IR EMISSION SPECTROSCOPY OF AMMONIA: LINELISTS AND ASSIGNMENTS

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We present high resolution intensity-calibrated linelists of ammonia (NH_3) at high temperatures obtained from Fourier transform emission spectra recorded using a tube furnace. Individual calibrated linelists are presented for 12 temperatures ($300 - 1300^\circ$C in 100°C intervals and 1370°C). Each linelist covers the 800–2200 cm^{-1} range and includes the majority of the ν_2 bending mode and the complete ν_4 mode regions. We also demonstrate the useful technique of obtaining empirical lower state energies from spectra at different temperatures. We expect our hot NH_3 linelists to find direct application in modeling of the spectra of extrasolar planets and brown dwarfs.

Quantum number assignments in the experimental linelists are difficult because of extensive perturbations and the poor convergence of traditional Hamiltonians based on perturbation theory. A new theoretical linelist, known as BYTe, was computed variationally to assign and model spectra with ammonia temperatures up to 1500 K. It was computed using the NH3-2010 spectroscopically-determined potential energy surface and the TROVE rovibrational computer program. Intensities were calculated using an ab initio dipole moment surface. BYTe comprises more than 1.1 billion transitions in the wavenumber range from 0 to 12 000 cm^{-1}, constructed from 1.3 million energy levels lying below 18 000 cm^{-1}. Given an accurate potential energy surface, variational calculations are able to account automatically for perturbations.