INFRARED SIMULATIONS DERIVED FROM SUBMILLIMETER WAVE ANALYSES

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The analysis of infrared spectra of heavy molecules is challenging due to partially resolved transitions and overlapping hot bands. Quite often it is necessary to analyze jet-cooled spectra, perform a band contour analysis, or empirically measure the cross sections to provide analyses for inclusion into spectral databases for atmospheric remote sensing applications. The specificity of the pure rotational spectra in the submillimeter wave region enables the determination of the rotational manifolds of many thermally populated vibrational states. The resulting analyses provide spectral constants to directly simulate the infrared spectrum and model the Q/P/R branch transitions, account for the temperature dependence of the spectrum, and aid in the assignment and determination of band centers and transitions moments of both the fundamental and the associated hot bands. We will demonstrate the utility of this approach by discussing recent advances in the simulation of the infrared spectrum of nitric acid and chlorine nitrate.