ACCURATE POTENTIAL ENERGY SURFACE, ROVIBRATIONAL ENERGY LEVELS, AND TRANSITIONS OF AMMONIA C_{3v} ISOTOPOLOGUES: $^{14}NH_3$, $^{15}NH_3$, $^{14}ND_3$ and $^{14}NT_3$

XINCHUAN HUANG, *MS 245-6, NASA Ames Research Center, Moffett Field, CA, 94035*; DAVID W. SCHWENKE, *MS T27B-1, NASA Ames Research Center, Moffett Field, CA, 94035*; TIMOTHY J. LEE, *MS 245-1, NASA Ames Research Center, Moffett Field, CA, 94035*.

A further refined, global potential energy surface (PES) is computed for the C_{3v} symmetry isotopologues of ammonia, including $^{14}NH_3$, $^{15}NH_3$, $^{14}ND_3$ and $^{14}NT_3$. The refinement procedure was similar to that used in our previously reported PES[a], but now extends to higher J energy levels and other isotopologues. Both the diagonal Born-Oppenheimer correction and the non-adiabatic correction were included. $J = 0 - 6$ rovibrational energy levels and transition frequencies of $^{14}NH_3$ computed on this PES are in excellent agreement with HITRAN data. Statistics on nearly 4100 transitions and more than 1000 energy levels demonstrate the accuracy achieved by the state-of-the-art "Best Theory + Experiment" strategy. Most transition frequencies are of $\pm 0.01 - 0.02$ cm^{-1} accuracy. Similar accuracy has been found on $^{15}NH_3$ $J = 0 - 3$ rovibrational energy levels. Several transitions and energy levels in HITRAN have been identified as unreliable or suspicious, and some have been re-assigned. For $^{14}ND_3$ and $^{14}NT_3$, $J = 0 - 3$ calculations have been performed. Agreement for pure rotation-inversion transitions is nearly perfect, with more reliable energy levels presented. On the other hand, our $J = 0$ results suggest a re-analysis on the $^{14}ND_3$ ν_1 band origin is needed. Finally, we will discuss possible future refinements leading to an even better final PES for Ammonia.

[a] X. Huang, D.W. Schwenke, and T.J. Lee, *J. Chem. Phys.* **129**, 214304 (2008).