ELECTRONIC STRUCTURE AND SPECTROSCOPY OF NH⁺

G. J. VÁZQUEZ, and J. M. AMERO, Centro de Ciencias Físicas, Universidad Nacional Autónoma de México (UNAM), 62251 Cuernavaca, México (vaztor@s.unam.mx).

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. 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^2Π, a^4Σ⁻, A^2Σ⁻, B^2Δ, C^2Σ⁺) are found in good agreement with experiment.

We find four new bound electronic states of NH⁺, namely, three doublets (2Δ, 3Σ⁺, 5Σ⁺) and one sextet (6Π). A fifth bound electronic state, a quartet (4Π) which was reported schematically in an early SCF study 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, as well as vertical de-excitation energies for emission from the novel states to lower lying bound states. The potential energy curve of NH₂⁺ (X¹Σ⁺) 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.