

ACCURATE $^{14}\text{NH}_3$ ROVIBRATIONAL IR ANALYSIS AT 6000 CM^{-1}

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Ammonia is an important “weed” molecule in interstellar medium, planetary and exoplanetary atmosphere studies. In last ten years, new experimental IR analysis have been reported in the extended region between 5000 cm^{-1} (or $2\ \mu\text{m}$) and $10,000\text{ cm}^{-1}$ (or $1\ \mu\text{m}$). But reliable line list is still missing for the 6000 cm^{-1} (or $1.63\ \mu\text{m}$) region. Combining the JPL experimental measurements with the line positions predicted on our Ames-Pre3 potential energy surface and the 296K intensity predicted by the UCL-C2018 line list, we have been able to successfully assign more than 1300 transitions in that range. The transitions belong to following bands: $\nu_2+\nu_3+\nu_4$ (0111), $\nu_1+\nu_2+\nu_4$ (1101), $3\nu_2+\nu_3$ (0310), $\nu_1+3\nu_2$ (1300), $6\nu_2$ (0600s), and a “hot” band $2\nu_2+\nu_3+\nu_4$ (0211) – ν_2 (0100). The combination difference for the determined experimental energy levels are about $1\text{E-}3\text{ cm}^{-1}$, close to the resolution of lab measurements. Our Ames-Pre3 predictions for most $J=0\text{-}10$ transitions are found to be accurate within $\pm 0.05\text{ cm}^{-1}$, better than the C2018 line positions. Newly determined band origins and rovibrational levels will be presented along with band-by-band simulations comparing to the observed spectra. More complete Effective Hamiltonian model analysis is the target due for future work.

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