

12-15-1979

Rates of dissociative attachment of electrons to excited H₂ and D₂

J. M. Wadehra

University of Pittsburgh, ad5541@wayne.edu

Recommended Citation

Wadehra JM. Rates of dissociative attachment of electrons to excited H₂ and D₂. *Appl. Phys. Lett.* 1979;35(12):917-919. doi:
[10.1063/1.91023](https://doi.org/10.1063/1.91023)

Available at: http://digitalcommons.wayne.edu/phy_astro_frp/111

This Article is brought to you for free and open access by the Physics and Astronomy at DigitalCommons@WayneState. It has been accepted for inclusion in Physics and Astronomy Faculty Research Publications by an authorized administrator of DigitalCommons@WayneState.

changes in the refractive indices and phases [η, η', ϕ , and ϕ' in Eq. (11)], which result in a change in the output power [Eq. (11)]. The experiments clearly demonstrated the feasibility of constructing a sensitive all-fiber interferometric sensor (gyro, acoustic, temperature, magnetic field). Further technical detail on the performance of these new sensors will be presented in subsequent publications.

- ¹R.A. Steinberg and T.G. Giallorenzi, *Appl. Opt.* **15**, 2440 (1976).
²A. Simon and R. Ulrich, *Appl. Phys. Lett.* **33**, 517 (1977).
³R. Ulrich and M. Johnson, *Opt. Lett.* **4**, 152 (1979).
⁴A.W. Snyder, *J. Opt. Soc. Am.* **62**, 1267 (1972).
⁵H. Kogelnik and Schmidt, *IEEE J. Quant. Elect.* **QE-12**, 396 (1976).
⁶S.K. Sheem and T.G. Giallorenzi, *Opt. Lett.* **4**, 29 (1979).
⁷S.K. Sheem and T.G. Giallorenzi, *Appl. Phys. Lett.* **34**, 131 (1979).
⁸M.F. Brace, A.L. Cullen, E.F.F. Gillespie and J.A. Staniforth, *IRE Trans. Antennas and Propag.* **AP-7**, S219 (1959).

Rates of dissociative attachment of electrons to excited H₂ and D₂

J. M. Wadehra

Department of Physics, University of Pittsburgh, Pittsburgh, Pennsylvania 15260

(Received 14 July 1979; accepted for publication 5 October 1979)

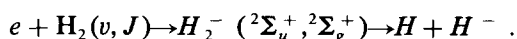
Calculations are reported of the contributions of the lowest $^2\Sigma_u^+$ and $^2\Sigma_g^+$ resonant states to the rates of dissociative attachment of electrons to H₂ and D₂. For all electron temperatures, the rate is significantly enhanced by vibrational and rotational excitation of the initial molecule.

Typically, for an electron temperature of 1.5 eV, the attachment rates for various (v, J) levels are, in $\text{cm}^3 \text{sec}^{-1}$, 5.4×10^{-15} for (0,0), 7.2×10^{-11} for (0,20), and 7.8×10^{-9} for (8,0), for H₂; and 4.5×10^{-17} for (0,0), 1.4×10^{-14} for (0,20), and 6.0×10^{-9} for (11,0), for D₂.

PACS numbers: 34.80.Gs, 34.90.+q, 34.10.+x

It has been suggested that dissociative attachment of electrons to excited molecules might be responsible for the high negative ion production recently found in low-density hydrogen plasmas¹⁻³. Recent calculations^{4,5} using resonant scattering theory indeed showed a significant enhancement of the dissociative attachment cross section by vibrational or rotational excitation of the initial molecule. However, calculations of attachment rates are needed before any definite conclusion regarding the interpretation of high negative ion densities in hydrogenic plasmas can be made. The purpose of this letter is to present the rates of dissociative electron attachment to excited H₂ and D₂ at average electron energies up to 5 eV, for which only the contributions of the $(1\sigma_g)^2(1\sigma_u)^2\Sigma_u^+$ and $(1\sigma_g)(1\sigma_u)^2\Sigma_g^+$ resonances are presumably significant.

In the usual resonant scattering theory, the process of dissociative attachment proceeds via an intermediate resonant state:



The radial nuclear wave function $\xi_J(R)$ for the resonant state of the negative ion satisfies the equation

$$\left[-\frac{1}{2M} \frac{d^2}{dR^2} + \frac{J(J+1)}{2MR^2} + V^-(R) - \frac{i}{2}\Gamma(R) - E \right] \times \xi_J(R) = \zeta_{v,J}(R) [\Gamma_0(R)/2\pi k_0(R)]^{1/2},$$

in which J and E are the total angular momentum and energy, M is the reduced mass of the nuclei, $V^-(R)$ and $\Gamma(R)$ are the potential energy and width of the appropriate resonant state, and $\zeta_{v,J}(R)$ is the radial nuclear wave function of the initial vibrational and rotational state of the neutral molecule. The function $k_0(R)$, which is defined in terms of the potential energy $V_0(R)$ for the ground state of the neutral

molecule by

$$\frac{1}{2}k_0^2(R) = V^-(R) - V_0(R),$$

gives the wave number of the electrons that can be captured or emitted when the nuclei are at the separation R without a change in the nuclear velocity. The dissociative attachment cross section can then be obtained from the asymptotic behavior of $\xi_J(R)$ through

$$\sigma_{DA} = \frac{2\pi^2 K}{k M} \lim_{R \rightarrow \infty} \left| \xi_J(R) \right|^2,$$

where k and K are the wave numbers describing the incident

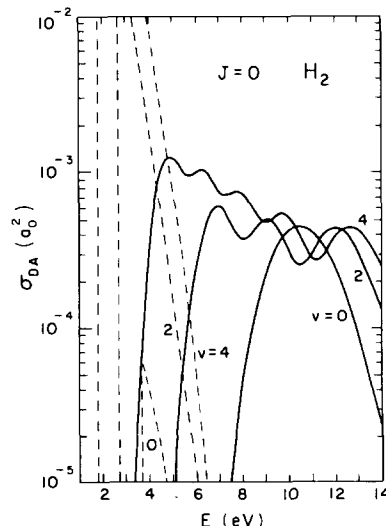


FIG. 1. Contributions of the $^2\Sigma_u^+$ and the $^2\Sigma_g^+$ resonant states to the dissociative attachment cross sections for various rotationless vibrational states of H₂:— $^2\Sigma_g^+$, - - - $^2\Sigma_u^+$.

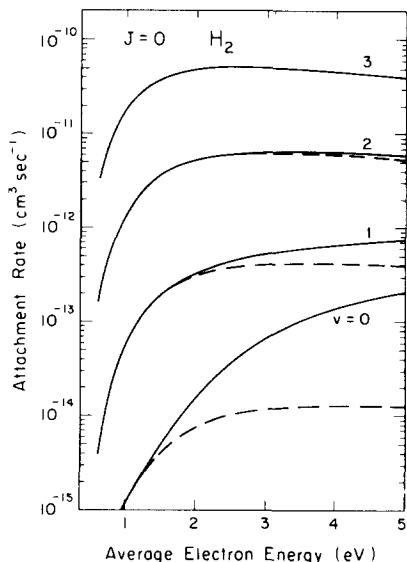


FIG. 2. Rate of dissociative electron attachment to various rotationless vibrational states of H_2 ; ---- $^2\Sigma_u^+$, —total $^2\Sigma_u^+ + ^2\Sigma_g^+$.

electronic motion and the outgoing ion motion in the center-of-mass frame.

The electron energy distribution is taken to be Maxwellian,

$$f(E) = \frac{2}{\pi^{1/2}} \left(\frac{3}{2\bar{E}} \right)^{3/2} E^{1/2} \exp\left(-\frac{3E}{2\bar{E}} \right),$$

where \bar{E} , the average electron energy, is related to the electron temperature T by $\bar{E} = \frac{3}{2} kT$. The rate coefficient for dissociative attachment is obtained by convoluting the cross section $\sigma_{DA}(E)$ with the above distribution function $f(E)$,

$$k(\bar{E}) = \left(\frac{2}{m} \right)^{1/2} \int_0^\infty E^{1/2} \sigma_{DA}(E) f(E) dE.$$

Figure 1 shows the contributions of the $^2\Sigma_u^+$ and $^2\Sigma_g^+$ resonances to the dissociative attachment cross section. The

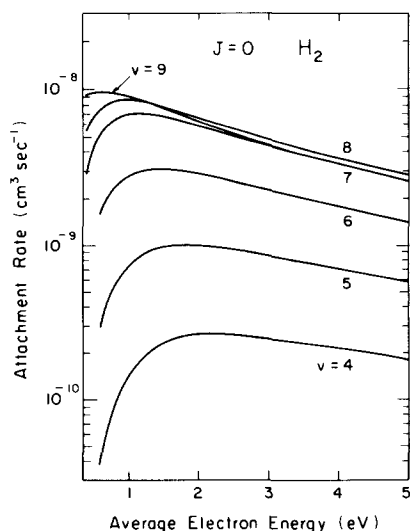


FIG. 3. Total contribution of the $^2\Sigma_u^+$ and $^2\Sigma_g^+$ resonant states to the rate of dissociative electron attachment to higher rotationless vibrational states of H_2 .

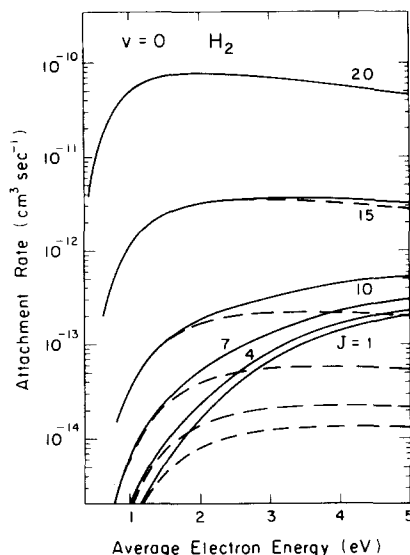


FIG. 4. Rate of dissociative electron attachment to various rotational levels of the ground vibrational state of H_2 ; ---- $^2\Sigma_u^+$, —total $^2\Sigma_u^+ + ^2\Sigma_g^+$.

contribution of the $^2\Sigma_g^+$ resonance shows structure which is related to the oscillations in the initial vibrational wave function of neutral molecule. This structure corresponding to a transition between a continuum and a dissociating resonant state seems to be related to Condon's diffraction bands⁶ and has been observed in previous experimental and theoretical studies.⁷⁻⁹

Figures 2-7 show the attachment rate $k(\bar{E})$ as a function of average electron energy \bar{E} for various vibrational and rotational levels of H_2 and D_2 . The fact that the average electron energy \bar{E} and the electron temperature T are related in a linear fashion, namely, $\bar{E} = \frac{3}{2} kT$, makes it simple to obtain the attachment rate for any electron temperature from Figs. 2-7 in a straightforward manner. In a previous analysis¹ of negative ion densities in a hydrogen plasma, the attachment

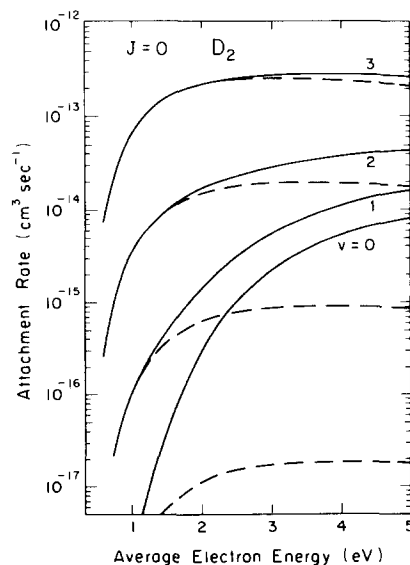


FIG. 5. Rate of dissociative electron attachment to various rotationless vibrational states of D_2 ; ---- $^2\Sigma_u^+$, —total $^2\Sigma_u^+ + ^2\Sigma_g^+$.

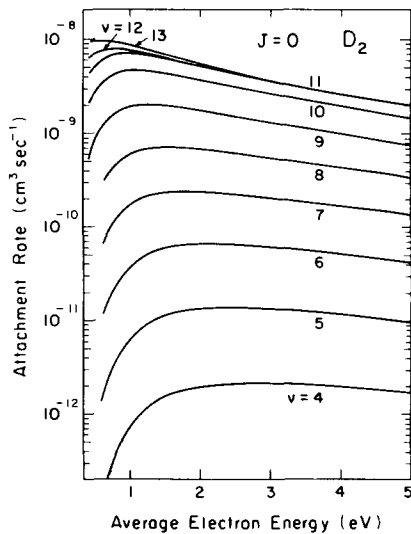


FIG. 6. Total contribution of the ${}^2\Sigma_u^+$ and ${}^2\Sigma_x^+$ resonant states to the rate of dissociative electron attachment to higher rotationless vibrational states of D_2 .

rate at the gas temperature of 1.5 eV was taken to be $\sim 10^{-15} \text{ cm}^3 \text{ sec}^{-1}$. The present results, however, indicate that this rate could be as high as $\sim 10^{-8} \text{ cm}^3 \text{ sec}^{-1}$ if the molecules are heated. Even a modest heating of the plasma can, therefore, lead to significant ion production.

The enhancement of the attachment rate is a direct consequence of the enhanced attachment cross sections associated with the vibrationally and rotationally excited states of the molecule. The enhancement of the cross section arises from an increase in the survival factor, which is the probability that the resonant state dissociates without autoionization. This factor is increased because electron capture can occur at larger values of R due to the larger amplitude of the vibrational motion in excited vibrational levels, and to the centrifugal stretching in excited rotational levels.

The attachment rates are shown up to vibrational levels $v = 9$ for H_2 and $v = 13$ for D_2 . For molecules in higher vibrational levels, the dissociative attachment process becomes exothermic and the attachment rate is not expected to depend strongly on the initial vibrational state of the molecule.

The attachment rates for $v = 9$ for H_2 , and for $v = 12$

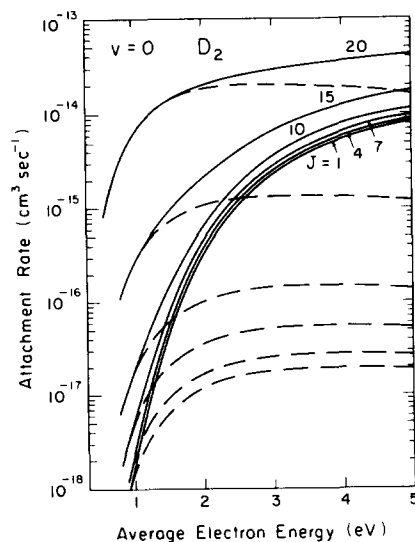


FIG. 7. Rate of dissociative electron attachment to various rotational levels of the ground vibrational state of D_2 . ---- ${}^2\Sigma_u^+$, — total ${}^2\Sigma_u^+ + {}^2\Sigma_g^+$.

and 13 for D_2 , at high electron temperature are smaller than those for lower vibrational levels. This could possibly be due to breakdown of Born-Oppenheimer approximation since in higher vibrational states the nuclear velocities become comparable to electronic velocities.

Special thanks are due Professor J. N. Bardsley for many helpful conversations and for constant encouragement throughout this work. This research was supported, in part, by the Advanced Research Projects Agency and monitored by the Office of Naval Research under Contract No. N000-14-76-C-0098.

¹E. Nicolopoulou, M. Bacal, and H. J. Doucet, *J. Phys. (Paris)* **38**, 1399 (1977).

²M. Bacal and G. W. Hamilton, *Phys. Rev. Lett* **42**, 1538 (1979).

³J. R. Hiskes, M. Bacal, and G. W. Hamilton, Lawrence Livermore Laboratory Report No. UCID-18031, 1979.

⁴J. M. Wadehra and J. N. Bardsley, *Phys. Rev. Lett.* **41**, 1795 (1978).

⁵J. N. Bardsley and J. M. Wadehra, *Phys. Rev. A* **20**, 1398 (1979).

⁶E. U. Condon, *Phys. Rev.* **32**, 858 (1928).

⁷D. J. Ehrlich and R. M. Osgood, Jr., *Phys. Rev. Lett* **41**, 547 (1978).

⁸A. Dalgarno, G. Herzberg, and T. L. Stephens, *Astrophys. J.* **162**, L49 (1970).

⁹C. Derkits, J. N. Bardsley, and J. M. Wadehra, *J. Phys. B* **12**, L529 (1979).