Relaxation of ArH+ by collision with He: Isotopic effects

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Context. The study of noble gas compounds has gained renewed interest thanks to the recent detection of ArH+ in the interstellar medium (ISM). The analysis of physical-chemical conditions in the regions of the ISM where ArH+ is observed requires accurate collisional data of ArH+ with He, H2, electrons, and H. Aims. The main goals of this work are to compute the first three-dimensional potential energy surface (PES) to study the interaction of ArH+ with He, analyze the influence of the isotopic effects in the rate coefficients, and evaluate the rovibrational relaxation rates. Methods. Two ab initio grids of energy were computed at the coupled cluster with single, double, and perturbative triple excitations (CCSD(T)) level of theory using the augmented correlation consistent polarized quadruple, and quintuple zeta basis sets (aug-cc-pVQZ, and aug-cc-pV5Z) and a grid at the complete basis set limit was determined. The analytical representation of the PES was performed using the reproducing kernel Hilbert space (RKHS). The dynamics of the system was studied using the close coupling method. Results. The differences in the rate coefficients for the isotopes 36ArH+38ArH+, and 40ArH+ in collision with He are negligible. However, the rotational rates for the collision of ArD+ with He cannot be estimated from those for ArH++He. Comparison with previous rates for the 36ArH++He collision showed discrepancies for ?j > 2, and in the case of high initial rotational states of 36ArH+ differences were found even for ?j = 1. The rates for transitions between different vibrational states were also examined. Finally, new sets of rotational rates for 36ArH++He and 36ArD++He are reported. © 2019 ESO.

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