

# HIGH ACCURACY POTENTIAL ENERGY SURFACE, DIPOLE MOMENT SURFACE, ROVIBRATIONAL ENERGIES AND LINE LIST CALCULATIONS FOR $^{14}\text{NH}_3$

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We present a new spectroscopic potential energy surface (PES) for  $^{14}\text{NH}_3$ , produced by refining a high accuracy *ab initio* PES<sup>a</sup> to experimental energy levels taken predominantly from MARVEL<sup>b</sup>. The PES reproduces 1722 matched J=0-8 experimental energies with a root-mean-square error of 0.035 cm<sup>-1</sup> under 6000 cm<sup>-1</sup> and 0.059 under 7200 cm<sup>-1</sup>. In conjunction with a new DMS calculated using multi reference configuration interaction (MRCI) and H=aug-cc-pVQZ, N=aug-cc-pWCVQZ basis sets, an infrared (IR) line list has been computed which is suitable for use up to 2000 K. The line list is used to assign experimental lines in the 7500 - 10,500 cm<sup>-1</sup> region and previously unassigned lines in HITRAN in the 6000-7000 cm<sup>-1</sup> region.

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<sup>a</sup>Oleg L. Polyansky, Roman I. Ovsyannikov, Aleksandra A. Kyuberis, Lorenzo Lodi, Jonathan Tennyson, Andrey Yachmenev, Sergei N. Yurchenko, Nikolai F. Zobov, *J. Mol. Spec.*, 327 (2016) 21-30

<sup>b</sup>Afaf R. Al Derzia, Tibor Furtenbacher, Jonathan Tennyson, Sergei N. Yurchenko, Attila G. Császár, *J. Quant. Spectrosc. Rad. Trans.*, 161 (2015) 117-130