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Radiative charge transfer in collisions of H^+ with Na at very low energies

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The radiative charge transfer for H^++Na($3s$) collisions has been investigated by using both the optical-potential and semiclassical methods in the energy ranges of $10^{-6}-10$ and $10^{-2}-100$ eV, respectively, which are in agreement in the overlapping energy region. The relevant molecular potentials and dipole matrix elements were obtained from the multireference single- and double-excitation configuration interaction approach. The radiative charge-transfer cross sections display rich resonance structures, due to the formation of quasibound rotational-vibrational molecular states, in the energy range below 0.2 eV. The present radiative charge-transfer cross-section results disagree with the calculations of Watanabe *et al.* [Phys. Rev. A **66**, 044701 (2002)]. The rate coefficient is obtained for temperatures between 0.1 and 20 000 K. Below 7000 K, it has a nearly constant value of approximately 1.7×10^{-13} cm^3 s^{-1}, which is about 1/3 of that of Watanabe *et al.* The nonradiative charge transfer becomes dominant at energies above 4 eV.

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I. INTRODUCTION

The distribution of sodium between its ionized and neutral forms is important for the interpretation of observations of the resonance line of sodium atoms in the atmospheres of planets and comets [1]. Charge transfer between neutral sodium atoms and protons may modify the ionization distribution in stellar winds [2]. Nonradiative charge transfer of Na to H^+ has been investigated extensively for energies from eV to keV [1,3–11]. However, at low temperatures such as in interstellar space [12] or in cold and ultracold experiments [13], the collision energies are much less than 1 eV, and radiative charge transfer may become dominant over nonradiative charge transfer. The radiative charge-transfer process

$$\mathrm{Na}(3s) + \mathrm{H}^+ \rightarrow \mathrm{Na}^+ + \mathrm{H}(1s) + h\nu \tag{1}$$

was previously investigated by Watanabe *et al.* [14] using an optical-potential method and the molecular data were obtained by a pseudopotential approach. The radiative cross sections they computed have a $1/E$ dependence at energies above 10^{-2} eV, and the rate coefficient changes slowly with temperatures below 10^2 K, but decreases rapidly above 10^2 K. On the other hand in the Langevin formula for a polarization potential, the cross section behaves as $1/E^{1/2}$. For collisions of Li with H^+, Kimura *et al.* [15] also found that the cross section has a $1/E$ dependence. But the calculations of Stancil and Zygelman [16] showed that the cross section scaling is the same as in the Langevin formula.

In order to re-examine this energy dependence and provide the exact radiative charge-transfer parameters for applications, we perform an investigation of the radiative charge-transfer process in collisions of ground-state Na atoms with H^+ ions using both the optical-potential and the semiclassical methods. The molecular potentials and dipole matrix elements are calculated by an *ab initio* multireference single- and double-excitation configuration interaction (MRD-CI) package [17,18]. The obtained cross sections and rate coefficients are compared with those of Watanabe *et al.* [14]. Atomic units will be used in the remaining part of this paper, unless explicitly indicated otherwise.

II. THEORETICAL METHOD

An optical-potential method for treating radiative decay, including radiative charge transfer and radiative association, induced by ion-atom collisions was described in detail by Zygelman and Dalgarno [19] and successfully applied to calculations of some collision systems [16,20–23]. Here we only outline the optical-potential method and relevant formulas. During the ion-atom collisions, the transition probability per unit time, i.e., the Einstein coefficient, is represented by the imaginary part of a complex optical potential. The scattering wave $F_A(\vec{R})$, where R is the internuclear distance and the subscript A denotes the initial upper molecular state ($A\ ^2\Sigma^+$), is obtained by solving the Schrödinger equation

$$\left[-\frac{1}{2\mu}\nabla_{\vec{R}}^2 + V_A(R) - E\right]F_A(\vec{R}) = \frac{i}{2}A(R)F_A(\vec{R}), \tag{2}$$

where E is the collision energy in the entrance channel, μ is the reduced mass, and $A(R)$ is the transition probability for the radiative transition given by

$$A(R) = \frac{4}{3}D^2(R)\frac{|V_A(R) - V_X(R)|^3}{c^3}, \tag{3}$$

where c is the speed of light, and $V_A(R)$ and $V_X(R)$ are the adiabatic potential energies for the upper $A\ ^2\Sigma^+$ and the lower $X\ ^2\Sigma^+$ states, respectively. $D(R)$ is the dipole-transition-moment matrix element between the $A\ ^2\Sigma^+$ and $X\ ^2\Sigma^+$ states. For large R values, the $A\ ^2\Sigma^+$ state separates asymptotically into the atomic states Na($3s$) and H^+, while

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the $X\,{}^2\Sigma^+$ state separates into the atomic states Na^+ and $\mathrm{H}(1s)$.

The cross section for collision-induced radiative decay can be written as

$$\sigma(E) = \frac{\pi}{k_A^2}\sum_J^\infty (2J+1)[1-\exp(-4\eta_J)], \tag{4}$$

where η_J is the imaginary part of the phase shift for the Jth partial wave of the radial Schrödinger equation which is given in the distorted-wave approximation by

$$\eta_J = \frac{\pi}{2}\int_0^\infty dR |f_J^A(k_A R)|^2 A(R), \tag{5}$$

where $k_A = \sqrt{2\mu[E - V_A(\infty)]}$, and $f_J^A(k_A R)$ is the regular solution of the homogeneous radial equation

$$\left\{\frac{d^2}{dR^2} - \frac{J(J+1)}{R^2} - 2\mu[V_A(R) - V_A(\infty)] + k_A^2\right\} f_J^A(k_A R) = 0, \tag{6}$$

and is normalized asymptotically according to

$$f_J^A(k_A R) = \sqrt{\frac{2\mu}{\pi k_A}}\sin\left(k_A R - \frac{J\pi}{2} + \delta_J^A\right). \tag{7}$$

In order to extend the calculation to higher energy, by replacing the summation in Eq. (4) and applying the JWKB approximation, one obtains the expression for the semiclassical cross section,

$$\sigma(E) = 2\pi\sqrt{\frac{2\mu}{E}}\int p\,dp \int_{R_A^{\mathrm{ctp}}}^\infty dR \frac{A(R)}{\sqrt{1 - V_A(R)/E - p^2/R^2}}, \tag{8}$$

where p is the impact parameter and R_A^{ctp} is the classical turning point in the incoming channel [19,24]. For large energies ($E \gg V_A$), the double integral is nearly energy independent, and therefore $\sigma(E)$ varies as $1/E^{1/2}$ [16,22,23].

III. RESULTS AND DISCUSSION

As in our previous work [7], an *ab initio* CI calculation is carried out for potential curves of four Σ^+ plus one Δ electronic states in A_1 symmetry and two electronic Π states in B_1 symmetry of the $(\mathrm{NaH})^+$ system by using the MRD-CI package [17,18]. A $(6s,3p,2d,1f)$ contracted to $[4s,3p,2d,1f]$ basis set is employed for hydrogen. An effective core potential (ECP) adapted basis set $(4s,4p,2d,1f)$ [25] is used for the Na atom. A diffuse $(2s2p)$ basis set centered on the Na atom is employed to describe its Rydberg states, while a diffuse $(2s3p)$ set is used for H atom. The adiabatic potential energies and dipole matrix elements are calculated for internuclear distance $R = 1.4-30$ a.u., as shown in Fig. 1. The adiabatic potentials $X\,{}^2\Sigma^+$, $A\,{}^2\Sigma^+$, $B\,{}^2\Sigma^+$, and $C\,{}^2\Pi$ correspond to $\mathrm{Na}^+ + \mathrm{H}(1s)$, $\mathrm{Na}(3s) + \mathrm{H}^+$, $\mathrm{Na}^+ + \mathrm{H}(2p\sigma^+)$, and $\mathrm{Na}^+ + \mathrm{H}(2p\pi)$ states in the asymptotic regions, respectively. The initial state is $\mathrm{Na}(3s) + \mathrm{H}^+$ ($A\,{}^2\Sigma^+$), so we only need to consider the radiative charge-transfer process between $A\,{}^2\Sigma^+$ and the lower state $X\,{}^2\Sigma^+$.

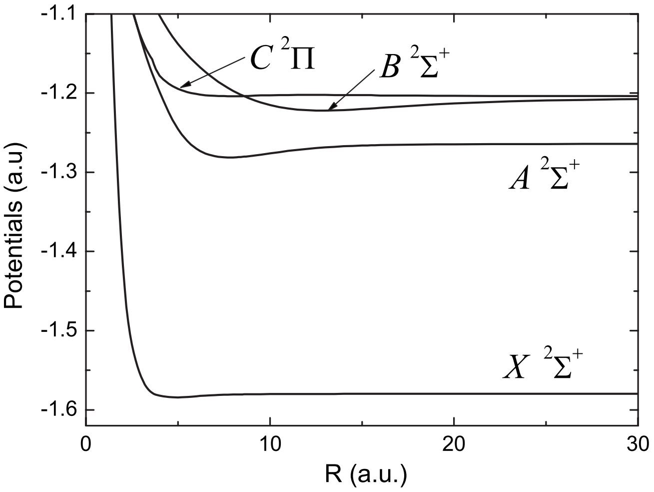

FIG. 1. Adiabatic potentials of $(\mathrm{NaH})^+$ as a function of internuclear distance. The $X\,{}^2\Sigma^+$, $A\,{}^2\Sigma^+$, $B\,{}^2\Sigma^+$, and $C\,{}^2\Pi$ correspond to $\mathrm{Na}^+ + \mathrm{H}(1s)$, $\mathrm{Na}(3s) + \mathrm{H}^+$, $\mathrm{Na}^+ + \mathrm{H}(2p\sigma^+)$, and $\mathrm{Na}^+ + \mathrm{H}(2p\pi)$ states in the asymptotic regions, respectively.

The dipole matrix elements between the $X\,{}^2\Sigma^+$ and $A\,{}^2\Sigma^+$ states are given in Fig. 2, and comparison with the results of Watanabe *et al.* [14] shows good agreement within a deviation of 5% except for $R < 2.6$ a.u. We calculate the transition probability $A(R)$ from Eq. (3), as shown in Fig. 3. The $A(R)$ value increases as the internuclear distance increases, reaching a maximum near $R = 4.8$ a.u., and then decreases gradually thereafter. Our calculated $A(R)$ is similar in shape to that of Watanabe *et al.* [14]. The unit of $A(R)$, shown as 10^{-8} s^{-1}, in Ref. [14] is apparently in error, however, so that our $A(R)$ cannot be compared to it.

Beyond $R = 30$ a.u., the potential of the $A\,{}^2\Sigma^+$ state can be described by the long-range form

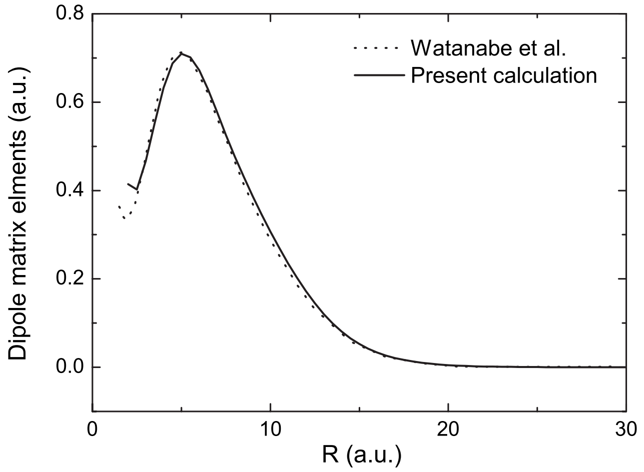

FIG. 2. Dipole matrix element between the $X\,{}^2\Sigma^+$ and $A\,{}^2\Sigma^+$ states as a function of internuclear distance. Dotted line: Watanabe *et al.* [14]; solid line: present calculation.

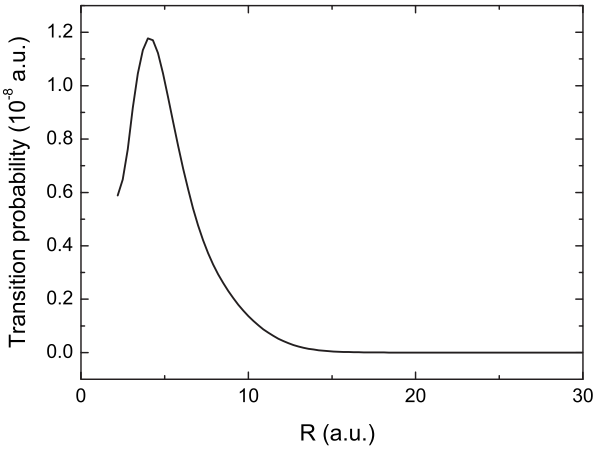

FIG. 3. Transition probability $A(R)$ between the $X\ ^2\Sigma^+$ and $A\ ^2\Sigma^+$ states as a function of internuclear distance.

$$V_L(R) = -\frac{1}{2}\left[\frac{C_4}{R^4} + \frac{C_6}{R^6} + \frac{C_8}{R^8}\right], \tag{9}$$

where C_4, C_6, and C_8 are the dipole, quadrupole, and octupole polarizabilities of the Na(3*s*) atom, respectively, and are chosen to be same as those used in Ref. [14]. For the ground state $X\ ^2\Sigma^+$, the form of the long-range potential is $V_L(R)=-(1/2)(\alpha_d/R^4)$, where α_d is the dipole polarizability of the H(1*s*) atom. The long-range asymptotic behavior of the dipole matrix element is fitted to the form d_0/R^n.

Using the optical-potential method described above, we calculate the radiative decay cross sections. Because in the present system of interest, the lower $X\ ^2\Sigma^+$ state only has a very shallow well (~0.125 eV) at short range, contributions from radiative association to collision-induced radiative decay can be very small and it is assumed that the radiative decay only contributes to the charge-transfer process [22]. The computed radiative cross sections are given in Fig. 4. The cross section decreases as the collision energy increases. Rich resonance structures appear in the energy region of 10^{-5}–0.2 eV. These resonances are attributed to the presence of quasi-bound or virtual rotational-vibrational levels in the entrance channel, and may give rise to an enhancement in the rate coefficients [16,23]. It is interesting to check the effects of the long-range form of potentials on the radiative charge-transfer cross sections by applying the first dipole term in Eq. (9), and the cross section is plotted in Fig. 4 with a dashed line. Comparison shows that the quadrupole and octupole terms in Eq. (9) only influence the position of the resonance structures at very low collision energies. This is because the quadrupole and octupole terms can change the shape of the potentials, which modifies the positions of the vibrational levels in the entrance channel. The discrepancy will become smaller if the *ab initio* molecular calculation is extended to a larger internuclear distance, say 50 a.u. For practical purposes, this effect changes the radiative charge-transfer rate coefficients by less than 2% and can be neglected.

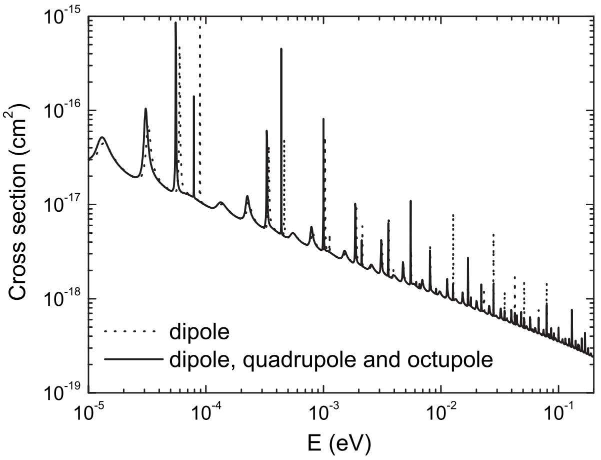

FIG. 4. Comparison of the radiative charge-transfer cross sections by considering different asymptotic behaviors for potentials when $R>30$ a.u. Solid line includes dipole, quadrupole, and octupole terms as shown in Eq. (9), and dotted line includes only the dipole term.

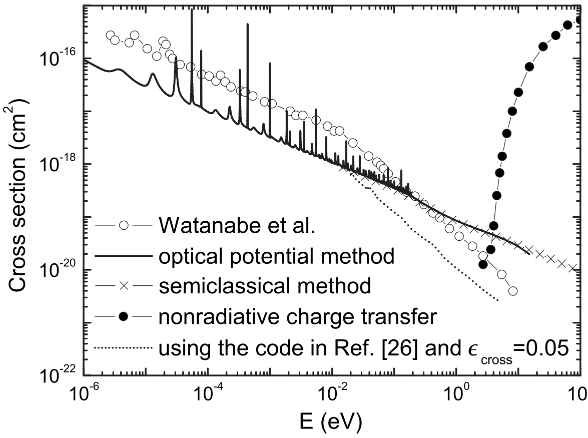

FIG. 5. Radiative charge-transfer cross sections for H^++Na(3*s*) collisions. Solid line: the present results employing an optical-potential method; crosses: the present results using the semiclassical method; dotted line: the present results using the code in Ref. [26] and cross-section convergence parameter $\epsilon_{\text{cross}}=0.05$; open circles: Watanabe *et al.* [14]; filled circles: nonradiative charge-transfer cross sections [7].

In Fig. 5, we compare our radiative charge-transfer cross section with that of Watanabe *et al.* [14] in the energy range between 10^{-6} and 10 eV. Perhaps because of the fewer calculated energy points, Watanabe *et al.* [14] did not find the rich resonance structures. In addition, for collision energy $E<10^{-2}$ eV, their calculated cross sections are about three to four times larger than ours except at the positions of resonances. For $E>10^{-2}$ eV, their calculated cross sections decrease much faster than ours. For $E>0.3$ eV, our cross sections become larger than theirs. Our cross section has an energy dependence of $1/E^{1/2}$, which is consistent with the Langevin cross-section behavior for a polarization potential. The cross section of Watanabe *et al.* [14] has a $1/E$ dependence at energies above 10^{-2} eV, however. This $1/E$ dependence also appears in the work of same group for calculating H^++Li(2*s*) collisions [15]. In a later study, Stancil and Zygelman [16] found the radiative charge-transfer cross section behaving as $1/E^{1/2}$. In order to clarify this discrepancy,

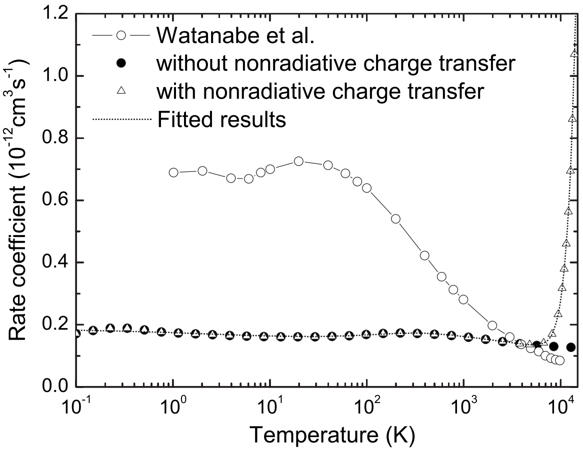

FIG. 6. Radiative and nonradiative charge-transfer rate coefficients as functions of temperature. Only the radiative charge-transfer process is included: present calculation (filled circles); Watanabe *et al.* [14] (open circles). Both radiative and nonradiative charge-transfer processes included: present calculation (triangles); fitted present results (dotted lines).

we repeated the cross-section calculations by using the code in Ref. [26], the same as that of Watanabe *et al.* [14]. In this code, because the wave function is complex in Eq. (2), we can obtain two coupled differential equations. By solving the coupled equations, the radiative decay cross section can be expressed in terms of the imaginary component of the phase shift. When running this code, we chose the convergence parameters for cross section ϵ_{cross} and phase shift ϵ_{phase} to be 10^{-3} and 10^{-4}, respectively. The cross sections obtained in this way are almost identical to our present results. In the work of Watanabe *et al.* [14], the ϵ_{cross} value was chosen to be 0.05. If we also choose ϵ_{cross} to be 0.05, then the slope of the cross section is similar to that of Watanabe *et al.* [14], as shown in Fig. 5. Therefore, it can be concluded that the calculation precision in Refs. [14,15] was probably not sufficient, and this results in the incorrect energy dependence of the cross sections.

Even if we choose $\epsilon_{\text{cross}}=0.05$ using the code in Ref. [26], the slope of the cross section is similar to the result of Watanabe *et al.* [14], but the magnitude of the cross sections is still a few times smaller than theirs except at the position of resonances. This discrepancy may come from the difference in the transition probability $A(R)$. But the $A(R)$ unit of 10^{-8} s^{-1}, as we have mentioned before, in Ref. [14] may be an error, so that our results cannot be compared directly to it. On the other hand, the molecular data of Watanabe *et al.* [14] are obtained by a pseudopotential approximation, and the calculation accuracy may therefore be lower than our *ab initio* MRD-CI results.

In order to extend the treatment to higher energy, we have also performed a semiclassical calculation using Eq. (8) for collision energy between 10^{-2} and 100 eV, and give the results in Fig. 5. In the overlapping energy range of $10^{-2}-10$ eV, our optical-potential cross sections are in fair agreement with the semiclassical results. Also given in Fig. 5 are the nonradiative charge-transfer cross sections which have been published in Ref. [7]. There is a weak avoided crossing between the $A\ ^2\Sigma^+$ and $B\ ^2\Sigma^+$ states at $R=12$ a.u., as shown in Fig. 1, which induces the charge transfer at an energy of approximately 2 eV. As the collision energy increases, the rotational coupling between $A\ ^2\Sigma^+$ and $C\ ^2\Pi$ becomes the dominant mechanism and the nonradiative charge-transfer cross sections increase rapidly. When $E<3$ eV, the radiative charge-transfer cross section is much larger than the nonradiative one. But when $E>4$ eV, the nonradiative charge transfer becomes dominant over the radiative charge-transfer process.

TABLE I. Rate coefficients for radiative and nonradiative charge transfers in $H^+/Na(3s)$ collisions. Note: units for a_i and c_i are 10^{-12} cm^3 s^{-1} and K, respectively.

T (K)	$\alpha(T)$ (10^{-12} cm^3 s^{-1})
0.1	0.171
0.2	0.187
0.3	0.189
0.5	0.183
0.7	0.178
1.0	0.174
3.0	0.167
5.0	0.164
7.0	0.162
10	0.161
30	0.161
50	0.163
70	0.165
100	0.169
300	0.172
500	0.169
700	0.166
1000	0.161
3000	0.143
5000	0.136
7000	0.145
10000	0.278
20000	5.115
a_1	10.59
b_1	7.6175
c_1	5311.3
a_2	1.338
b_2	−0.0895
c_2	71835
a_3	−0.2825
b_3	0.167
c_3	177.2

The rate coefficients for temperatures between 0.1 and 20 000 K are obtained by averaging the optical-potential radiative charge-transfer cross sections in Fig. 5 over a Maxwellian velocity distribution. The results are displayed in Fig. 6 and compared to those of Watanabe *et al.* [14]. In Ref.

[14], the unit of rate coefficients 10^{12} cm^3 s^{-1} is apparently a typographical error, and we have modified it in Fig. 6. Our rate coefficient approaches a constant value of about 1.7×10^{-13} cm^3 s^{-1} at $T < 7000$ K, which is similar to the results for collisions of Li with H$^+$ [16] and O with He$^+$ [22]. This is because the cross section behaves as $1/E^{1/2}$. When $T > 7000$ K, the rate coefficients increase quickly because the contribution from the nonradiative charge-transfer process becomes dominant. In contrast to the present study, the rate coefficients of Watanabe *et al.* [14] vary smoothly for $T < 100$ K, and then decrease sharply for $T > 100$ K. Our rate coefficients are about three to four times smaller than those of Watanabe *et al.* [14] for $T < 100$ K; at 2000 K, the two calculations come into close agreement.

For convenience in future applications, we also give the rate coefficients for temperatures between 0.1 and 20 000 K, including both the radiative and nonradiative charge-transfer processes, in Table I. Finally, the rate coefficients are fitted to the form

$$\alpha(T) = \sum_i a_i \left(\frac{T}{10\,000}\right)^{b_i} \exp\left(-\frac{T}{c_i}\right). \qquad (10)$$

The fitting parameters are also provided at the end of Table I. Units for a_i and c_i are 10^{-12} cm^3 s^{-1} and kelvin, respectively. The fitting is reliable to within 3% over the temperature range of 0.5–20 000 K, and to no more than 6% from 0.1 to 0.5 K. The fitted data are also plotted in Fig. 6.

IV. CONCLUSION

In the present study we have re-examined the radiative charge-transfer cross sections in collisions of protons with Na($3s$) atoms for collision energies from 10^{-6} to 10 eV using the optical-potential method and from 0.01 to 100 eV using the semiclassical method. The results of these calculations are consistent in the overlapping energy region, but they differ significantly from the results of Watanabe *et al.* [14]. The discrepancy in the magnitude of the cross sections may come from the differences of transition probability. The distinction in the energy dependence of the cross section may be due to the inadequate precision in the calculation of Watanabe *et al.* [14]. Our optical-potential calculation shows that the asymptotic form of the potentials will influence the position of the resonance structures. The rate coefficient is also presented and is found to have a nearly constant value below 7000 K. The nonradiative charge-transfer process becomes the dominant contributor to the rate coefficients above 7000 K.

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[1] C. Courbin, R. J. Allan, P. Salas, and P. Wahnon, J. Phys. B **23**, 3909 (1990).
[2] T. Royer, D. Dowek, J. C. Houver, J. Pommier, and N. Andersen, Z. Phys. D: At., Mol. Clusters **10**, 45 (1988).
[3] V. S. Kushawaha, Z. Phys. A **313**, 155 (1983).
[4] H. Croft and A. S. Dickinson, J. Phys. B **29**, 57 (1996).
[5] C. M. Dutta, P. Nordlander, M. Kimura, and A. Dalgarno, Phys. Rev. A **63**, 022709 (2001).
[6] A.-T. Le, C.-N. Liu, and C. D. Lin, Phys. Rev. A **68**, 012705 (2003).
[7] C. H. Liu, Y. Z. Qu, L. Liu, J. G. Wang, Y. Li, H.-P. Liebermann, P. Funke, and R. J. Buenker, Phys. Rev. A **78**, 024703 (2008).
[8] M. Gieler, F. Aumayr, P. Ziegelwanger, H. Winter, and W. Fritsch, Phys. Rev. A **43**, 127 (1991).
[9] K. Finck, Y. Wang, Z. Roller-Lutz, and H. O. Lutz, Phys. Rev. A **38**, 6115 (1988).
[10] A. Jain and T. G. Winter, Phys. Rev. A **51**, 2963 (1995).
[11] R. Shingal and B. H. Bransden, J. Phys. B **20**, 4815 (1987).
[12] D. M. Meyer and J. T. Lauroesch, Astrophys. J. **520**, L103 (1999).
[13] T. C. Killian, M. J. Lim, S. Kulin, R. Dumke, S. D. Bergeson, and S. L. Rolston, Phys. Rev. Lett. **86**, 3759 (2001).
[14] A. Watanabe, C. M. Dutta, P. Nordlander, M. Kimura, and A. Dalgarno, Phys. Rev. A **66**, 044701 (2002).
[15] M. Kimura, C. M. Dutta, and N. Shimakura, Astrophys. J. **430**, 435 (1994); **454**, 545 (1995).
[16] P. C. Stancil and B. Zygelman, Astrophys. J. **472**, 102 (1996).
[17] R. J. Buenker and S. D. Peyerimhoff, Theor. Chim. Acta **35**, 33 (1974); **39**, 217 (1975); R. J. Buenker, Int. J. Quantum Chem. **29**, 435 (1986).
[18] R. J. Buenker, in *Proceedings of the Workshop on Quantum Chemistry and Molecular Physics*, Wollongong, Australia, edited by P. G. Burton (Wollongong University Press, Wollongong, Australia, 1980); in *Study in Physical and Theoretical Chemistry*, Current Aspects of Quantum Chemistry Vol. 21, edited by R. Carbo (Elsevier, Amsterdam, 1981), p. 17; R. J. Buenker and R. A. Phillips, J. Mol. Struct.: THEOCHEM **123**, 291 (1985); S. Krebs and R. J. Buenker, J. Chem. Phys. **103**, 5613 (1995).
[19] B. Zygelman and A. Dalgarno, Phys. Rev. A **38**, 1877 (1988).
[20] B. Zygelman, A. Dalgarno, M. Kimura, and N. F. Lane, Phys. Rev. A **40**, 2340 (1989).
[21] B. W. West, N. F. Lane, and J. S. Cohen, Phys. Rev. A **26**, 3164 (1982).
[22] L. B. Zhao, P. C. Stancil, J. P. Gu, H.-P. Liebermann, Y. Li, P. Funke, R. J. Buenker, B. Zygelman, M. Kimura, and A. Dalgarno, Astrophys. J. **615**, 1063 (2004).
[23] L. B. Zhao, J. G. Wang, P. C. Stancil, J. P. Gu, H.-P. Liebermann, R. J. Buenker, and M. Kimura, J. Phys. B **39**, 5151 (2006).
[24] D. R. Bates, Mon. Not. R. Astron. Soc. **111**, 303 (1951).
[25] L. Fernandez Pacios and P. A. Christiansen, J. Chem. Phys. **82**, 2664 (1985).
[26] A. C. Allison, Comput. Phys. Commun. **3**, 173 (1972).