EXTENDED MEASUREMENTS AND AN EXPERIMENTAL ACCURACY EFFECTIVE HAMILTONIAN MODEL FOR THE $3\nu_2$ AND $\nu_2 + \nu_4$ STATES OF AMMONIA

JENIVEVE PEARSON, SHANSHAN YU, JOHN PEARSON, KEEYOON SUNG, BRIAN DROUIN, *Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA, USA*; OLIVIER PIRALI, *AILES beamline, Synchrotron SOLEIL, Saint Aubin, France*.

The infrared spectrum of ammonia has proven to be highly problematic for effective Hamiltonian analysis. As a result, previous studies failed to model the $3\nu_2$ and $\nu_2 + \nu_4$ bands of the spectrum close to experimental accuracy. To remedy this a global fit of the $3\nu_2$ and $\nu_2 + \nu_4$ bands has been undertaken using SPFIT. The analysis includes about 1000 newly assigned vibrational transitions in $3\nu_2$ to $2\nu_2$ as well as inversion transitions in $3\nu_2$ to $3\nu_2$. The spectra were a long path infrared absorption spectrum recorded with the Synchrotron light source at SOLEIL, with a path length of 180 m and a resolution of 0.0011 cm^{-1} at room temperature and 1 Torr of pressure, and a mid-infrared discharge spectrum recorded similarly at SOLEIL, with a path length of 0.7 m and resolution .004 cm^{-1} at 10 Torr and 900 K. Our fit has achieved experimental accuracy through the use of a number of terms that had not previously been in the Hamiltonian proving that ammonia is tractable to effective Hamiltonians despite previous beliefs.