ELECTRONIC STRUCTURE AND SPECTROSCOPY OF NH^+

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Ab–initio SCF MRSD–CI electronic structure calculations were carried out on the NH^+ cation. A basis set of DZ+POL quality augmented with Rydberg and bond functions was employed together with an extensive treatment of electron correlation. More than fifty electronic states of NH^+ are reported, including doublets, quartets and sextets[a]. Leading configurations, vertical ionization energies of NH, vertical excitation energies of NH^+ and potential energy curves are reported. Spectroscopic properties calculated for the five known bound electronic states of NH^+ ($X^2\Pi$, $a^4\Sigma^-$, $A^2\Sigma^-$, $B^2\Delta$, $C^2\Sigma^+$) are found in good agreement with experiment.
We find four new bound electronic states of NH^+, namely, three doublets ($^2\Delta$, $^2\Sigma^+$, $^2\Sigma^+$) and one sextet ($^6\Pi$). A fifth bound electronic state, a quartet ($^4\Pi$) which was reported schematically in an early SCF study[b] is calculated for the first time over a wide range of N–H distances. Adiabatic excitation and ionization energies and spectroscopic constants are also reported for these five states[c], as well as vertical de–excitation energies for emission from the novel states to lower lying bound states. The potential energy curve of $NH^{2+}(X^1\Sigma^+)$ was also calculated to aid in the discussion of a Rydberg bound state of NH^+. It is hoped that the information reported in the present work will be helpful in guiding the laboratory and/or astrophysical search for these species.

[a] J. M. Amero, G. J. Vázquez, *Int. J. Quantum Chem.*, **101**, 396 (2005).
[b] H. P. D. Liu, G. J. Verhaegen, *J. Chem. Phys.*, **53**, 735 (1970).
[c] J. M. Amero, G. J. Vázquez, *Int. J. Quantum Chem.*, **99**, 353 (2004).