RADIATIVE RECOMBINATION RATE and PHOTOIONIZATION CROSS SECTIONS FOR (C IV, C V and C VI) IONS

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Abstract

Radiative recombination rate coefficient and photoionization cross sections as inverse process have been investigated for three Carbon ions (C IV, C V, C VI). The theory which has been adopted by us is based on analytic fit formula, to calculate the rate coefficient and photoionization cross sections. The agreement of the rate coefficient for our calculations compared with other theoretical data depending on the single-electron model that utilizes Dirac-Slater wave function, is very good for C IV-ion and excellent for (C V& C VI)-ions. There were no measurements available to compare our data with them for the rate coefficient, also no calculations or measurements were available for the photoionization cross sections.

Keywords : recombination rate - photoionization - cross sections

INTRODUCTION

From a fundamental point of view, photoionization of ionic systems provides the opportunity to investigate the dynamic interplay among many body electron-electron correlation and relativistic effects. Cross sections are also important as applied data, because photoionization takes place in many physical systems, including a large variety of astrophysical systems, the upper atmosphere and different types of laboratory plasma ^[1].

Photoionization and recombination of ions are of particular interest in X-ray astronomy, X-ray photoionization models in general require these parameters prevalent in high-temperature sources such as active galactic nuclei, supernova remnant, and hot stellar coronae^[2].

The theoretical treatment of (e + ion) recombination subsumes both the non-resonant recombination (i.e. radiative recombination, RR), and the resonant recombination (i.e. di-electronic recombination, DR) processes in a unified scheme. Radiative recombination rate along with photoionization cross sections are required for estimates of ionization equilibrium and thermal balance in terrestrial and astrophysical plasmas contaminated by various ions ^[3].

Recently we published two researches about single and double photoionization of atoms ^[4,5]. A number of calculations exists for photoionization cross sections and radiative recombination rate for ions ^[2,3,6-10].

Sixteen years ago there was a significant problem because the calculations could only in a few cases be tested by experiments, as a result of a distinct lack of experimental photoionization cross section data. The situation has now changed, thanks to the experimental development described above and the high-quality data it has brought along. Thus it has become possible to benchmark the calculations in many cases, and thereby to stimulate further development of the theoretical models and improve our understanding of fundamental atomic physics ^[1].

In this research, we present the calculations and analytic fits to the rates of radiative recombination and photoionization cross sections toward C IV, CV & C VI ions ^[11,12]. Barfield ^[6]

depended on the single-electron model that utilizes Dirac-Slater wave function for the same ions, where he discussed the ionization balance calculations for high-temperature plasmas that occur in the solar corona and in some controlled thermonuclear reactors. Other researchers like Trzhaskovskaya et.al ^[3] depended on the multipole and relativistic effects which are of great importance in consideration of photoionization and radiative recombination at high electron energies, especially for heavy and highly-charged ions.

THEORY

Recombination of an incoming electron to the target ion may occur through non-resonant, background continuum, usually referred to as radiative recombination (RR)^[8],

$$e + X^{++} \rightarrow hv + X^{+} \qquad \dots \qquad (1)$$

This is the inverse process of direct photoionization.

An analytic fit to the radiative recombination rates which we have depended it in our calculations for (C IV, C V, C VI) ions ^[11].

$$\alpha_r(T) = a \left[\sqrt{T/T_{\circ}} \left(1 + \sqrt{T/T_{\circ}} \right)^{1-b} \left(1 + \sqrt{T/T_{1}} \right)^{1+b} \right]^{-1} \qquad \dots \qquad (2)$$

Where T is the temperature, a, b, T_0 , T_1 are the fitting parameters.

Concerning the photoionization cross sections, we has use a non-relativistic formula to calculate it for the same ions ^[12].

$$\sigma_{ph}(E) = \sigma_{\circ}F(y) \quad \text{Mb} \quad \dots \quad (3)$$
$$F(y) = \left[(x-1)^2 + y_w^2 \right] y^{0.5p-5.5} (1 + \sqrt{y/y_a})^{-p} \quad \dots \quad (4)$$

Where $x = \frac{E}{E_{\circ}} - y_{\circ}$, $y = \sqrt{x^2 + y_1^2}$, E is the photon energy in eV, and $\sigma_{\circ}, E_{\circ}, y_w, y_a, p, y_{\circ}$, and y_1

are fit parameters $(1Mb = 10^{-18} cm^2)$.

Tables (1) and (2) show the fitting parameters which have been used in getting our data of radiative recombination rate and photoionization cross sections for (C IV, C V, C VI) ions.

RESULTS AND DISCUSSION

In this paper we describe the analytic fit calculations of photoionization and photorecombination, as inverse processes, and RR, to obtain the (e + ion) recombination rates and cross sections of (C IV, C V, C VI) ions.

In Figure (1), we present our calculations of the radiative recombination rate coefficient $\alpha_r(T)$ for (C IV)-ion compared with the data of Barfield ^[6]. We notice that the rate coefficient is decreases slowly so-them with the increasing of temperature and the comparison is very good, specially at high temperatures we get matching.

In figure (2), our comparison of $\alpha_r(T)$ for (C V)-ion is in excellent agreement with Barfield^[6] data. Our fits are accurate in a much wider temperature range, however, since our fitting formula has correct at low-temperature and high-temperature asymptotes.

In figure (3), we also compare our data of RR rate coefficient with Barfield ^[6] data for (C VI)-ion. Here the comparison is in excellent agreement, and we notice that it decreases with the increasing temperature as shown in figure.

In table (3), we show the photoionization cross sections of (C IV, C V, C VI) ions in the energy range $(1-10^3)eV$. Unfortunately there were no theoretical or experimental data to make a comparison with them. Also, , to our knowledge there were no measurements for radiative recombination rate coefficient to compare it with our data.

In figure (1) we notice that the discrepancies between our method and Barfield's ^[6] method who used the single-electron model are less than 1% at $T \le 10^2 K$, since the main contribution to the total rate at these temperatures comes from the recombination to highly excited levels. At T $>10^2 K$, the discrepancies begins to decrease and vanish, since the main contribution to the total rate at high temperature comes from the ground state recombination. Although the calculations are computationally intensive, they yield nearly all photoionization and recombination parameters needed for astrophysical photoionization models with higher precision than hitherto possible. Previous calculations of (e + ion) recombination rates, reported in the present series on photoionization and recombination, were carried out in LS coupling. There were two reasons. First, the calculations are extremely complex and involve both radiative photoionization and collisional electron-ion scattering calculations. Second, the effect of relativistic fine structure was expected to be small for these light elements.

As is evidence, our calculations are in excellent agreement over the wide range of temperature (10-3000)K with no relativistic nor multipoles be included. In each case, our values of $\alpha_r(T)$ coincide with an accuracy with the results of Barfield^[6]. The maximum difference between calculations is ~1% at low temperatures. The reason for the difference at low temperatures is not clear. It is possible that this is the influence of method of calculation used in Ref.[6], or due to a combination of neglect of the higher multipoles and semi-relativistic approximation. The formula has been factorized giving rise to the temperature-dependent relativistic correction factor for which the usual non-relativistic expression for the rate coefficient must be multiplied. This factor has been naturally absent in all calculations, even though the rate coefficient has been calculated at high temperature.

CONCLUSION

From precedence we conclude that the fitting formula we had depended on was very good in calculating the radiative recombination rate. Also, we must mention that our dependence on the fitting parameter was for reason, which is those parameters has been putting after the ensuring of its validity by comparing the photoionization cross sections results with the experimental measurements, which represent the exact norm in such cases. The differences in the energy range which was not sequent to show that the random choices of energies not effect in the calculated data.

Ion	$a(cm^3s^{-1})$	b	$T_{\circ}(K)$	$T_1(K)$
C IV	8.54×10^{-11}	0.5247	5.014×10 ²	1.479×10 ⁷
C V	2.765×10^{-10}	0.6858	1.535×10^{2}	2.556×10 ⁷
C VI	6.556×10 ⁻¹⁰	0.7567	6.523×10 ¹	2.446×10 ⁷

TABLE (1): FIT PARAMETERS FOR RADIATIVE RECOMBINATION RATE.

TABLE (2): FIT PARAMETERS FOR PHOTOIONZATION CROSS SECTIONS.

Ion	$E_{\circ}(eV)$	$\sigma_{\circ}(Mb)$	У _а	р	<i>Y</i> _{<i>w</i>}	y _°	<i>Y</i> ₁
C IV	3.506	106.8	14.36	7.457	0.0	0.0	0.0
C V	46.24	234.4	21.83	2.581	0.0	0.0	0.0
C VI	15.48	1521	32.88	2.963	0.0	0.0	0.0

$E_{Ph}(eV)$	$\sigma_{_{Ph}}(Mb)$					
	C IV	C V	C VI			
1	188.387	-	-			
10	3.664	71012.2	748.07			
20	2.826	1829.94	27.105			
40	1.338	4.918	40.433			
60	0.738	3.947	22.677			
80	0.456	6.554	13.359			
100	0.304	6.081	8.481			
200	0.0731	2.017	1.749			
240	0.0484	1.440	1.118			
280	0.0338	1.025	0.760			
300	0.0287	0.876	0.638			
350	0.0197	0.610	0.429			
400	0.0142	0.442	0.302			
450	0.0105	0.330	0.221			
500	0.0080	0.253	0.167			
550	0.0063	0.199	0.129			
600	0.0050	0.159	0.102			
650	0.0040	0.129	0.082			
700	0.0033	0.106	0.066			
750	0.0027	0.088	0.055			
800	0.0023	0.074	0.046			
850	0.0019	0.063	0.039			
900	0.0016	0.054	0.033			
1000	0.0012	0.04	0.024			

TABLE (3): PHOTOIONIZATION CROSS SECTION FOR (C IV, C V, C VI) IONS.



FIG.(1): RADIATIVE RECOMBINATION RATE FOR (C IV)-ION





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معدل اعادة الاتحاد المشع والمقاطع العرضية للتأين الضوئي لآيونات (C IV, C V, C VI) علاء عبد الحسن خلف قسم الفيزياء – كلية العلوم – جامعة البصرة

خلاصة

تمت دراسة معامل اعادة الاتحاد والعملية العكسية المتمثلة بالتأين الضوئي وحساب المقاطع العرضية لها لآيونات عنصر الكاربون (C IV, C V, C VI). قمنا باعتماد صيغة التلائم التحليلي لحساب معامل المعدل والمقاطع العرضية للتأين الضوئي لهذه الايونات. كان التوافق بين نتائجنا والحسابات النظرية الاخرى التي اعتمدت نموذج الالكترون-المنفرد المستند على دوال موجة ديراك-سليتر، جيدا جدا لحالة ايون- (C IV) وممتازة لحالة ايونات (C V & C VI) . لم تتوافر لدينا قياسات عملية لمعامل المعدل لغرض مقارنة نتائجنا معها، ولا حسابات نظرية أو قراءات عملية للمقاطع العرضية للتأين

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