NO_3 STATES ACCESSED BY PHOTODETACHMENT AND DARK-STATE SPECTROSCOPY: WHAT DO WE KNOW?

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A good argument can be made that the atmospherically relevant NO_3 radical is the most complicated tetraatomic molecule. Five electronic states (the ground $\tilde{X}^2A_2'$ state, and the two degenerate $\tilde{A}^2E''$ and $\tilde{B}^2E'$ states) lie within 2 eV, and are coupled by several strong interactions. Amongst these is a strong linear and quadratic Jahn-Teller effect in the $\tilde{A}^2E''$ state, and a profound pseudo-Jahn-Teller interaction which couples the $\tilde{X}^2A_2'$ ground state with the second excited state. The latter is almost strong enough to break the D_{3h} equilibrium symmetry of the ground state, and severely perturbs vibrational levels associated with the two in-plane modes of e' symmetry. This talk will report *ab initio* calculations based on the equation-of-motion coupled cluster model, its application to parametrize various vibronic model Hamiltonians, and simulations of the photodetachment spectrum of NO_3^- as well as the recent experiments of Okumura and coworkers in which the (dipole forbidden) $\tilde{A}^2E''$ state is accessed by direct absorption from the ground state.