EXPLORING THE HIGH-RESOLUTION SPECTROSCOPY OF MOLECULES THAT CAN AFFECT THE QUALITY OF YOUR LIFE

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Few things affect your quality of life more than the air you breathe and the temperature of your immediate environment. Since more than 80% of the energy used in the industrialized world today is still derived from fossil fuels, these two quantities are not unrelated. Most organic molecules injected into the troposphere are degraded via oxidative processes involving free radical intermediates, and many of these intermediates are the same as the ones involved in the combustion of fossil fuels. Key oxidizing intermediates are hydroxyl, OH (day), and nitrate, NO$_3$ (night), and early intermediates of oxidized organic compounds include the alkoxy (RO) and peroxy (RO$_2$) families of radicals. Recently we have explored the spectroscopy of RO, RO$_2$, and NO$_3$ radicals both for diagnostic purposes and to characterize their molecular properties and benchmark quantum chemistry calculations.

We have utilized moderate resolution cavity ringdown spectroscopy (CRDS) to study ambient temperature radicals and high resolution CRDS and laser induced fluorescence (LIF) to study jet-cooled radicals. Peroxy radicals and NO$_3$ have weak $A - \bar{X}$ electronic transitions in the near infrared which we have studied with CRDS. Comparable LIF measurements have been made for the alkoxy species in the UV. Both vibrational and rotational resolution of the electronic spectra is observed. Data obtained from the spectral observations provide information about both the geometric and electronic structure of these radicals as well as their dynamics and also provide the capability for unambiguous diagnostics of their concentrations and reactions.