LETTERS TO THE EDITOR

REACTION RATE COEFFICIENT FOR RADIATIVE ELECTRON ATTACHMENT TO ATOMS

R. K. JANEV

Institute of Physics, Beograd

and

LJ. PETKOVSKI

Institute of Physics, Skopje

Received 10 April 1973

It has been found recently that the process of radiative electron attachment to atoms is one of the most important sources of continuous radiation from some astrophysical and laboratory plasmas¹⁻³). Direct experimental measurements of the cross section σ_{att} for this process are extremely difficult³) and still not performed. In this situation the averaged value of the cross section over the electron distribution f(v), namely the reaction rate coefficient

$$a = \int_{0}^{\infty} v \,\sigma_{att}(v) f(v) \,\mathrm{d}v \tag{1}$$

could serve an important information about the process.

In this letter we shall calculate the coefficient a for radiative electron attachment to atoms with ${}^{2}S_{1/2}$ ground state configuration. The cross section in this case is given by⁴ (atomic units are used)

$$\sigma_{att} = \frac{4\pi}{3c^3} \frac{\omega^3}{k} M_{ok}^2, \qquad (2)$$

where k is the electron wave number, ω is the frequency of the emitted photon and M_{0k} is the electric dipole matrix element. In one – electron approximation, which is applicable in our case, dipole matrix element has the form

$$M_{0k} = \int_{0}^{\infty} P_{0}(r) r u_{k}(r) dr, \qquad (3)$$

where $P_0(r)$ and $u_k(r)$ are the radial wave functions of the bound and free electron states, respectively. As the considered proces in a $p \rightarrow s$ free — bound transition, the initial state wave function is

$$u_{k}(r) = \cos \delta_{1} j_{1}(kr) - \sin \delta_{1} n_{1}(kr), \qquad (4)$$

with δ_1 being the scattering phase shift of the p-partial wave and $j_1(x)$ and $n_1(x)$ are the spherical Bessel and Neumann functions, respectively. The bound state wave function is correctly represented by

$$P_0(r) = A \sqrt{2\gamma} e^{-\gamma r}, \quad A = (1 - \gamma r_0)^{-1/2}, \quad (5)$$

where $-\gamma^2/2$ is the binding energy and r_0 is the effective range of the Hartree-Fock atomic field. The wave function (5) has exact asymptotic behaviour ⁵⁾ and the constant A serves for satisfying the relevant boundary condition imposed on $P_0(r)$ at the radius r_0 of the short ranged atomic field. For hydrogen and alk ali atoms parameters γ and r_0 are given in Table 1.

ion	Н-	Li⁻	Na-	К-	Rb⁻	Cs-
γ	0.236	0.215	0.160	0.149	0.141	0.130
ro	2.65	3.36	4.08	4.87	5.86	6.10

Table 1

With the above wave functions the dipole matrix element M_{0k} can be calculated analytically and for the electron attachment cross section we obtain

$$\sigma_{ott} = \sum_{n=1}^{3} B_n \frac{k^{2n-1}}{\gamma^2 + k^2}, \quad B_n = a_n B, \tag{6}$$

where

$$B = \frac{4\pi\gamma}{3c^3} A^2, \quad a_1 = 1 + g\gamma^3 + g^2 \frac{\gamma^6}{4}, \quad a_2 = -\left(g + g^2 \frac{\gamma^3}{2}\right), \quad a_3 = g^2 \frac{\gamma^2}{4}$$

and g being a small quantity⁴).

Assuming for f(v) the Maxwellian distribution function, the integral in (1) with σ_{att} in the form (6) can be calculated in closed form

$$a = \sum_{n=1}^{3} c_n I_n, \quad I_n = \frac{1}{2} \lambda^3 \Gamma \left(n + \frac{3}{2} \right) \Psi \left(n + \frac{3}{2}, \quad n + \frac{3}{2}; \quad \lambda^2 \right), \quad (7)$$
$$\lambda^2 = \frac{\gamma^2}{2 \kappa T}, \quad C_n = \frac{4}{\sqrt{\pi}} B_n,$$

where \varkappa is the Boltzman's constant, T is absolute temperature and $\Psi(a, b; x)$ is the second solution of Kummer's equation.

Now we note that the radiative electron attachment cross section is dominantely distributed at small energies. Therefore in (6) the first term (n = 1) is a leading one and for $k^2 \leq 1$ we can neglect other terms in (6). Having in mind that in the case of negative ions always is $\gamma^2 \leq 1$ we may take $a_1 = 1$. Now the expression for α reduces to

$$a_0 = \frac{2B}{\sqrt{\pi}} \lambda^3 \Gamma\left(\frac{5}{2}\right) \Psi\left(\frac{5}{2}, \frac{5}{2}; \lambda^2\right). \tag{8}$$

The coefficient a_0 corresponds to the plane wave approximation ($\delta_1 = 0$) of the initial state wave function $u_k(r)$. We note that λ^2 is a dimensionless parameter and that all characteristics of the atom and the corresponding negative ion are included only in the constant *B*. So the temperature dependence of a_0 will be the same for all electron attachment reactions with $2_{51/2}$ atoms. The coefficient a_0 can be expressed in terms of the more usual first solution F(a, b; x) of the Kummer's equation. After some manipulations we get

$$a_0 = 2B\lambda^2 \left[\frac{1}{2\lambda^2} + \sqrt{\pi} \lambda e^{\lambda^2} - F\left(1, \frac{1}{2}; \lambda^2\right) \right], \qquad (9)$$

where the function $F(1, \frac{1}{2}; x)$ is already tabulated⁶). Using this form, we have calculated a_0 for hydrogen and alkali atoms case for

$$T = 300$$
 °K, 1000 °K, 3000 °K, 6000 °K and 10 000 °K.

The results are given in Table 2 (in units of 10⁻¹⁴ cm³/sec).

Atom T (°K)	н	Li	Na	K	Rb	Cs
300	0.968	1.75	1.23	1.63	3.04	2.48
1000	2.72	4.88	3.36	4.32	7.55	5.97
3000	6.05	10.6	6.23	7.81	12.9	10.6
6000	8.77	15.1	8.36	10.2	16.4	12.4
10000	11.0	18.6	9.65	11.7	18.5	14.5

Table 2

The low and high temperature behaviours of the reaction rate coefficient α_0 are

$$a_0 \underset{T \to 0}{\approx} 3B \frac{\varkappa T}{\gamma^2}, \quad a_0 \underset{T \to \infty}{\sim} B\left(1 - \frac{\gamma^2}{\varkappa T}\right).$$
 (10)

References

- L. M. Branscomb, in »Atomic and Molecular Processes*, ed. D. R. Bates, Academic Press, New York, 1962, p. 100;
- 2) O. Weber, Z. Phys., 152 (1958) 281;
- 3) G. Boldt, Z. Phys., 154 (1959) 319;
- 4) R. K. Janev, Ph. D. Thesis, Beograd (1968);
- 5) L. D. Landau and E. M. Lifshits, »Quantum Mechanics», ed. Fizmatgiz, Moscow (1963);
- 6) L. J. Slater, *Confluent Hypergeometric Functions*, ed. University Press. Cambridge (1960).