LIF SPECTROSCOPY OF AlNC/AlCN IN SUPERSONIC FREE EXPANSIONS

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The $^1A' - \tilde{X}\ ^1\Sigma^+$ electronic transition of AlNC/AlCN has been observed for the first time using the laser induced fluorescence (LIF) technique. Prior to our experiments, *ab initio* calculations extending the original work of Ma *et al* [a] were carried out at CCD/6-31G(d) and QCISD/6-311+G(3df) levels to elucidate the structures and molecular constants of the ground and excited states for spectroscopic searching. As reported by Ma *et al*, AlNC is found to be the lower lying species in the ground state, at about 2000 cm^{-1} below AlCN. We also find that the singlet excited state has a bent structure while the singlet ground states are linear. Guided by the predictions, the LIF excitation spectrum, LIF dispersed spectra from single vibronic levels (SVL), and LIF temporal profiles have been measured and analyzed. The species of current interest were generated by reacting the CN fragments from CH_3CN in an Ar plasma with Al atoms evaporated using laser ablation of the metal surface. The dispersed fluorescence (DF) spectra show two kinds of vibronic bands: isolated sharp bands and congested bands. For the sharp features, the vibrational frequencies obtained from the vibronic structure show good agreement with the *ab initio* calculations and therefore the spectral carrier is assigned to AlNC/AlCN. Possible predissociation in the excited state is expected based on the following observations: (1) Rotational structures of the vibronic bands in the excitation spectrum are not resolved at the instrumental resolution of our laser source, ~ 0.04 cm^{-1}; (2) The fluorescence time profiles follow the excitation laser pulse; and (3) Al atomic lines, $^2S - {}^2P$, are observed in some of the DF spectra. The congested vibronic bands in the DF spectra show the progressions of the stretching between Al and CN group starting at 1364 and 2710 cm^{-1}, but the exact causes of these progressions are not clear. A more complete analysis is underway and will be discussed in the presentation.

[a] B. Ma, Y. Yamaguchi, H. F. Schaffer III, Mol. Phys. **86**, 1331 (1995)