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Interaction Cross Section of C_S^+ Ions

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August 11, 1976

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Interaction Cross Section of C_S^+ Ions

J. R. Hiskes

Abstract

Some estimates of the shape of C_S ion and C_S atom interaction potentials suggests that the $C_S^+ + C_S^+$ charge transfer cross section may be less than 10^{-15} cm^2 .

In the selection of an ion for use in a heavy-ion-pellet-fusion system, care must be taken such that the ion selected not have charge-changing reactions with like ions during the storage time. More specifically, what is desired is a singly charged positive ion of large mass ($A > 120$) with a charge-changing cross section no greater than 10^{-15} cm^2 for relative kinetic energies less than 100 keV (500 eV per nucleon). Presented in this note are some considerations relevant to the C_S^+ ion, developments which are an extension of some earlier ideas presented by Y. K. Kim pertaining to the U^+ ion.

At these low energies per nucleon the charge transfer cross section

is determined by the intersection of the interaction potentials of the ions on the left and on the right, respectively. At large separations the ions on the left in reaction (1) interact through coulomb and polarization forces. The polarizability of the C_S^+ ion is equal¹ to $18.8a_0^3$. Expressed in atomic units (energy units = $e^2/a_0 = 27.2 \text{ eV}$; lengths in a_0) the interaction potential at large separations is

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$$V(R) = \frac{1}{R} - \frac{18.8}{R^4} \quad (2)$$

As the ions move close together the polarization forces increase until the outermost electrons are near to being stripped off, at which point the polarization forces become saturated. The closed shell configuration of the C_s^+ is somewhat larger than a_0 , and with an ionization potential of 25.1 eV. The dimensions are somewhat larger than that of the hydrogen atom, but the ionization potential is also larger; the electric field for stripping is expected to be comparable to that for the ground state of hydrogen,² i.e. $\mathcal{E} \approx 3 \times 10^8$ Volts/cm. For this stripping field the polarization forces saturate near $R = 4$.

At small separations the potential is expected to show the hard-core interaction of the $X_e - X_e$ closed shell configurations. These potentials have been derived from scattering data by Amdur and Mason³, and calculated by M. Gardner and A. Karo⁴, for $R \geq 5$. For closer separations, the hard core potential is assumed to have the form

$$V_{\text{CORE}}(R) = 0.0897 \left(\frac{5}{R}\right)^8, \quad (3)$$

suggested by reference (3). The total interaction potential, including the terms in (2) and (3) and with the polarization term saturating at $R = 4$, is shown in the figure.

In the case of the cesium atom the polarizability is large,⁵ $403a_0^3$, but saturates at much larger ion-atom separations. The outer regions of the C_s wavefunction are closely approximated by a $H(2s)$ function⁶; the ionization potentials are 3.89 and 3.4 eV, respectively. It follows that the electric

stripping field² for $C_S(6s)$ is close to that for $H(2s)$, $\mathcal{E}^0 = 3 \times 10^7$ Volts/cm. In the presence of a C_S^{++} ion, saturation and stripping of C_S occur at $R = 17$; for interatomic spacings closer than this the electron passes from the atom to the ion and the coulomb part of the interaction potential for the reactants on the right hand side of reaction (1) becomes equal to $1/R$.

For these close-in separations at least one of the electrons must be in an excited state and we would expect the hard core to be "softer" than in the previous case. Ignoring the hard core entirely, the potential is shown in the figure and labeled as a π state.

Taking the intersection point as the interaction radius would suggest a reaction cross section equal to $1.2 \times 10^{-15} \text{ cm}^2$. But the crossing is a σ - π crossing, and although rotational couplings will contribute to a transition, the transition probability is expected to be small.

The first excited state of C_S can couple with the ground state of C_S^{++} to form a σ state. The polarization and core considerations here are similar to those for the π state. The potential shown in the figure gives rise to a σ - σ crossing at essentially the same radius.

At the σ - σ crossing the transition probability is most likely to be no smaller than one-tenth but no larger than one-half, to give an interaction cross section less than 10^{-15} cm^2 .

The $C_S^+ + C_S^+$ system can easily be handled using conventional Hartree-Fock molecular orbital codes. The availability of such potentials and electronic functions would make possible the direct calculation of the charge transfer cross section.

The inverse reaction,

would be expected to be appreciably larger than reaction (1). Many of the excited states of C_S^+ lie close to the $C_S^{++} + C_S$ potential curve and several may cross at larger inter-nuclear separations. These excited states are indicated schematically by the dotted curve in the figure.

REFERENCES

1. R. M. Sternheimer, Phys. Rev. 115, 1198 (1959).
2. D. S. Bailey, J. R. Hiskes, and A. C. Riviere, Nuclear Fusion 5, 41 (1965).
3. I. Amdur and E. A. Mason, J. Chem. Phys. 23, 624 (1956).
4. M. Gardner and A. Karo, Lawrence Livermore Laboratory Biannual Status Report VIII-2, Chemical Modeling Group, December, 1973.
5. R. W. Molof, H. L. Schwartz, T. M. Miller, and B. Bederson, Phys. Rev. A10, 1131 (1974).
6. J. W. Gadzuk, Surface Science 6, 133 (1967).

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GEORGE EASTMAN COMPANY, RUTHERFORD, N.J.

Inverse γ_{10M} Energy (Atomic Units, 27.2 eV)

2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0

R , (atomic units, a_0)

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