DIPOLE MOMENT AND ROVIBRATIONAL INTENSITIES IN THE ELECTRONIC GROUND STATE OF NH_3: BRIDGING THE GAP BETWEEN *AB INITIO* THEORY AND SPECTROSCOPIC EXPERIMENT.

SERGEI N. YURCHENKO, JINGJING ZHENG, WALTER THIEL, *Max-Planck-Institut für Kohlenforschung, Kaiser-Wilhelm-Platz 1, D–45470 Mülheim an der Ruhr, Germany*; MIGUEL CARVAJAL, *Departamento de Fisica Aplicada, Facultad de Ciencias Experimentales, Avda. de las FF.AA. s/n, Universidad de Huelva, 21071, Huelva, Spain*; HAI LIN, *Department of Chemistry, University of Minnesota, 207 Pleasant St. SE. Minneapolis, Minnesota 55455*; PER JENSEN, *FB C – Theoretische Chemie, Bergische Universität, D–42097 Wuppertal, Germany*.

We report theoretical values for the transition moments of an extensive set of vibrational bands in the electronic ground state of $^{14}NH_3$. 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[a] 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_3. 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_3 pyramidal molecules prior to observation with sufficient accuracy to facilitate the observation of t hese 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.

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