SHOCKGAS-IR: A HIGH-TEMPERATURE AND HIGH-PRESSURE ABSORPTION CROSS-SECTION DATABASE

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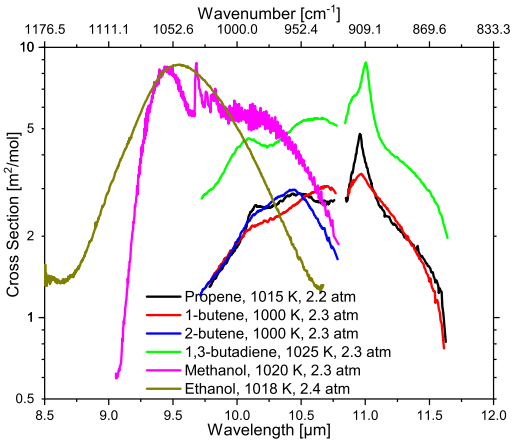

An infrared absorption cross-section database for gas-phase molecules at high-temperatures and high-pressures is under construction to address a growing cross-disciplinary need for experimental data at these conditions. Recently developed broad-scan, rapid-tuning external-cavity quantum cascade lasers (QCL) have enabled the application of shock tube facilities, commonly used to study high-temperature chemical kinetics, to the efficient acquisition of absorption spectra under short-duration shock-heated test gas conditions. Available shock tube facilities can produce temperatures from 500 to 10,000 K and pressures from 0.1 to 1000 atm with test time durations ranging from 500 μs to 50 ms. Uncertainties in the known thermodynamic conditions as low as $\pm 1\%$ can be achieved. Presently available laser systems enable the rapid acquisition ($<$ 10 ms) of approximately 300 cm^{-1} wide spectral regions at any location within the QCL-accessible wavelength region of 3.6 -11.7 μm (850 - 2800 cm^{-1}). The resulting spectra are composed of discrete data points at a spectral interval ranging from 0.3 - 0.6 cm^{-1} and an instrument broadening function defined by the laser linewidth ($\leq$ 0.0033 cm^{-1}).

Present efforts are focused on studying large polyatomic molecules (4+ atoms) dilute in a bath gas of argon under conditions for which dissociation is negligible and test time durations are favorable (T $<$ 1600K and P $<$ 5atm). The database currently includes ethylene, methanol, and ethanol with over a dozen more species measured and being prepared for inclusion soon. Database permanent URL: https://purl.stanford.edu/cy149sv5686