AB INITIO CALCULATION OF NH$_3$ SPECTRUM

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An ab initio potential energy surface (PES) for NH$_3$ is computed using the methodology pioneered for water (Polyansky et al. J. Phys. Chem. A, 117, 9633 (2013)). A multireference configuration calculations are performed at 50000 points using quadruple and 5z basis sets to give a complete basis set (CBS) extrapolation. Relativistic and adiabatic surfaces are also computed. The points are fitted to an analytical PES. The rovibrational energy levels are computed using the program TROVE in both linearized and curvilinear coordinates. Better convergence is obtained for the higher energy levels using curvilinear coordinates: an accuracy of about 1 cm$^{-1}$ is achieved for the levels up to 12 000 cm$^{-1}$. The levels up to 18 000 cm$^{-1}$ are reproduced with the accuracy of a few cm$^{-1}$. These results are used to assign the visible spectrum of $^{14}$NH$_3$ recorded by Coy and Lehmann (J. Chem. Phys., 84, 5239 (1988)). Predicted rovibrational levels for NH$_3$D, NHD$_2$, ND$_3$ and $^{15}$NH$_3$ are given.