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Calculation of elastic integral and differential collision cross-sections for low energy Ne^+, Ar^+, Kr^+ and Xe^+ ions with neutral He atoms

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There are very few published results, either experimental or theoretical, for elastic integral and differential scattering cross-sections of Ne^+, Ar^+, Kr^+ and Xe^+ ground state ions with ground state neutral He atoms at low energies. This information is important in radiation detector physics studies. In the present work, we present results of calculated cross sections for these collisions at centre-of-mass energies from about 1 meV up to 5 eV. The method of calculation uses a modified Tang–Toennies model from Siska (1986) for the ion–atom potential energy curves of the He–Ne^+, He–Ar^+, He–Kr^+ and He–Xe^+ molecular states $X\,^2\Sigma_{1/2}$ and $A_1\,^2\Pi_{3/2}$, arising from the He atom in its ground state $^1S_0$ and noble-gas ion in its $^2P_{3/2}$ ground electronic state. The potentials are of the form

$$V(r) = A\exp(-br) - B\exp(-br/2) - \sum_{n=2}^{3} f_{2n}(r)C_{2n}r^{-2n},$$

Table 1
Parameters for the modified Tang–Toennies potential

System	State	D_e (eV)	r_e (10^{-10} m)	σ (10^{-10} m)	A (eV)	B (eV)	b (10^{-10} m^{-1})
$HeNe^+$	$X\,^2\Sigma_{1/2}$	0.794[a]	1.341[a]	1.159[a]	35918.33	170.32	8.125
	$A_1\,^2\Pi_{3/2}$	0.035[b]	2.381[b]	2.011[b]	570.7951	1.0079	4.220
$HeAr^+$	$X\,^2\Sigma_{1/2}$	0.035[a]	2.565[a]	2.187[a]	845.9262	2.3817	4.0369
	$A_1\,^2\Pi_{3/2}$	0.020[b]	2.963[b]	2.593[b]	5710.831	3.9113	4.4212
$HeKr^+$	$X\,^2\Sigma_{1/2}$	0.0298[b]	2.911[b]	2.514[b]	1378.527	6.0718	3.7692
	$A_1\,^2\Pi_{3/2}$	0.020[b]	3.175[b]	2.778[b]	3153.945	7.0809	3.8708
$HeXe^+$	$X\,^2\Sigma_{1/2}$	0.050[b]	2.646[b]	2.249[b]	725.7040	5.3246	3.6589
	$A_1\,^2\Pi_{3/2}$	0.0185[b]	3.175[b]	2.778[b]	3856.770	3.9499	3.9873

For all systems $C_4 = 1.4761\times10^{-40}$ eV m^4 and for $HeNe^+$ $C_6 = 1.7606\times10^{-60}$ eV m^6, for $HeAr^+$ $C_6 = 4.8568\times10^{-60}$ eV m^6, for $HeKr^+$ $C_6 = 5.2040\times10^{-60}$ eV m^6 and for $HeXe^+$ (the gas dipole and quadrupole polarizabilities were taken from the compilation of Shevelko (1997) and Mason and McDaniel (1988)).
[a] Siska (1986).
[b] Hausamann and Morgner (1985).

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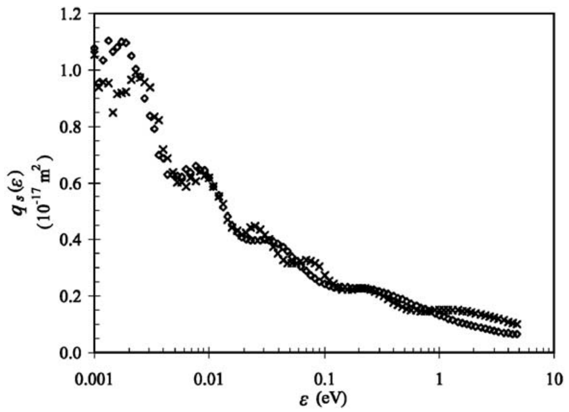

Fig. 1. Calculated (Xe^+,He) integral elastic scattering cross sections $q_s(\varepsilon)$ for the states $X\,^2\Sigma_{1/2}(\times)$ and $A_1\,^2\Pi_{3/2}(\diamond)$ of $HeXe^+$.

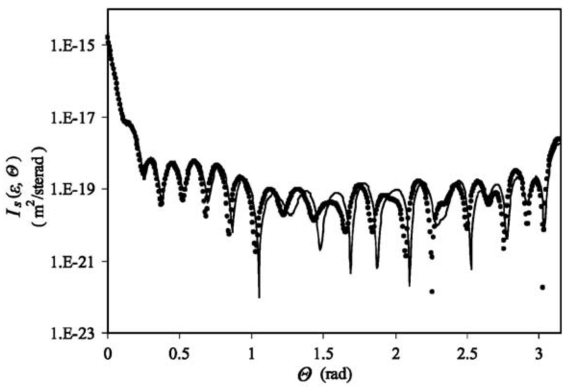

Fig. 2. Calculated differential elastic scattering cross sections $I_s(\varepsilon,\Theta)$ for 10 meV Xe^+ ions onto He for the states $X\,^2\Sigma_{1/2}$ (continuous line) and $A_1\,^2\Pi_{3/2}$ (dots) of $HeXe^+$.

where the damping function is given by

$$f_{2n}(r) = 1 - \exp(-br)\sum_{k=0}^{2n}\frac{(br)^k}{k!}.$$

In this model the constants A, B and b are adjusted to reproduce spectroscopic data or ab initio calculations, using the well depth D_e, location of the minimum r_e, and the zero crossing position σ of the interaction potential. This model, additionally, reproduces the correct long-range behavior of the potential by incorporating the C_4 and C_6 coefficients. The parameters for the potentials $V_X(r)$ and $V_A(r)$ for the molecular states $X\,^2\Sigma_{1/2}$ and $A_1\,^2\Pi_{3/2}$, respectively, are listed in Table 1.

The elastic integral and differential collision cross-sections are calculated using this potential model and the JWKB (Jeffreys–Wentzel–Kramers–Brillouin) semi-classical approximation for the phase shifts and the scattering amplitude calculations for the range 1 meV–5 eV, which falls within the range of applicability of the JWKB method. The number of phase shifts used in the calculation was very large (up to about 5000 in Xe^+–He for 5 eV in the CM frame). The overall integral cross sections decrease from about $10^{-17}\,m^2$ at 1 meV to $10^{-18}\,m^2$ at 5 eV. The calculated integral cross sections show interference effects for all interactions of the noble-gas ions with the He atom. Curves with detailed results of elastic integral and differential collisions cross sections for Xe^+ in He are present in Figs. 1 and 2.

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