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Charge transfer of C^{3+} ions in atomic hydrogen

S. Bienstock
Harvard-Smithsonian Center for Astrophysics, Cambridge, Massachusetts 02138

T. G. Heil
Department of Physics and Astronomy, University of Georgia, Athens, Georgia 30602

C. Bottcher
Physics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37830

A. Dalgarno
Harvard-Smithsonian Center for Astrophysics, Cambridge, Massachusetts, 02138
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Cross sections are calculated for the charge transfer of C^{3+} ions in atomic hydrogen at impact energies up to 5 keV. Agreement is satisfactory with both the low-energy data below 250 eV and the high-energy data above 2 keV. The calculations show that the cross-section behavior is largely due to capture into the $1s^2 2s3s\ ^3S$ state of C^{2+} for which the cross sections pass through a minimum at an energy near 250 eV and increase rapidly beyond the minimum out to 5 keV.

Charge transfer in collisions of multiply charged ions with neutral hydrogen atoms affects significantly the thermal and ionization structure of beam-injected hydrogen plasmas and modifies substantially the transport of impurity ions. Measurements of charge transfer cross sections for C^{3+} ions colliding with H atoms at impact energies between 11 and 250 eV/amu have been reported by Phaneuf[1] and at impact energies between 2 and 5 keV/amu by Gardner *et al.*,[2] Crandell *et al.*,[3] and Phaneuf *et al.*[4] The low-energy measurements yield cross sections which decrease to a value of $6 \times 10^{-16}\ \text{cm}^2$ at 250 eV/amu, whereas the higher-energy data are consistent with cross sections of about $1.6 \times 10^{-15}\ \text{cm}^2$.

We present here a theoretical interpretation which demonstrates that the low- and high-energy data can be reconciled, a rapid increase in the cross sections occurring between 250 and 4000 eV/amu.

A quasimolecular adiabatic description of the collision of C^{3+} with H has been given by Heil, Butler, and Dalgarno[5] in which the charge-transfer process is driven by the off-diagonal elements of a diabatic potential energy matrix $\underline{V}(R)$ whose diagonal elements are diabatic potential-energy surfaces of either $^1\Sigma^+$ or $^3\Sigma^+$ symmetry. The cross section $\sigma(E)$ at an energy E can be written as the weighted sum

$$\sigma(E) = \tfrac{1}{4}[\sigma_0(E) + 3\sigma_1(E)] \ ,$$

where σ_S is the cross section for charge transfer in the $^{2S+1}\Sigma^+$ symmetry. In the theory used by Heil *et al.*[5] the nuclear motion is described by a decomposition into partial waves corresponding to nuclear angular quantum numbers J and the cross sections are expressed as summations

$$\sigma_S(E) = \frac{\pi\hbar^2}{2\mu E} \sum_j \sum_J (2J+1)|S_{ij}^J|^2 \ ,$$

where μ is the reduced mass, E is the energy of relative motion, and S_{ij}^J is the scattering matrix element connecting the initial state i formed by the approach of C^{3+} and H to a final state j formed by charge transfer and separating to C^{2+} and H^+.

In our calculations only those states were retained for which the adiabatic coupling is strong. For the $^3\Sigma^+$ symmetry, the final states separating to C^{2+} $1s^2 2s3s\ ^3S$ and H^+ and to C^{2+} $1s^2 2s3p\ ^3P^0$ and H^+ are strongly coupled and for the $^1\Sigma^+$ symmetry, the two final states separating to C^{2+} $1s^2 2p^2\ ^1S$ and H^+ and to C^{2+} $1s^2 2p^2\ ^1D$ and H^+ are strongly coupled.[5]

For transitions which are driven by strong localized couplings, translation factors may not be necessary[5] and the scattering equations may be written in the form

$$\left[\frac{\hbar^2}{2\mu}\nabla_R^2 \underline{I} - \underline{V}(R) + E\underline{I}\right]\underline{F}(\vec{R}) = 0 \ .$$

We solved them by numerical integration.[5] With increasing energy the method quickly becomes too laborious and our closing-coupling calculations are impracticable above about 500 eV. We have developed a unitarized distorted-wave approximation which can be readily carried through to second order in the coupling strength and which improves rapidly in accuracy as E and J increase. We have constructed a systemat-

TABLE I. Charge-transfer cross sections $\frac{1}{4}(2S+1)\sigma_S$ and σ in units of 10^{-16} cm^2 for $C^{3+}+H \rightarrow C^{2+}+H^+$.

Energy E (eV)	Final state of C^{2+} $1s^22p^2\,{}^1D$	$1s^22p^2\,{}^1S$	$1s^22s3s\,{}^3S$	$1s^22s3p\,{}^3P^0$	Total
10		3.1	11.1	0.09	14.3
20		3.4	8.4	0.18	11.9
30		3.6	6.9	0.19	10.6
50	0.02	3.4	5.1	0.12	8.65
75	0.06	2.8	4.1	0.09	7.00
125	0.16	2.3	3.2	0.18	5.85
250	0.28	1.9	2.4	0.32	4.96
375	0.26	2.4	2.6	0.27	5.55
500	0.27	2.7	3.2	0.38	6.57
1000	0.27	2.7	5.1	1.2	9.22
2000	0.27	1.9	8.5	3.8	14.5
5000	0.34	1.0	11.2	4.6	17.1

ic procedure in which for a given value of E close-coupling results are obtained for small J, second-order distorted-wave results for intermediate J, and first-order distorted-wave results for high J, each method giving way to the simpler approximation as it acquires sufficient accuracy.[6] The procedure gives results which are identical to those obtained from a complete solution of the coupled scattering equations. With the procedure it becomes possible to extend the calculations of Heil *et al.*[5] to energies of 5 keV.

Figure 1 illustrates the ${}^1\Sigma^+$ and ${}^3\Sigma^+$ cross sections $\frac{1}{4}(2S+1)\sigma_S(E)$ and the total charge transfer cross section $\sigma(E)$ as functions of the energy E. The calculated cross sections agree with the measured values within the experimental errors and demonstrate the mutual consistency of the low- and high-energy data. Table I lists the cross sections for the individual channels. At low energies charge transfer occurs largely into the C^{2+} $1s^22p^2\,{}^1S$ and C^{2+} $1s^22s3s\,{}^3S$ states but with increasing energy all four states are significant. The rapid increase above 250 eV implied by the low- and high-energy cross-section measurements is mostly attributable to the ${}^3S$ capture cross section which passes through a minimum at 250 eV and then increases out to 5 keV.

The detection of emissions from the charge transfer states would be a valuable test of the theoretical predictions of the cross sections for the different channels.[5]

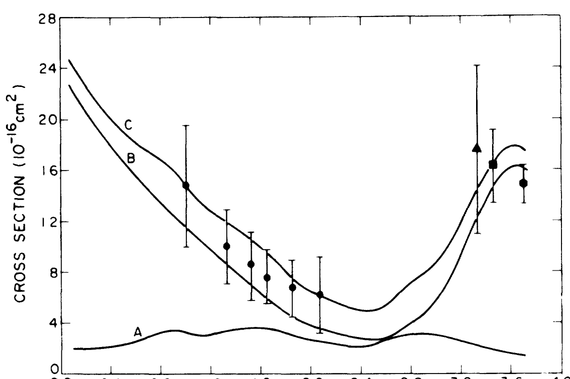

FIG. 1. Cross sections $\frac{1}{4}\sigma_0(E)$, $\frac{3}{4}\sigma_1(E)$, and their sum, $\sigma(E)$, for $C^{3+}+H \rightarrow C^{2+}+H^+$ as a function of the impact energy in eV/amu. Curve (A) refers to the calculated ${}^1\Sigma^+$ cross-section sum, curve (B) to the ${}^3\Sigma^+$ cross-section sum, and curve (C) to the calculated total charge transfer cross section. The experimental points ●, ▲, ■, and ● refer to the total charge-transfer cross section $\sigma(E)$ presented in Refs. 1–4, respectively.

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