Seminar

Friday, 19 March 2004

2:00 Pursley Hall Room 211

"The Amazing 21st Century Chemistry of Silver Nitrate!"

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One would not expect that much exciting chemistry would be left to investigate in the 21st century for a compound as anciently known and as ubiquitous in the chemistry lab as silver nitrate! But the talk will illustrate new findings of rich excited-state chemistry and photophysics for silver nitrate in areas that include metal-metal bonding and electronic spectroscopy. Excimers and exciplexes are well known species in organic molecules, but their inorganic counterparts have not been studied as much. Exciplexes involving diatomic and polyatomic units of neutral heavy metals such as mercury are known and have led to proposing mercury vapor as a gas-phase laser. However, exciplex formation between *cationic* heavy metal atoms has not been studied. Preliminary spectroscopic and computational results suggest that $*[Ag^+]_n$ exciplexes do form, indeed. Computational data suggest that an exciplex is reasonable as a result of a transition from a $\sigma_u^*(4d_{z^2})$ antibonding HOMO to a $\sigma_g(5sp)$ bonding vacant orbital. If an excited monomer cation collides in solution with a ground-state cation, the excited-state covalent bonding between these two species may be strong enough to compete with the electrostatic repulsion. Preliminary *ab initio* calculations showed no minimum for the ground state of the $[Ag^+]_2$ dimer, while for triplet $*[Ag^+]_2$, an R_e value of 2.90 Å was determined. The talk will also show solid-state examples of emitting materials that exhibit phosphorescence due to the formation of M-M bonded excimers and exciplexes in complexes of closed-shell transition metal ions. These systems exhibit a variety of fascinating optical phenomena, including luminescence thermochromism, solvatochromism, and concentration luminochromism.