Quantitative Infrared and Near-infrared Gas-Phase Spectra for Pyridine: Absolute Intensities and Vibrational Assignments

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Highlights

- The gas-phase quantitative spectrum for pyridine in the IR and near-IR are reported for the first time for atmospheric and other monitoring applications.

- In addition, we have had to reassign many of the fundamental modes compared to previously literature assignments, in particular ν_1, ν_2, ν_3, ν_4, ν_{14}, and ν_{20}. Many are assigned via use of vapor phase profiles and combination bands.

- Based on the new fundamental assignments, over two hundred combination and overtone bands are assigned.

- Frequency calculations were carried out using both Gaussian03 and CFOUR, while intensities were computed using GAMESS; these theoretically calculated frequencies and intensities aided in the assignments of combination and overtone bands.

- Using the newly derived absorption cross-sections, spectral features of pyridine for potential utility for atmospheric monitoring are identified and discussed.