THE NON-LTE SPECTROSCOPY OF MOLECULAR REACTIONS USING THE EXOMOL DATABASE

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This talk describes our recent development of two robust methods for calculating non-local thermal equilibrium (non-LTE) spectra of polyatomic molecules. Specifically, we look at molecules produced in reactive or dissociative environments, with vibrational populations outside local thermal equilibrium (LTE). The methodology is based on ExoMol's accurate and extensive ro-vibrational line lists containing transitions with high vibrational excitations and relies on the detailed ro-vibrational assignments. Two approaches for non-LTE vibrational populations of the product are introduced: a simplistic 1D approach based on the Harmonic approximation, and full 3D model incorporating accurate vibrational wavefunctions computed variationally with the TROVE (Theoretical ROVibrational Energy) program. The developed methodology is applied to two molecules, silylene (SiH_2) produced in a decomposition of disilane (Si_2H_6), and carbon monoxide (CO) produced by formamide (CH_3NO) glow discharge. We show how the two approaches compare well to each other and to experimentally obtained spectra, and how their non-LTE spectral signatures can be used to trace different reaction channels of molecular dissociations.

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