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Charge transfer of N^{3+} ions in collisions with atomic hydrogen

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Cross sections are calculated for the charge transfer of N^{3+} ions in collisions with atomic hydrogen at impact energies up to 5 keV/amu. The calculated cross sections exceed the values measured between 860 and 5080 eV/amu by about 20%. The charge-transfer process results in the emission of extreme-ultraviolet radiation at 45 nm whose detection would serve as a measure of the detailed mechanism by which charge transfer proceeds.

Charge transfer is an important process in high-temperature plasmas into which neutral atoms are injected. We have previously described calculations for collisions of C^{3+} (Ref. 1) and O^{3+} (Ref. 2) ions at energies up to 5 keV/amu with atomic hydrogen and compared the results with experimental data. Measurements of charge-transfer cross sections for N^{3+} ions in collisions with H atoms at center-of-mass impact energies above 857 eV have been reported by Phaneuf, Meyer, and McKnight,[3] Crandall, Phaneuf, and Meyer,[4] and Seim, Muller, Wirkner-Bott, and Salzborn.[5] We present here cross sections calculated by *ab initio* quantal methods for energies up to 5 keV and compare them with the experimental data. Our calculations indicate that charge transfer leads to the emission of spectral lines whose intensities provide a detailed probe of the charge-transfer mechanisms.

At low energies, the charge-transfer process can be described as a transition between electronic states of the quasimolecule NH^{3+}. The approach of ground-state N^{3+} ions and ground-state H atoms produces $^2\Sigma^+$ molecular states which undergo avoided crossings with curves of the same symmetry separating to N^{2+} + H^+. Using *ab initio* configuration-interaction methods,[6] Heil, Butler, and Dalgarno[7] have calculated the adiabatic interaction potentials $\epsilon_i(R)$ and the matrix elements of the nuclear momentum operator $A_{ij}(R)$ which couples the adiabatic $^2\Sigma^+$ molecular states of NH^{3+}. Starting with these potentials and coupling matrix elements, they[7] performed a unitary transformation to a diabatic basis chosen so that the coupling matrix elements of $\underline{C}^{-1}(R)\underline{A}(R)\underline{C}(R)$ vanish.[8] The diabatic nuclear eigenfunctions satisfy the set of coupled equations[8]

$$\left[\frac{1}{2\mu}\nabla_R^2\underline{I}-\underline{V}(R)+E\underline{I}\right]\underline{F}^d(\vec{R})=\underline{0}\ , \tag{1}$$

where μ is the reduced mass of the colliding system, and $\underline{V}(R)=\underline{C}^{-1}(R)\underline{\epsilon}(R)\underline{C}(R)$ is a diabatic potential matrix whose diagonal elements are potential-energy surfaces, and whose off-diagonal elements drive transitions between molecular states of the same symmetry. Equation (1) was solved by expanding $\underline{F}^d(\vec{R})$ in an orthonormal set of total angular momentum eigenfunctions and the resulting coupled differential equations

$$\left[\frac{d^2}{dR^2}+2\mu E-\frac{J(J+1)}{R^2}\right]\underline{I}\underline{f}^J(R)-2\mu\underline{V}(R)\underline{f}^J(R)=\underline{0} \tag{2}$$

were integrated numerically from threshold energies to 10 eV,[7] a procedure which becomes impractical at high energies. We use here a unitarized, multichannel distorted-wave approximation[1,9] which can be carried through readily to second order in the coupling strength to extend these calculations to energies of 5 keV. This distorted-wave approximation[1,9] improves rapidly in accuracy as the energy of relative motion and the nuclear angular momentum quantum number J increase. For a given value of E, close-coupling results were obtained for low values of the angular momentum J, unitarized 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 became sufficiently accurate. The procedure gives results which are identical to those obtained from a complete close-coupled solution of the scattering equations. The cross sections are expressed as summations

$$\sigma(E)=\frac{\pi}{k_i^2}\sum_j\sum_J(2J+1)|S_{ij}^J|^2\ , \tag{3}$$

where k_i is the wave number of relative motion in the entrance channel and S_{ij}^J is the scattering matrix element connecting the initial state i formed by the approach of N^{3+} and H to a final state j formed by charge transfer and separating to N^{2+} and H^+.

The adiabatic potential-energy functions and coupling matrix elements which determine the charge transfer of N^{3+} with H at low and intermediate energies have been given by Heil *et al.*[7] Only those states were retained for which the adiabatic radial coupling is strong. The $^2\Sigma^+$ symmetry involves four molecular states, the entrance channel, and product channels dissociating, respectively, to $N^{2+}(2s2p^2,\ ^2D)+H^+$, $N^{2+}(2s2p^2,\ ^2S)$ + H^+, and to N^{2+} ($2s^23s,\ ^2S$) + H^+. Several avoided crossings occur, each of which is associated with a peak in one of the adiabatic coupling elements. The transformation to a diabatic basis maps the complex behavior of the adiabatic coupling elements into a set of much simpler diabatic coupling functions.[7]

With the omission of momentum translation factors,[10] the coupling matrix elements, the transformation matrix, and the diabatic interaction matrix depend upon the origin of coordinates. The dependence is weak in cases where the coupling between the adiabatic states is localized at avoided crossings. Charge transfer of N^{3+} in H is such a case, as has been demonstrated by Gargaud, Hansen, McCarroll, and Valiron[11] by explicit calculations of the cross sections at

TABLE I. Cross section in 10^{-16} cm^2 for $N^{3+} + H \rightarrow N^{2+}(2s2p^2,\ ^2D;\ 2s2p^2,\ ^2S;\ 2s^23s,\ ^2S) + H^+$. 5.04($-$11) is an abbreviated notation for 5.04×10^{-11}.

Center-of-mass energy	Channel			
	$(2s2p^2,\ ^2D)$	$(2s2p^2,\ ^2S)$	$(2s^23s,\ ^2S)$	Total
0.278	5.04(−11)	1.34(−6)	9.41	9.41
1.50	5.32(−11)	5.60(−5)	21.5	21.5
3.91	1.37(−9)	1.34(−3)	29.1	29.1
8.10	8.96(−8)	3.00(−2)	33.3	33.3
10	· · ·	6.52(−2)	33.9	33.9
25	1.50(−5)	0.375	34.2	34.6
50	1.50(−4)	0.706	33.2	33.9
75	7.60(−4)	0.902	31.4	32.3
125	4.50(−3)	1.14	29.1	30.3
250	2.20(−2)	1.41	26.2	27.6
500	8.37(−2)	1.50	24.4	26.0
1000	0.176	1.29	24.3	25.8
2000	0.220	1.17	23.5	24.9
5000	0.324	0.757	19.3	20.4

center-of-mass energies up to 136 eV for different choices of origin.

Table I lists the calculated cross sections for the individual final states of N^{2+}. Our calculation indicates that the charge transfer occurs almost exclusively into $N^{2+}(2s^23s,\ ^2S)$, for which the crossing with the entrance channel occurs at $8.8a_0$. The cross section reaches a maximum of 34×10^{-16} cm^2 at 25 eV and is relatively flat thereafter, having decreased to 19×10^{-16} cm^2 at 5 keV. The next largest cross section is that for capture into $N^{2+}(2s2p^2,\ ^2S)$, which is negligible at low energies and increases to about 4% of the total by 5 keV. The cross section for capture into $N^{2+}(2s2p^2,\ ^2D)$ increases rapidly with energy above 25 eV but its magnitude remains less than 2% of the total out to 5 keV.

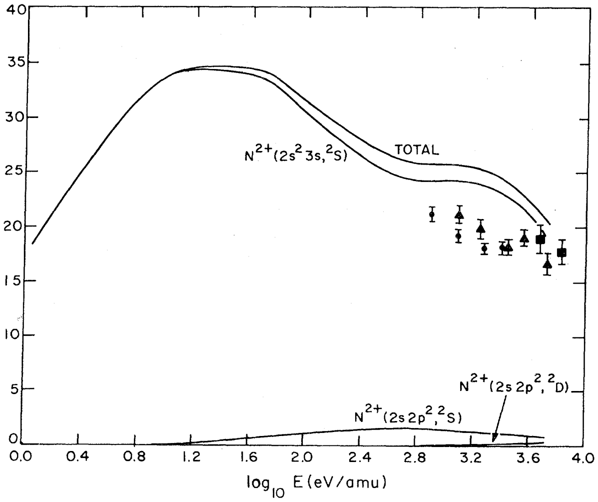

FIG. 1. Cross sections for the charge-transfer processes $N^{3+} + H \rightarrow N^{2+}(2s2p^2,\ ^2D;\ 2s2p^2,\ ^2S;\ 2s^23s,\ ^2S) + H^+$, labeled by the final N^{2+} state. Their sum is labeled "total." The experimental data are Δ [Crandall *et al.* (Ref. 4)], ■ [Phaneuf *et al.* (Ref. 3)], ● [Seim *et al.* (Ref. 5)].

Gargaud *et al.*[11] have carried out similar calculations up to center-of-mass energies of 136 eV. They used a model potential method to calculate the adiabatic potential energies and coupling matrix elements and included the $^2\Sigma^+$ molecular states separating to H^+ and N^{2+} $(2s^23s,\ ^2S)$, $N^{2+}(2s^23p,\ ^2P^0)$, and $N^{2+}(2s^23d,\ ^2D)$. Their method is not suitable for the inclusion of the states separating to $N^{2+}(2s2p^2,\ ^2S)$ and $N^{2+}(2s2p^2,\ ^2D)$. Christensen, Watson, and Blint[12] and Watson and Christensen[13] had earlier carried out two-state calculations including in the final states only the state separating to $N^{2+}(2s^23s,\ ^2S)$ and restricted to energies below 7 eV.

Figure 1 compares the individual and the total calculated cross sections with the data of Phaneuf *et al.*,[3] Crandall *et al.*,[4] and Seim *et al.*[5]

The calculated cross sections exceed at all energies the cross sections obtained from the ion beam measurements between 857 and 5000 eV. The differences are about 20%, which is well within the theoretical uncertainties. The beam may contain metastable $N^{3+}(2s3p,\ ^3P)$ ions but they are probably as reactive as the ground-state ions and are unlikely to be the cause of the discrepancies.

A valuable diagnostic probe of the charge-transfer mechanism and of the probable contribution from metastable species is provided by the spectral lines emitted by the product ions. Capture into the $(2s^23s,\ ^2S)$ level of N^{2+} is followed by the emission of a doublet at 45.187 and 45.223 nm.

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