Quantum study of noble gas molecules of astrophysical interest in collision with He

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The recent detections of HeH^+ [1] and ArH^+ [2] in the interstellar medium (ISM) have shown that noble molecules exist in nature. In the last years, the formation and destruction mechanisms of many other molecules bearing noble atoms in the ISM have been studied. (e.g., $HeHHe^+$, and $HeHNe^+$[3], and $ArHAr^+$, $NeHNe^+$ and $ArHNe^+$ [4]). New searches for these kinds of compounds are certainly underway[5].

In typical molecular clouds, the analysis of the physic-chemical conditions of the regions where the molecules are detected should be performed with non-local-thermal equilibrium (non-LTE) models. Such models require the knowledge of the collisional rate coefficients with the most common colliders in the ISM, e.g., He, H_2, H, and e. However, these rates are not available for most of the noble gas molecules proposed to be detectable.

Therefore, our work focuses on the theoretical and computational study of the collision of several triatomic noble gas-bearing molecules with He. For each system, a new two-dimensional potential energy surface was developed from a grid of *ab initio* energies computed at the CCSD(T) level of theory at the complete basis set limit. Such surfaces were used in close coupling calculations.

The computed rate coefficients for $HeHHe^+$+He, $NeHNe^+$+He, and $ArHAr^+$+He are shown in Figure 1. The larger rate coefficients were found for the collision of $HeHHe^+$+He[6]. The rates for $HeHNe^+$+He and $ArHNe^+$+He are lower than those for HeH^+ and ArH^+. Finally, a large set of rotational de-excitation rate coefficients that can be used in future non-LTE calculations have been reported for five noble gas molecules.

Index Terms: molecular collisions, potential energy surface, close coupling calculations

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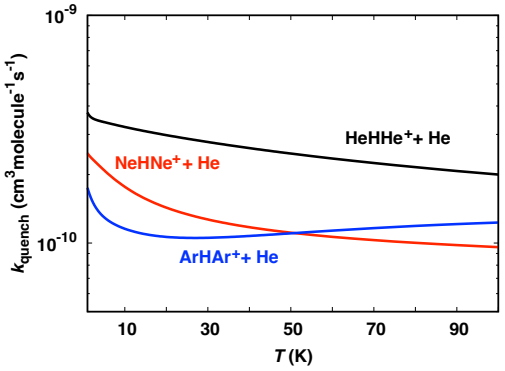

Figure 1: *Quenching rate coefficients of $HeHHe^+$+He, $NeHNe^+$+He, and $ArHAr^+$+He.*

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