

DIPOLE MOMENT AND ROVIBRATIONAL INTENSITIES IN THE ELECTRONIC GROUND STATE OF NH<sub>3</sub>: BRIDGING THE GAP BETWEEN *AB INITIO* THEORY AND SPECTROSCOPIC EXPERIMENT.

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We report theoretical values for the transition moments of an extensive set of vibrational bands in the electronic ground state of <sup>14</sup>NH<sub>3</sub>. For selected bands, we have further made detailed simulations of the rotational structure. The calculations are carried out by means of recently developed computational procedures for describing the nuclear motion<sup>a</sup> and are based on a high-level *ab initio* potential energy surface, and high-level dipole moment surfaces, for the electronic ground state of NH<sub>3</sub>. The reported theoretical intensity values are compared to, and found to agree very well with, corresponding experimental results. It is believed that the computational method, in conjunction with high-quality *ab initio* potential energy and dipole moment surfaces, can simulate rotation-vibration spectra of XY<sub>3</sub> pyramidal molecules prior to observation with sufficient accuracy to facilitate the observation of these spectra. By degrading the accuracy of selected elements of the calculations, we have also investigated the influence of customary approximations on the computed intensity values.

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<sup>a</sup>S. N. Yurchenko, M. Carvajal, P. Jensen, H. Lin, J. Zheng, and W. Thiel, *Mol. Phys.* **103**, 359-378 (2005) and references therein.