SILVER TRIMER: AN INTERESTING COINAGE-METAL SYSTEM WITH JAHN-TELLER ACTIVITY

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Silver trimer Ag_3 is believed to exhibit large amplitude motions away from the symmetrical configuration of D_{3h} symmetry attributable to the single e' mode that shows linear and quadratic Jahn-Teller activity. Both laser-induced fluorescence (LIF) and dispersed fluorescence (DF) spectra have been reported for Ag_3.[a] Preliminary Jahn-Teller analyses for the $\widetilde{B}^2E''$ and $\widetilde{X}^2E'$ states have been based, respectively, on the LIF and DF data. However the interpretation has been subject to some ambiguity. For the $\widetilde{X}^2E'$ state, extensive *ab initio* computations were carried out to calculate the linear and quadratic Jahn-Teller 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 effects for this heavy system was also determined. For the $\widetilde{B}^2E''$ state, the Jahn-Teller constants were obtained. For the theoretical calculations we utilized our newly constructed basis set for Ag. The Jahn-Teller simulations of the LIF and DF spectra were carried out by means of the SOCJT program[b] which calculates the positions of the spin-vibronic energy levels in the presence of Jahn-Teller and spin orbit effects. The analysis of the Jahn-Teller distorted ground PES of Ag_3 and its vibronic structure will be discussed.

[a] A. M. Ellis, E. S. J. Robles, and T. A. Miller *Chem. Phys. Lett.* **201**, 132, 1993.
[b] T. A. Barkholtz, and T. A. Miller *Int. Rev. Phys. Chem.* **17**, 435, 1998.