§7. Electron Capture Rates in Collisions of H^+ Ions with Si Atoms: Capture by the Ground and Excited State

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Observation of the silicon spectral lines has been widely used as a diagnostic means of the physical conditions in astrophysical plasmas[1]. Specifically, Baliunas and Butler[1] examined the effect of charge transfer in conjunction with the silicon spectral lines, and estimated the value of the rate coefficient as 10^{-11} cm^3/s for the charge transfer process in collisions of H^+ ions with $Si(^3P)$ ground state atoms. From this, they suggested a possible importance of the ionization process of silicon atoms. There is no other theoretical or experimental determination of the charge transfer cross section for the $[H^+ + Si]$ system.

We have carried out a theoretical investigation for charge transfer in collisions of H^+ ions with neutral Si atoms both in the ground and metastable states at collision energies from 10^{-3} eV to 10 keV, using molecular states for the SiH^+ obtained earlier[2]. The processes we have studied are as follows, with corresponding asymptotic energy defects:

i) Ground state Si ions:

$$H^+ + Si(^3P) \text{ ---> } H + Si^+(^4P) + 1112\ cm^{-1} \quad (1)$$
$$\text{---> } H + Si^+(^2P) + 43936\ cm^{-1},$$

and

ii) Metastable Si ions:

$$H^+ + Si(^1D) \text{ ---> } H + Si^+(^2D) - 5069\ cm^{-1} \quad (2)$$

The metastable ^1D state in Eq.(2), which lies at 50235 cm^{-1} higher in energy than the $[Si^+(^2P) + H]$ state, is considered to compete more and more in collision dynamics with the ground state as the collision energy increases to higher-eV or -keV regime. Hence, it is important to understand the electron capture mechanism of the both ground and metastable states, and to determine each cross section accurately. The adiabatic potential curves of SiH^+ are obtained by employing the *ab initio* multireference single- and double-excitation configuration interaction (MRD-CI) method[2]. From the bottom of adiabatic potentials, they correspond asymptotically to the atomic states $[H + Si^+(^2P)$: $^3\Pi$ $^1\Sigma^+]$, $[H + Si^+(^4P)$: $^3\Pi, ^3\Sigma^-]$ and $[H^+ + Si(^3P)$: $^3\Pi, ^3\Sigma^-]$ for triplet manifold, and $[H^+ + Si(^1D)$: $^1\Pi, ^1\Sigma^+]$ and $[H + Si^+(^2D)$: $^1\Pi, ^1\Sigma^+]$ for singlet manifold. It should be noted that the $3^1\Sigma^+$ and $2^1\Sigma^+$ states have a sharp avoided crossing near internuclear separation (R) = 5 a.u. On the other hand, for the triplet, there is no such a sharpe avoided crossing. A semiclassical MO expansion method with a straight-line trajectory of the incident ion was employed to study the collision dynamics. The MO's included in the dynamical calculations are the two sets of states: separating to $[H^+ + Si(^3P)]$ $(2^3\Sigma^-, 3^3\Pi)$, $[H + Si^+(^4P)]$ $(1^3\Sigma^-, 2^3\Pi)$, $[H + Si^+(^2P)]$ $(1^3\Sigma^+, 1^3\Pi)$ for the charge transfer from the initial ground state, and $[H^+ + Si(^1D)]$ $(2^1\Sigma^+, 2^1\Pi)$, $[H + Si^+(^2D)]$ $(3^1\Sigma^+, 3^1\Pi)$ for the electron capture from the initial metastable state. A fully quantum mechanical representation of the MO expansion method was employed for collision energies below 30 eV. The molecular states included are two sets of channels: (i) $[Si^+(^4P) + H]$ $(3^3\Pi)$ and $[Si(^3P) + H^+]$ $(2^3\Pi)$ and (ii) $[Si^+(^2D) + H]$ $(3^1\Pi)$ and $[Si(^1D) + H^+]$ $(2^1\Pi)$.

Because of a small asymptotic energy defect between the initial and closest electron capture channels, and because of the exothermicity in nature for the transition, the electron capture process from the ground state $Si(^3P)$ atoms is extremely efficient. Therefore, the present cross section for the $Si^+(^4P)$ formation are found to have a broad peak with a value of 1×10^{-14} cm^2 between 10 eV and 10 keV. It gradually decreases as the collision energy decreases, but it still has a value of 10^{-15} cm^2 even at 1 eV. (1b) The present cross section for the $Si^+(^2P)$ formation is comparable with those of the $Si^+(^4P)$ formation above 1 keV, but it sharply decreases below 0.5 keV because of a larger energy defect from the initial state. The $Si^+(^2D)$ formation in the singlet-state collision is also large with the charge transfer cross section of 3×10^{-15} cm^2 above 1 eV.

References

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1). S. L. Baliunas and S. E. Butler, Astrophys. J. 235, L45 (1980).

2). A. B. Sannigrahi, R. J. Buenker, G. Hirsch and J. P. Gu, Chem. Phys. Lett. 237, 204 (1995).