## §2. Electron Capture in Collisions of Al^{2+} Ions with He Atoms at Low-to Intermediate Energies

Watanabe, A., Sato, H. (Ochanomizu University)
Suzuki, R. (Hitotsubashi University)
Kimura, M. (Yamaguchi University)
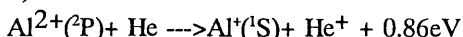Gu, J.P., Hirsch, G., Buenker, R.J. (Universiater fuer Wuppertal)
Kato, T.

We have carried out a theoretical investigation for charge transfer in collisions of Al^{2+} ions with He atoms both in the ground and metastable states at collision energies below 10 keV. Al ions are present in astrophysical environment as well as in fusion plasma, and hence the understanding of scattering dynamics and accurate determination of cross sections is essential for application. The theoretical studies are based on a molecular orbital (MO) expansion method within a semiclassical formalism. The processes we have studied are as follows, with corresponding asymptotic energy defects:

i) ground state atoms:

Al^{2+}(^{2}S) + He ---> Al$^+$(^{1}S) + He$^+$ + 12.5 eV

---> Al$^+$(^{3}P) + He$^+$ + 22.9 eV
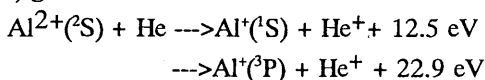
and

ii) excited atoms

Al^{2+}(^{2}P)+ He ---> Al$^+$(^{1}S)+ He$^+$ + 0.86eV

The excited ^{2}P state, which lies at 6.66 eV higher in energy than the [Al^{2+}(^{2}S)+ He] state, is considered to be produced in astrophysical environment where high-energy ions and γ rays constantly interact, and hence, compete in collision dynamics with the ground. Therefore, it is useful if accurate knowledge of charge transfer mechanisms of both the ground and excited states is known for further understanding of the ionization balance in astrophysics.

In the present ab initio calculations, the AO basis set employed for the Al atom is (16s9p4d3f), contracted to [12s7p4d2f], augmented by two d and one f polarization functions. For the He atom, we employ the same basis set that was used earlier. The potential curves are obtained by the multireference single and double excitation (MRD-CI) configuration interaction method [1]. A semiclassical MO expansion method with a straight-line trajectory of the incident ion was employed to study the collision dynamics below 10 keV [2]. Transitions between the molecular states are driven by nonadiabatic couplings. By solving the resulted first-order coupled equations with respect to time t, we obtain the scattering amplitudes for transitions: the square of the amplitude gives the transition probability, and integration of the probability over the impact parameter gives the cross section. Adiabatic potentials for the AlHe^{2+} system are shown in Fig.1. First two lowest leveles correspond to the initial channels, followed by a series of the charge transfer [Al$^+$ + He$^+$] channels. At higher above, there is another series of excited charge transfer channels. We have carried out scattering calculations both from the ground and metastable states.

References:

[1] R. J. Buenker and S. D. Peyerimhoff, Theor. Chim. Acta, 35, 33 (1975).
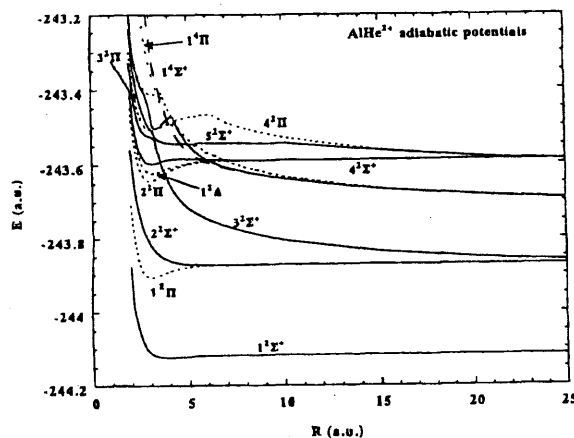[2] M. Kimura and N. F. Lane, Adv. At. Mol. Phys. 26, 76 (1989).

Fig.1 Adiabatic potentials for the AlHe^{2+}.