Title:	Ab Initio Potential Energy Curves for the Ground and Low Lying Excited States of NH– and the Effect of 2Σ± States on Λ-Doubling of the Ground State X2Π
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Abstract:	Complete basis set extrapolated ab initio potential energy curves obtained from multireference configuration interaction (MRCI) level calculations for the ground state (X2Π) and the a4Σ– state of NH– and the ground state (X3Σ–) of NH are reported. The potential energy curves for the A′2Σ– and A2Σ+ states of NH– have been computed using the V6Z basis set at the MRCI level. Λ-doubling parameters p and q are calculated for the ground and the first excited vibrational states of the ground electronic state of NH– using second-orderperturbation theory. The effect of the 2Σ+ and 2Σ– states on the Λ-doubling values is discussed. Earlier experiments had not considered the influence of the 2Σ– state on p and q while fitting the spectral data. Using the computed potential energy curves and the ro-vibrational spectra including the fine splitting, we have computed the threshold for electron detachment. The result is in agreement with the experimental values of Neumark et al. [J. Chem. Phys. 1985, 83, 4364] and Farley et al. [Phys. Rev. A 1987, 35, 1099].
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