both laser-induced fluorescence (LIF) and dispersed fluorescence (DF) spectra have been reported for Ag_3 .¹ Preliminary JT analyses for the B $^2E''$ and X $^2E'$ states have been based, respectively, on the LIF and DF data. However, the interpretation has been subject to some ambiguity. For the X $^2E'$ state, extensive *ab initio* computations were carried out to calculate the linear and quadratic JT constants, the geometries and symmetries of the global minima and saddle points as well as the barrier to pseudorotation around the moat of the potential energy surface (PES). The magnitude of the spin-orbit (SO) effects for this heavy system was also determined. For the B $^2E''$ state, the JT constants were obtained. For the theoretical calculations we utilized our newly constructed basis set for Ag. The JT simulations of the LIF and DF spectra were carried out by means of the SOCJT program² which calculates the positions of the spin-vibronic energy levels in the presence of JT and SO effects. The analysis of the JT distorted ground and excited PES's of Ag_3 and their vibronic structure will be reported. ¹A. M. Ellis, E. S. J. Robles, and T. A. Miller *Chem. Phys. Lett.* **201**, 132, 1993. ²T. A. Barkholtz, and T. A. Miller *Int. Rev. Phys. Chem.* **17**, 435, 1998.

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