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CROSS SECTIONS FOR THE DISSOCIATION OF H_2^+ AND D_2^+ BY A VACUUM CARBON ARC

R. G. Alsmiller, Jr.

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Neutron Physics Division

CROSS SECTIONS FOR THE DISSOCIATION OF H_2^+ and D_2^+ BY A VACUUM CARBON ARC

R. G. Alsmiller, Jr.

Date Issued

OCT 6 1959

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ABSTRACT

The cross section for the dissociation of the H_2^+ and D_2^+ molecule by a particle of charge ze is calculated. The calculation is carried out in Born approximation using exact two-center wave functions, the Frank-Condon principle, and a classical average over molecular orientations.

The cross section is compared with the cross section calculated by Ivash[1] using L.C.A.O. wave functions and it is found that the two cross sections are in good agreement over the entire velocity range considered.

The calculated results are compared with experimental results obtained from the dissociation of H_2^+ and D_2^+ by a vacuum carbon arc. The theoretical and experimental results are found to agree within a factor of two.

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1. E. V. Ivash, Phys. Rev. 112, 155 (1958).

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I. INTRODUCTION

An essential feature of the ORNL thermonuclear apparatus is the dissociation of the deuteron molecular ion by a carbon arc. The mechanism of this dissociation is uncertain. However, recent experimental results indicate that there is a significant amount of highly ionized carbon in the arc and the possibility exists that the dissociation may be caused by these highly charged ions. To test this hypothesis a calculation of the dissociation cross section has been carried out.

A calculation of the cross section for the dissociation of H_2^+ and D_2^+ by a heavy particle of charge ze has previously been given by Ivash.[1] In this calculation only the excitation to the lowest lying repulsive state, $2p\sigma_\mu$, was included and approximate electronic wave functions (i.e., L.C.A.O. wave functions) were used.

In the present work calculations very similar to those of Ivash are carried out. The only significant difference is that contributions from the $2p\sigma_\mu$ and $2p\pi_\mu$ states are included and exact two-center wave functions are used. The calculations are done in Born approximation; the Frank-Condon principle is assumed throughout; and a classical average over molecular orientations is used.

II. EXPRESSION FOR THE CROSS SECTION

In this section we wish to obtain an expression for the dissociation cross section suitable for numerical computation. Since, in the approximation we use, the cross sections for D_2^+ and H_2^+ are the same we shall no longer specify which molecule we are considering.

Treating the molecular nuclei as fixed, the cross section for the excitation of the molecule from an initial state i to a final state f by a particle of charge ze (e = magnitude of electronic charge) may be written in Born approximation as (using atomic units, i.e., $\hbar = m = e = 1$)

$$\sigma_{fi} = \left(\frac{\mu_R}{2\pi}\right)^2 \frac{K_f}{K_i} \int \left|V_{fi}\right|^2 d\Omega_f \tag{1}$$

$$V_{fi} = \int e^{-i\vec{K}_f\cdot\vec{R}} \psi_f^*(\vec{r}) \frac{z}{\left|\vec{R} - \vec{r}\right|} e^{i\vec{K}_i\cdot\vec{R}} \psi_i(\vec{r}) d\vec{R} d\vec{r} \tag{2}$$

where

$\vec{K}_f, \vec{K}_i$ = wave vectors of outgoing and incident particle, respectively,

$d\Omega_f$ = differential solid angle of $\vec{K}_f$ with respect to $\vec{K}_i$,

μ_R = reduced mass of incident particle with respect to molecule,

ψ_f, ψ_i = final and initial wave functions of the molecular electron.

From the conservation of energy we have

$$K_f^2 = K_i^2 - 2\mu_R \Delta E_{fi} \tag{3}$$

where

ΔE_{fi} = excitation energy of molecule.

In Eq. (2) the interaction energy between the incident particle and the molecular nuclei has been omitted because of the orthogonality of the electronic wave functions.

Equation (1) gives the total cross section for the excitation of a given state of the molecule when the molecular axis has a given orientation with respect to $\vec{K}_i$. We assume that all orientations of the molecule are equally likely and define $\bar{\sigma}_{fi}$ by averaging over all direction of the molecular axis, $\vec{a}$, with respect to $\vec{K}_i$. This is, of course, the same as averaging over all direction of $\vec{K}_i$ with respect to $\vec{a}$ so we have

$$\bar{\sigma}_{fi} = \frac{1}{4\pi} \int \sigma_{fi} d\Omega_i \tag{4}$$

where

$d\Omega_i$ = differential solid angle of $\vec{K}_i$ with respect to $\vec{a}$.

The quantity $\bar{\sigma}_{fi}$ is now the total excitation cross section to the state f; if f is not a bound state for the molecule it may be identified with the contribution to the dissociation cross section from the state f. Finally the total dissociation cross section, $\bar{\sigma}_T$, may be written

$$\bar{\sigma}_T = \sum_f \bar{\sigma}_{fi} \tag{5}$$

where the sum includes only those states of the molecule which are not bound and the bar is used to indicate that a classical average over molecular orientations has been performed.

To evaluate the cross section we must specify the form of the wave functions. We use exact two-center wave functions which may be written in the form[2]

$$\psi_{n\lambda\mu} = N_{n\lambda\mu} X_{n\lambda\mu}(\xi) M_{\mu\lambda}(\eta) \begin{Bmatrix} \cos \mu\phi \\ \sin \mu\phi \end{Bmatrix} \tag{6}$$

where

n, λ, μ = quantum numbers which replace the subscripts f,i;

$n = 1,2\ldots,\ \lambda = 0,1\ldots,\ \mu = 0,1\ldots\lambda,$

ξ, η, ϕ = prolate spheroidal coordinates[3]

$N_{n\lambda\mu}$ = normalizing constant.

The function $X_{n\lambda\mu}(\xi)$ and $M_{\mu\lambda}$ are quite complicated and will not be reproduced here.[2] The normalization is such that

---

2. D. R. Bates, K. Ledsham, and A. L. Stewart, Royal Society of London Phil. Trans. 246, 215 (1953-1954).
3. P. M. Morse and H. Feshbach, Methods of Theoretical Physics, McGraw-Hill Book Company, Inc., New York (1953) p. 661.

$$N_{n\lambda\mu} = \left[\int_1^{\infty} \int_{-1}^{1} \int_0^{2\pi} X^2_{n\lambda\mu}(\xi) M^2_{\mu\lambda}(\eta) \begin{Bmatrix} \cos^2 \mu\phi \\ \sin^2 \mu\phi \end{Bmatrix} (\xi^2 - \eta^2) d\xi d\eta d\phi \right]^{-1/2} \tag{7}$$

In the present notation the ground state of the molecule, $1s\sigma_g$, is written

$$\psi_i = \psi_{100} = N_{100} X_{100}(\xi) M_{00}(\eta) \tag{8}$$

To evaluate the matrix element we first carry out the integration over $\vec{R}$ to obtain

$$V_{fi} = \frac{4\pi}{K^2} z \int e^{i\vec{K}\cdot\vec{r}} \psi^*_{n\lambda\mu}(\vec{r}) \psi_{100}(\vec{r}) d\vec{r} \tag{9}$$

where

$$\vec{K} = \vec{K}_i - \vec{K}_f.$$

We next expand $e^{i\vec{K}\cdot\vec{r}}$ in prolate spheroidal wave functions as[4,5]

$$e^{i\vec{K}\cdot\vec{r}} = 2 \sum_{\ell=0}^{\infty} \sum_{m=0}^{\ell} \frac{\epsilon_m i^\ell}{\Lambda_{m\ell}(h)} S_{m\ell}(h, \cos\theta_K) S_{m\ell}(h, \eta) \tag{10}$$

$$\cos m(\phi - \phi_K) j e_{m\ell}(h, \xi)$$

where

$h = (1/2)\, aK$,

a = distance between molecular nuclei,

θ_K, ϕ_K = polar angles of $\vec{K}$ with respect to $\vec{a}$,

---

4. P. M. Morse and H. Feshbach, op. cit., p. 1508.
5. J. A. Stratton, P. M. Morse, L. J. Chu, J. D. C. Little, F. J. Corbato, Spheroidal Wave Functions, The Technology Press of MIT and John Wiley and Sons, Inc., New York (1956).

$\epsilon_m = 1$ for $m = 0$

$= 2$ for $m \neq 0$,

$\Lambda_{m\ell}(h)$ = normalizing constant,[6]

$S_{m\ell}$ = linear combination of associated Legendre functions,*[7]

$je_{m\ell}$ = linear combination of spherical Bessel functions.[8]

Substituting in Eq. (9) from Eqs. (6), (8), and (10), we have

$$V_{fi} = \frac{4\pi z}{K^2} N_{n\lambda\mu} N_{100}\, 2 \sum_{m,\ell} \frac{\epsilon_m\, i^{\ell}}{\Lambda_{m\ell}(h)} \tag{11}$$

$$\int_1^{\infty} \int_{-1}^{1} \int_0^{2\pi} S_{m\ell}(h, \cos\theta_K) \cos m(\phi - \phi_K) \begin{Bmatrix} \cos \mu\phi \\ \sin \mu\phi \end{Bmatrix} S_{m\ell}(h,\eta) M_{\mu\lambda}(\eta) M_{00}(\eta)$$

$$je_{m\ell}(h,\xi) X_{n\lambda\mu}(\xi) X_{100}(\xi)(\xi^2 - \eta^2)\, d\phi\, d\eta\, d\xi$$

and carrying out the integration over ϕ

$$V_{fi} = \frac{4\pi z}{K^2} N_{n\lambda\mu} N_{100}\, 2 \sum_{\ell} \frac{\epsilon_\mu\, i^{\ell}}{\Lambda_{\mu\ell}(h)} S_{\mu\ell}(h, \cos\theta_K) \tag{12}$$

$$\int_1^{\infty} \int_{-1}^{1} S_{\mu\ell}(h,\eta) M_{\mu\lambda}(\eta) M_{00}(\eta) \begin{Bmatrix} \cos \mu\phi_K \\ \sin \mu\phi_K \end{Bmatrix} \pi 2 \delta_{\mu o}$$

$$je_{\mu\ell}(h,\xi) X_{n\lambda\mu}(\xi) X_{100}(\xi)(\xi^2 - \eta^2)\, d\eta\, d\xi.$$

---

*The functions $S_{m\ell}$ and $M_{\mu\lambda}$ are essentially the same functions evaluated at different values of the parameters involved in their definition.

6. Morse and Feshbach, op. cit., p. 1505.
7. Morse and Feshbach, op. cit., p. 1503.
8. Morse and Feshbach, op. cit., p. 1505.

Taking the absolute square we have

$$\left|V_{fi}\right|^2 = \left(\frac{4\pi z}{K^2}\right)^2 N^2_{n\lambda\mu} N^2_{100} 2^2 (\epsilon_\mu 2^{\delta_{\mu o}})^2 \sum_{\ell\ell'} \frac{i^{\ell}(-i)^{\ell'}}{\Lambda_{\mu\ell}(h)\Lambda_{\mu\ell'}(h)} \tag{13}$$

$$\int_1^\infty \int_1^\infty \int_{-1}^1 \int_{-1}^1 S_{\mu\ell}(h, \cos\theta_K) S_{\mu\ell'}(h, \cos\theta_K) \begin{Bmatrix} \cos^2 \mu\phi_K \\ \sin^2 \mu\phi_K \end{Bmatrix} \pi^2$$

$$S_{\mu\ell}(h,\eta) M_{\mu\lambda}(\eta) M_{00}(\eta)$$

$$S_{\mu\ell'}(h,\eta') M_{\mu\lambda}(\eta') M_{00}(\eta')$$

$$je_{\mu\ell}(h,\xi) X_{n\lambda\mu}(\xi) X_{100}(\xi)$$

$$je_{\mu\ell'}(h,\xi') X_{n\lambda\mu}(\xi') X_{100}(\xi')(\xi^2 - \eta^2)(\xi'^2 - \eta'^2)\, d\eta d\eta' d\xi d\xi'$$

where we have explicitly used the fact that the functions involved are real.[5]

We now substitute the above expression for the matrix element into Eqs. (4) and (1). Integration over $d\Omega_i\, d\Omega_f$ is most easily done by noting that it is equivalent to integrating over $d\Omega_K\, d\Omega_f$, where $d\Omega_K$ is the differential solid angle of $\vec{K}$ with respect to $\vec{a}$; i.e., $d(\cos\theta_K) d\phi_K$. Thus

$$\bar{\sigma}_{fi} = \left(\frac{\mu_R}{2\pi}\right)^2 \frac{K_f}{K_i} \frac{1}{4\pi} \int \left|V_{fi}\right|^2 d(\cos\theta_K) d\phi_K d\Omega_f \tag{14}$$

$$= \mu_R^2 \frac{K_f}{K_i} (4\pi z)^2 N_{n\lambda\mu}^2 N_{100}^2 \sum_{\ell} \frac{1}{\Lambda_{\mu\ell}(h)} \begin{Bmatrix} 2^{\delta_{\mu o}} \\ 1 - \delta_{\mu o} \end{Bmatrix}$$

$$\int \frac{d\Omega_f}{K^4} \left[\int_1^{\infty} \int_{-1}^{1} S_{\mu\ell}(h,\eta) M_{\mu\lambda}(\eta) M_{00}(\eta) \right.$$

$$\left. j e_{\mu\ell}(h,\xi) X_{n\lambda\mu}(\xi) X_{100}(\xi)(\xi^2 - \eta^2) d\eta d\xi \right]^2$$

where we have used[9]

$$\int_{-1}^{1} S_{\mu\ell}(h, \cos\theta_K) S_{\mu\ell'}(h, \cos\theta_K) d(\cos\theta_K) = \delta_{\ell\ell'} \Lambda_{\mu\ell}(h) \tag{15}$$

$$\epsilon_\mu 2^{\delta_{\mu o}} = 2 \text{ for all } \mu. \tag{16}$$

The integrand is not a function of $d\phi_f$ and the integration over $d(\cos\theta_f)$ may be changed to an integration over dK since

$$K^2 = K_i^2 + K_f^2 - 2K_i K_f \cos\theta_f \tag{17}$$

$$2KdK = -2K_i K_f d(\cos\theta_f).$$

Then adding the contribution from the two degenerate states we have

---

9. Morse and Feshbach, op. cit., p. 1503.

$$\bar{\sigma}_{fi} = \frac{1}{v^2} (4\pi)^3 z^2 N^2_{n\lambda\mu} N^2_{100} \int_{K_i-K_f}^{K_i+K_f} \frac{dK}{K^3} \sum_{\ell} \frac{1}{\Lambda_{\mu\ell}(h)} \tag{18}$$

$$\left[\int_1^{\infty} \left[T'_{\mu\ell\lambda}\xi^2 - U'_{\mu\ell\lambda} \right] je_{\mu\ell}(h,\xi) X_{n\lambda\mu}(\xi) X_{100}(\xi) d\xi \right]^2$$

where

$v \left(= \frac{K_i}{\mu_R} \right)$ = relative velocity of colliding particles

and

$$T'_{\mu\ell\lambda} = \int_{-1}^{1} S_{\mu\ell}(h,\eta) M_{\mu\lambda}(\eta) M_{00}(\eta) d\eta \tag{19}$$

$$U'_{\mu\ell\lambda} = \int_{-1}^{1} S_{\mu\ell}(h,\eta) M_{\mu\lambda}(\eta) M_{00}(\eta) \eta^2 d\eta.$$

From the form of the functions $S_{\mu\ell}(h,\eta)$ and $M_{\mu\lambda}(h,\eta)$ it is quite easy to show that

$$S_{\mu\ell}(h,\eta) = (-1)^{\ell+\mu} S_{\mu\ell}(h,-\eta) \tag{20}$$

$$M_{\mu\lambda}(\eta) = (-1)^{\lambda+\mu} M_{\mu\lambda}(-\eta)$$

and thus

$$\left.\begin{aligned} T'_{\mu\ell\lambda} &= 0 \\ U'_{\mu\ell\lambda} &= 0 \end{aligned}\right\} \quad \text{if } \ell + \lambda \text{ is odd.} \tag{21}$$

Letting

$$T_{\mu\ell\lambda} = \int_0^1 S_{\mu\ell}(h,\eta)M_{\mu\lambda}(\eta)M_{00}(\eta)d\eta \tag{22}$$

$$U_{\mu\ell\lambda} = \int_0^1 S_{\mu\ell}(h,\eta)M_{\mu\lambda}M_{00}(\eta)\eta^2 d\eta$$

we have

$$\left.\begin{aligned} T'_{\mu\ell\lambda} &= 2T_{\mu\ell\lambda} \\ U'_{\mu\ell\lambda} &= 2U_{\mu\ell\lambda} \end{aligned}\right\} \quad \text{if } \ell + \lambda \text{ is even.} \tag{23}$$

Then

$$\bar{\sigma}(1s\sigma \rightarrow n\lambda\mu) = N^2_{n\lambda\mu}N^2_{100}(4\pi)^3 \frac{4z^2}{v^2} \int_{K_i-K_f}^{K_i+K_f} \frac{dK}{K^3} \sum_{\ell=0}^{\infty} \frac{1}{\Lambda_{\mu,\alpha+2\ell}(h)} \tag{24}$$

$$\left[\int_1^{\infty} \left[T_{\mu,\alpha+2\ell,\lambda}\xi^2 - U_{\mu,\alpha+2\ell,\lambda}\right] je_{\mu,\alpha+2\ell}X_{n\lambda\mu}(\xi)X_{100}(\xi)d\xi\right]^2 \qquad \begin{aligned} &\alpha = 0 \text{ for even } \lambda \\ &\alpha = 1 \text{ for odd } \lambda. \end{aligned}$$

Equation (24) is now the contribution to the dissociation cross section from the state $n\lambda\mu$. In the case when $\mu \geq 1$ the contribution from the two degenerate states are included in Eq. (24).

III. NUMERICAL CALCULATIONS

Equation (24) is the expression used in the numerical calculations. The equilibrium separation distance for the molecular nuclei, a, was taken to be two Bohr radii throughout the calculations.

The terms in the sum over ℓ were obtained using an IBM 704. The spheroidal functions needed were computed from the coefficients given by Stratton and his coworkers,[5] and the wave functions were computed from the coefficients given by Bates.[3] The series converged quite rapidly and it was found that only four or five terms were needed to obtain sufficient accuracy.

Once the sum over ℓ was carried out the final integration over K was done with the aid of a planimeter. The use of the planimeter necessarily introduced slight inaccuracies in the final result, but on the other hand, the use of the planimeter resulted in an appreciable saving in machine time. The limits on the K integration may be obtained from

$$K_f^2 = K_i^2 \left[1 - \frac{2\mu_R \Delta E_{fi}}{K_i^2} \right]$$

and if

$$\frac{2\mu_R \Delta E_{fi}}{K_i^2} = \frac{\Delta E_{fi}}{\frac{1}{2}\mu_R v^2} << 1 \tag{25}$$

$$K_i - K_f \simeq \frac{\Delta E_{fi}}{v} \tag{26}$$

$$K_i + K_f \simeq 2K_i = 2\mu_R v \tag{27}$$

The approximation, Eq. (25), is quite good for the range of velocities we consider and thus Eqs. (26) and (27) may be used. Furthermore the integrand in the K integration goes to zero quite rapidly as K increases and for practical computation the integral may be cut off at a value $K << 2\mu_R v$.

This means that the cross section is essentially a function of the velocity only.

IV. RESULTS AND COMPARISON WITH EXPERIMENT

Calculations have been made for the $1s\sigma_g \rightarrow 2p\sigma_\mu$ and $1s\sigma_g \rightarrow 2p\pi_\mu$ transitions for a velocity range of from 1×10^8 cm/sec to 7.5×10^8 cm/sec. However, the Born approximation can be expected to give reasonably reliable results only at the largest of these velocities and probably fails quite badly at the lower velocities.

It should be noted that the $2p\pi_\mu$ state is really a bound state for the molecule[10] and contributes to the dissociation cross section only because we use the Frank-Condon principle. However, the binding is quite weak and occurs at such a large nuclear separation that unless the Frank-Condon principle is violated badly one can expect transitions to this state to lead to dissociation.

Transitions to the next few excited states were not calculated because the dipole matrix elements either vanish or are very small;[10] and thus, these states can not be expected to contribute appreciably to the cross section.

The results of the calculations are given in Table 1 and shown in Figs. 1 and 2. In all cases we give the cross section divided by z^2.

In Fig. 1 the cross section for the $1s\sigma_g$ - $2p\sigma_\mu$ transition is plotted as calculated here and as calculated by Ivash[1] using L.C.A.O. wave functions. The two curves are very nearly the same over the entire velocity range, thus justifying the use of the approximate wave functions.

In Fig. 2 the cross sections for the two transitions considered and the total cross section is shown.

We now wish to determine whether the cross section calculated here is adequate to explain the observed dissociation of the H_2^+ and D_2^+ molecules by the carbon arc. From the relation

---

10. D. R. Bates, R. T. S. Darling, S. C. Hawe, A. L. Stewart, Phys. Soc. of London, Proceedings 66, 1124 (1953), 67, 533 (1954).

Table 1

$v \cdot 10^8 \frac{cm}{sec}$	$\frac{\bar{\sigma}}{z^2} \cdot 10^{-16}$ cm^2 $1s\sigma_g \rightarrow 2p\sigma_\mu$	$\frac{\bar{\sigma}}{z^2} \cdot 10^{-16}$ cm^2 $1s\sigma_g \rightarrow 2p\pi_\mu$	$\frac{\bar{\sigma}_T}{z^2} \cdot 10^{-16}$ cm^2
.865	1.89	.10	1.99
1.057	2.37	.26	2.63
1.359	2.37	.40	2.77
2.106	1.93	.58	2.51
3.172	1.29	.56	1.85
5.360	.666	.372	1.04
7.579	.420	.251	.671

$$e^{-d \sum_i n_i \bar{\sigma}_{Ti}} = 1 - \beta$$

we have

$$\left(\frac{\bar{\sigma}_T}{z^2}\right) = \frac{1}{d \sum_i n_i z_i^2} \ln\left[\frac{1}{1 - \beta}\right] \tag{28}$$

where

n_i = density of ith kind of carbon ions,

z_i = charge number of ith kind of carbon ion,*

d = path length (= 2 cm),

β = breakup efficiency,

$\left(\frac{\bar{\sigma}_T}{z^2}\right)$ = cross section required to explain observed dissociation.

*In assigning these charge numbers we assume perfect screening, i.e., for c^{+++} we use $z = 3$, etc.

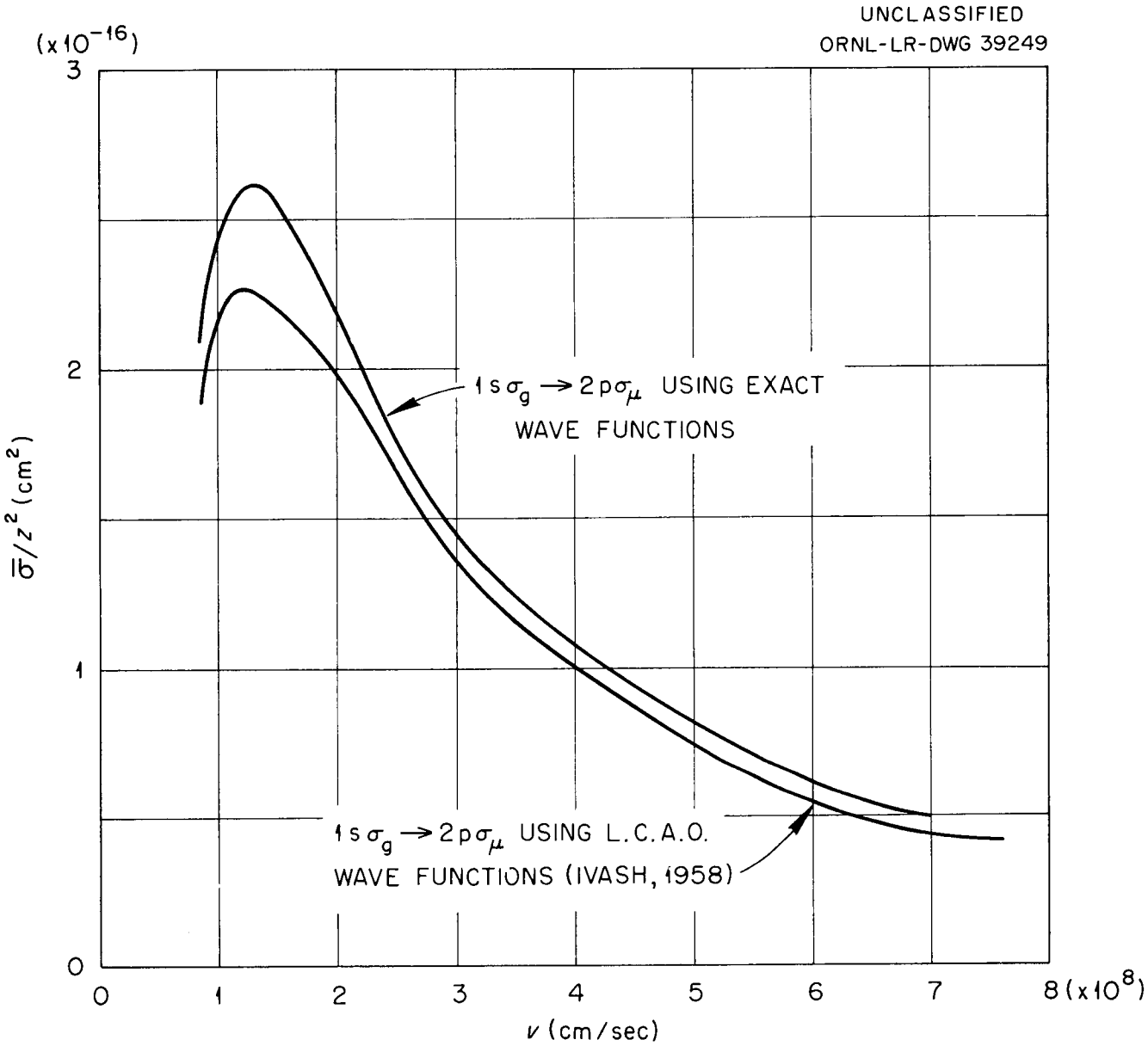
UNCLASSIFIED
ORNL-LR-DWG 39249
(x10^-16)
3
2
1
0
σ̄/z² (cm²)
1sσg → 2pσμ USING EXACT
WAVE FUNCTIONS
1sσg → 2pσμ USING L.C.A.O.
WAVE FUNCTIONS (IVASH, 1958)
0
1
2
3
4
5
6
7
8 (x10^8)
v (cm/sec)

Fig. 1.

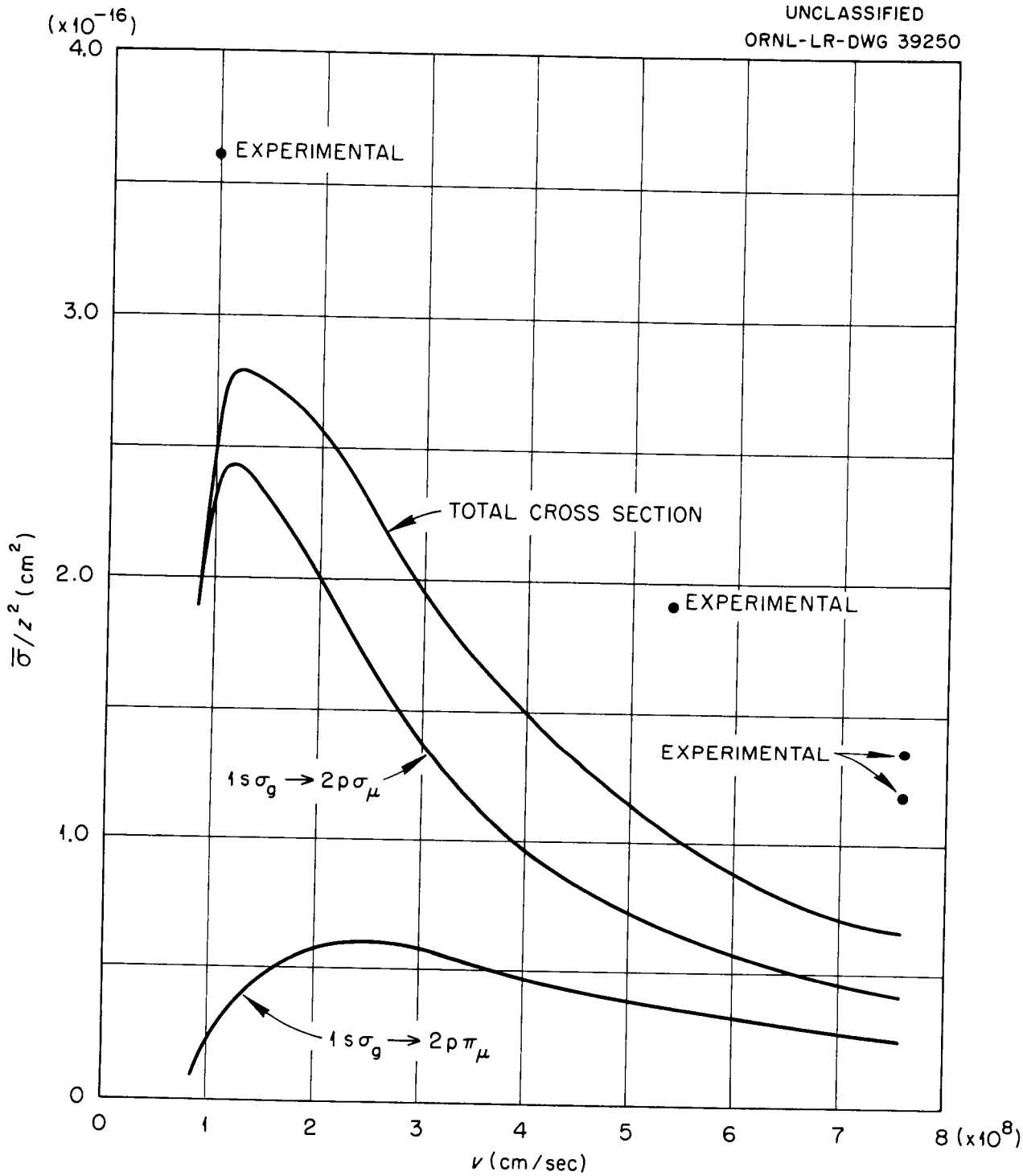
UNCLASSIFIED
ORNL-LR-DWG 39250
(x10^-16)
4.0
3.0
2.0
1.0
0
EXPERIMENTAL
TOTAL CROSS SECTION
EXPERIMENTAL
EXPERIMENTAL
1sσg → 2pσμ
1sσg → 2pπμ
σ̄/z² (cm²)
0
1
2
3
4
5
6
7
8 (x10^8)
v (cm/sec)

Fig. 2.

In an arc similar to that used in DCX a breakup efficiency of 30% for 600 kev H_2^+ molecules has been found. Furthermore, the density of the arc has been measured to be of the order of 10^{14} particles/cm^3 and by mass spectroscopic measurements the arc has been found to be 60% c^{++++} and 40% c^{+++}. Thus substituting into Eq. (28) we find that this data corresponds to an observed cross section of

$$\left(\frac{\bar{\sigma}_T}{z^2}\right) = 1.35 \times 10^{-16} \text{ cm}^2 \text{ for 600 kev } H_2^+.$$

Data on an arc somewhat different than that used in DCX has been taken[11] and a breakup efficiency of 10.6% for 600 kev H_2^+ molecules and 16.4% for 600 kev D_2^+ molecules was obtained. The density of this arc was measured[12] and found to be of order of 10^{14} particles/cm^3.

The population of the various charge states for the ions is not known for this arc, but the best available guess is that the arc is composed of 33-1/3% c^{+++}, 33-1/3% c^{++}, and 33-1/3% c^{+}. Thus from Eq. (28) we find that the observed cross sections are

$$\left(\frac{\bar{\sigma}_T}{z^2}\right) = 1.91 \times 10^{-16} \text{ cm}^2 \text{ for 600 kev } D_2^+$$

$$\left(\frac{\bar{\sigma}_T}{z^2}\right) = 1.19 \times 10^{-16} \text{ cm}^2 \text{ for 600 kev } H_2^+$$

Finally, measurements for the dissociation of 20 kev D_2^+ molecules have been taken and an efficiency of approximately 35% was obtained. The properties of the arc on which this result was obtained are not known; but presumably, they do not differ much from the properties of the arc discussed immediately above. Thus using

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11. C. F. Barnett, R. J. Mackin, Jr., and J. A. Ray, Dissociation of H_2^+ and D_2^+ by a Vacuum Carbon Arc, ORNL-2420 (1957).
12. A. M. Zuker, M. L. Halbert, and C. E. Humting, Bulletin of American Physical Society, Series II, 4, 40 (1959).

$$n = 10^{14}/cm^3$$

$$33\text{-}1/3\%\ c^{+++},\ 33\text{-}1/3\%\ c^{++},\ 33\text{-}1/3\%\ c^{+}$$

we find

$$\left(\frac{\bar{\sigma}_T}{z^2}\right) = 4.61 \times 10^{-16} \text{ for 20 kev } D_2^+$$

These observed cross section values are shown in Fig. 2.

The observed values differ from the calculated values by roughly a factor of two. Considering the somewhat rough character of the experimental data (and the calculated cross section) the agreement is probably as good as one could expect.

The situation seems to be worse at the lower velocities because the Born approximation probably over estimates the cross section by a considerable amount in this region. On the other hand, the experimental data at the lower velocities is much less reliable than at the higher velocities.

In considering the results it must be remembered that the calculated cross section does not include direct ionization and charge exchange, while the experimental results indicate that part of the dissociation (of the order of 20 or 30%) may be due to these processes.[11] Also, there may be a contribution due to the electrons in the arc.

In conclusion then, there seems to be reasonably good agreement between theory and experiment. The carbon ions account for most of the observed breakup. On the other hand, as the experiment improves this agreement could easily become worse rather than better. Certainly more work both experimental and theoretical is required before one can say with certainty that the dissociation of the molecular ion by the arc is completely understood.

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