$^{14}NH_3$ LINE POSITIONS AND INTENSITIES IN THE FAR-INFRARED: COMPARISON OF FT-IR MEASUREMENTS TO EMPIRICAL HAMILTONIAN MODEL PREDICTIONS

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We have analyzed multiple spectra of high purity (99.5%) normal ammonia sample recorded at room temperatures using the FT-IR and AILES beamline at Synchrotron SOLEIL, France. More than 2830 line positions and intensities are measured for the inversion-rotation and rovibrational transitions in the 50 – 660 cm^{-1}region. Quantum assignments were made for 2047 transitions from eight bands including four inversion-rotation bands (gs(a-s), ν_2(a-s), $2\nu_2$(a-s), and ν_4(a-s)) and four ro-vibrational bands (ν_2 – gs, $2\nu_2$ – gs, ν_4 – ν_2, and $2\nu_2$ –ν_4), as well as covering more than 300 lines of ΔK = 3 forbidden transitions. Out of the eight bands, we note that $2\nu_2$ – ν_4 has not been listed in the HITRAN 2012 database. The measured line positions for the assigned transitions are in an excellent agreement (typically better than 0.001 cm^{-1}) with the predictions from the empirical Hamiltonian model [S. Yu, J.C. Pearson, B.J. Drouin, et al.(2010)] in a wide range of J and K for all the eight bands. The comparison with the HITRAN 2012 database is also satisfactory, although systematic offsets are seen for transitions with high J and K and those from weak bands. However, differences of 20% or so are seen in line intensities for allowed transitions between the measurements and the model predictions, depending on the bands. We have also noticed that most of the intensity outliers in the Hamiltonian model predictions belong to transitions from gs(a-s) band. We present the final results of the FT-IR measurements of line positions and intensities, and their comparisons to the model predictions and the HITRAN 2012 database.[a]

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