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

ILIAS SIOUTIS, RUSSELL M. PITZER, and TERRY A. MILLER, *Laser Spectroscopy Facility, Department of Chemistry, The Ohio State University, Columbus, OH 43210*.

Silver trimer Ag_3 distorts away from the D_{3h} symmetrical configuration owing to the single e' vibrational mode that shows Jahn-Teller (JT) activity. Both laser-induced fluorescence (LIF) and dispersed fluorescence (DF) spectra have been reported for Ag_3. Preliminary JT 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. Potential energy curves representing cuts of C_{2v} symmetry have previously been calculated for the single e' mode of Ag_3 in the $\widetilde{X}\ ^2E'$ electronic state. Similar work but for the $\widetilde{B}\ ^2E''$ state has recently been undertaken as well. From these curves, the JT coupling parameters have been derived as well as general features of the potential energy surfaces (PES's). The spin-orbit (SO) interaction between the JT split states of the $\widetilde{B}\ ^2E''$ state has been calculated to be substantially smaller than in the $\widetilde{X}\ ^2E'$ state. Our theoretical calculations incorporated the state-averaging methodology and were done at the CISD and SO-CISD levels of theory using the COLUMBUS suite of programms. They were based on our newly constructed basis set for Ag. The JT simulations of the LIF and DF spectra were carried out by means of the SOCJT program which calculates the positions of the spin-vibronic energy levels in the presence of the JT and SO effects. The analyses of the JT-distorted ground and excited PES of Ag_3 and their vibronic structure will be discussed.