Inelastic cross sections for Ar*-He complex

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Collision-induced transfer between the excited states of rare gas atoms (He, Ne, Ar, Kr, Xe) is a topic that has been the focus of many experimental and theoretical studies (there is considerable literature on this topic, so we list just a few representative papers here 1–4). This is a subject of direct relevance to processes occurring in electric discharge excited rare gases and rare gas mixtures (including the dynamics of He/Ne, Ar^+ , Kr^+ , Xe, and excimer lasers). From a theoretical point of view, the mechanistic details of energy transfer induced by collisions with ground state rare gas atoms is a problem that is amenable to investigation using high-level computational techniques. The collision-pair potential energy curves (PECs) and interaction between energy levels are a central part of energy transfer models, and they also determine the rate constants of nonradiative transitions between excited states. The objective of this work was to get elastic and inelastic cross sections for this states from PECs and curves of nondiagonal matrix elements.

The calculations of PECs, spin-orbit interactions and nonadiabatic coupling matrix elements reported here were carried out using the MOLPRO 2015 (5) electronic structure program for 49 spin-orbit states in total. Matrices with these elements were transformed to matrices for different values of total angular momentum projection on internuclear axis and represented as block diagonal matrix.

Diagonal matrix elements with new PECs are used for calculation of elastic scattering cross sections and wavefunctions. These wavefunctions are used for calculation of inelastic scattering cross sections with distorted wave Born approximation.

Caclulated cross sections for inelastic processes can be used for calculation of rate constants of nonradiative transitions.

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