Charge transfer between S^{2+} and He: A comparative study of quantal and semiclassical approaches

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Abstract

A comparative study on charge transfer in collisions of ground-state S^{2+} ions with He has been performed within fully quantal and semiclassical molecular-orbit close-coupling approaches. The processes for capture into $S^+(^4S^o, ^2D^o, ^2P^o)$ + He^+ are taken into account. Quantal and semiclassical cross sections were evaluated, respectively, in the diabatic and adiabatic representations and found to be in good agreement. The calculations show that at collision energies below about 40 eV/u, the charge-transfer processes are dominated by $S^{2+}(^3P)$ + He → $S^+(^2D^o)$ + He^+, and capture into the $^2P^o$ and $^4S^o$ states become comparable with that into the $^2D^o$ state above 40 eV/u and 600 eV/u, respectively. The multireference single- and double-excitation configuration-interaction method was utilized to obtain adiabatic potentials and nonadiabatic coupling matrix elements. A detailed comparison of quantal and semiclassical transition probabilities is discussed. State-selective and total rate coefficients are presented with temperatures between 10, 000 K and 5.0×10^6 K.

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