CHARACTERIZATION OF Ca_2 THROUGH RESONANT EXCITATION AND DISPERSED LASER-INDUCED FLUORESCENCE (LIF) SPECTROSCOPY

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Alkali earth metal dimers, specifically Ca_2, are of theoretical interest [1,2] due to their weakly bound $X^1\Sigma_g$ ground state, arising from a fully occupied anti-bonding σ_u molecular orbital. Experimentally, alkali earth metals are of interest for ultra-cold chemical and physics applications. Due to their similar electronic structure to that of alkali metal atoms, alkali earth metal ions can be laser-cooled and readily formed in Coulomb crystals[3,4]. By inducing reactions, molecular ions can be generated within the Coulomb crystal, where they are translationally cooled by the surrounding atomic ions. Photodissociation techniques can then be used to detect the molecular ions via depletion. In the case of $Ca_2{}^+$, there are few available spectroscopic data that can be used to determine the frequencies of vibronic transitions that could be intermediates for photodissociation spectroscopy. To obtain such information, the neutral Ca_2 dimer should be spectroscopically characterized in greater detail. Previous spectroscopic efforts have observed vibronic emissions from the strongly perturbed $A^1\Sigma_u$ and $B^1\Sigma_u$ states to the ground state[1]. In this work, Ca_2 was created through laser ablation and supersonic expansion techniques, jet-cooled to 4K. Using an excimer-pumped dye laser, resonant and dispersed laser-induced fluorescence (LIF, DLIF) were performed. Dispersed LIF was detected by sending the fluorescence through a monochromator and detecting dispersed fluorescence with a photomultiplier tube (PMT). Lifetimes of emitting states were also measured. For the first time, the $c^3\Pi_u$-$X^1\Sigma_g$ vibronic transitions of Ca_2 were experimentally observed. Using DLIF, vibrational sequences in the $X^1\Sigma_g$ state were observed, confirming $X^1\Sigma_g$ as the emission's lower state.

[1] Bondybey, V. et al. Chem. Phys. Lett. 1984, 111, 195

[2] Allard, O. et al. Eur. Phys. J. D 2005, 35, 483

[3] Nguyen, J. et al. New. J. Phys. 2011, 13, 063023

[4] Calvin, A. et al. J. Phys. Chem. Lett. 2018, 9, 5797