Accurate Ne-H⁺ and Ar-H⁺ Interactions from Spectroscopic and Scattering States: a Comparison of Theory with Experiments (*).

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Summary. — The ground-state interaction potentials for the Ne(1S) and Ar(1S) systems with H⁺ as a partner have been obtained in a rather simple analytic form and with a parameter optimization that took into consideration a broad range of experimental data, thus extending and verifying earlier work which considered only scattering experiments. It is clearly shown by the present work that the available spectroscopic data on the location of the diatomic bound states and on the transitions between them, the measured differential cross-sections at various collision energies and the mobility coefficients at various $E/N$ values are all well reproduced by our final potential forms, as opposed to the poorer performances of earlier analytic potentials that had been suggested for the same systems. As a consequence of the present analysis very accurate, multiproperty potential functions are thus obtained and provided for the two systems under study.

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1. – Introduction.

The possibility of reliably knowing the interaction forces which exist between rare gases and the simple H⁺ ion is of great interest to many different areas of molecular physics and chemical physics.

(*) To speed up publication, the authors of this paper have agreed to not receive the proofs for correction.
In spite of their simplicity, in fact, such systems constitute attractive prototypes for a rather broad variety of studies like ion-molecule reactions, charge-exchange processes at near-thermal energy, spectroscopy of protonated gases and high-resolution laser photofragment spectroscopy (1). Moreover, the presence of ionic forces gives rise to a rather strong interaction between partners and therefore the relative abundance of bound states and predissociating states provides an extra element of richness and variety in the observed quantities, a fact which is ultimately very useful for an effective comparison between experiments and computed properties.

In the present study we will concentrate on the \( H^+\text{-Ne} \) and \( H^+\text{-Ar} \) protonated species in order to obtain rovibrational spectra associated to the reaction

\[
(H\text{-Rg})_m^+ + h\nu \rightarrow (H\text{-Rg})_n^+.
\]

discussing first the lower-lying bound states \((n, J)\) well below the dissociation thresholds of the various rotational states labelled by the usual \( J \) quantum number. Similar work on the lighter \( \text{He-H}^+ \) system has been already carried out earlier on (2) and will not be discussed here.

Moreover, the recent surge of interest in scattering experiments involving continuum states of these systems (3):

\[
\begin{align*}
\text{i) } & \quad H^+ + \text{Rg} \rightarrow H^+ + \text{Rg}, \\
\text{ii) } & \quad H^+ + \text{Rg} \rightarrow H^+ + \text{Rg}^*, \\
\text{iii) } & \quad H^+ + \text{Rg} \rightarrow H^+ + \text{Rg}^+,
\end{align*}
\]

where some of the investigated channels have been listed, also prompted us to obtain from \textit{ab initio} calculations the \( \text{Ne-H}^+ \) and \( \text{Ar-H}^+ \) interactions in the ground electronic states that are involved in generating angular distributions of channel i) in eq. (2) and to adjust the computed results by a best-fit procedure to elastic-scattering differential cross-sections at various relative energies (4).

Because the experimental quantities which are derived from reactions (1) and (2) sample different regions of the molecular interactions, one obviously expects that the corresponding potential functions will be sensitive in different ways to each set of data and therefore the final answer should be able to reproduce equally well all data available only if directly tested on each of them. In other words, even for such simple partners one can obtain a quantitatively reliable interaction potential function only by performing a multiproperty analysis of as

(2) W. Kolos and J. M. Peek: \textit{Chem. Phys.}, 12, 381 (1976). \\