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# Collisional Ionization Rates for Lithium- and Beryllium-Like Ions*

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Collisional ionization rates for C IV, N V, and O VI as well as for O V and Ne VII are deduced from the time history of spectral lines emitted by these ions in a hot plasma. The plasma (in the electron temperature range 100–260 eV) is produced in a 15-kJ theta-pinch device, and it is analyzed using the light-scattering technique. The results are consistent with theoretical calculations for O VI and with a semiempirical formula based on theoretical calculations for hydrogenic ions but smaller by factors 1.5–2.

## I. INTRODUCTION

Cross sections for ionization by electron impact have been measured now for many neutral and some singly ionized atoms.[1] The technique usually employed is the crossed-beam method. With increasing charge, such measurements become very difficult. Not only then are the cross sections decreasing rapidly, but it also is more difficult to obtain suitable high-current ion beams. The cross sections for ionization of some doubly ionized atoms[2,3] appear, at present, to be the only ones measured for higher ionization stages. Multiply ionized atoms, however, are important in many laboratory and astrophysical plasmas. In most of these applications only the corresponding rate coefficients are needed. Such ionization-rate coefficients can be deduced from the spectroscopic analysis of a well-diagnosed plasma, as was shown for neon ions in a stellarator discharge[4] and for heliumlike C V in a theta-pinch plasma.[5] (Excitation coefficients have been obtained by this method as well and will be the subject of another paper.) In Sec. II we present ionization rates for ions of the lithiumlike and berylliumlike isoelectronic sequences obtained with a theta-pinch device.

## II. THEORETICAL IONIZATION RATES

Theoretical cross sections for ionization from the ground state, specifically of lithiumlike and berylliumlike ions, have been calculated by Trefftz and Malik for O VI and O V using the Coulomb-Born-Oppenheimer method[6] and the distorted-wave approximation.[7] Recently, Schwartz[8] calculated the ionization cross sections for O VI for ionization from the ground state as well as from the 2$p$ excited level in the Coulomb-Born II approximation. The

calculations include distortion, which was found to increase the cross section by about 22% at 1.5 times the threshold energy and, to a lesser extent, at lower and higher impact energies (for example, only 13% at 5 times threshold).

The reduced cross section of Schwartz for the ionization from the 2$s$ level of O VI agrees to within 10% with the reduced cross section for ionization from the 1$s$ level of a hydrogenic ion of charge $Z = 128$ as calculated by Rudge and Schwartz[9] in the Born-exchange approximation. The reduced cross section for O VI as given by Trefftz[6] shows essentially the same maximum value; however, the peak is shifted to lower energies and her cross section is smaller at higher energies (e.g., by 30% at four times threshold.) Finally, the reduced cross section for ionization from the 2$p$ level as obtained by Schwartz[8] is somewhat larger than that for ionization from the 2$s$ level (by ~ 31% at 1.125 times threshold and by ~ 20% at 5 times threshold).

Using an empirical formula with three free parameters, Lotz[10] approximated all experimentally determined cross-section curves to within 10% and predicted many unknown cross sections. For ions four and more times ionized, his formula reduces to one with a single free parameter, and then essentially agrees with the calculations of Rudge and Schwartz[9] for a hydrogenlike ion with high $Z$ number. Rate coefficients derived from the predicted cross sections[10] have been computed and are tabulated in Ref. 11.

For many applications a simple expression of general validity for the ionization rates would be more desirable. A good starting point[12] is the well-known effective Gaunt-factor excitation rate, where the averaged Gaunt factor must now allow, of course, for all electric multipole transitions.

Summing over final states and assuming that the Gaunt factor scales proportionally to the principal quantum number in order to obtain the correct scaling law, this procedure suggests a rate coefficient for ionization from a state $i$ of the form

$$I_i = A(T) \frac{\eta_i}{E_i} \frac{(kT)^{1/2}}{E_i + 3kT} e^{-E_i/kT} . \tag{1}$$

Here $\eta_i$ is the number of electrons in the $i$th shell and $E_i$ the ionization energy. Both $kT$ and $E_i$ are in eV. The factor $A(T)$ consists, besides of a constant, essentially of the effective Gaunt factor. If we compare Eq. (1) with the rate coefficients derived from the Born-exchange approximation for hydrogenic ions[9] we can deduce the factor $A(T)$. We choose as a ~10% fit in the temperature range $\frac{1}{10} E_i \le kT \le 10 E_i$,

$$I_i \simeq 7.5 \times 10^{-8} \times \frac{\eta_i}{E_i} \left[ \left( \ln \frac{40 kT}{E_i} \right)^3 + 40 \right]$$

$$\times \frac{(kT)^{1/2}}{E_i + 3kT} e^{-E_i/kT} \text{ cm}^3/\text{sec} . \tag{2}$$

In the same temperature range, these rate coefficients agree with the predictions given by Lotz[11] to within 15% for all ions of the hydrogen, helium, lithium, and beryllium isoelectronic sequences of charge greater than three. The above formula approximates the rates for O VI derived from Schwartz's calculations[8] also to within ~10%, and agrees with the experimental rate coefficient obtained for heliumlike C V.[5] We finally can make a comparision with specific calculations for C v and C VI in the Coulomb-Born approximation.[13] The agreement for C v is very good (to better than 15%), whereas the rates for ionization from the ground state of C VI are larger by a factor of ~1.4 in Ref. 13.

Equation (2) may also yield ionization rates from excited levels. Beigman and Vainshtein[13] calculated the ionization rates from the 2s and 2p level of C VI. Over the whole temperature range $\frac{1}{10} E_i \le kT \le 10 E_i$, the rates averaged over s and p levels agree to within 25% with Eq. (2). A similar agreement is obtained for the ionization from the 2s level of hydrogenic ions as calculated in Ref. 9. Equation (2), of course, approximates the 2p ionization for O VI as calculated by Schwartz to within ~20%.

When considering the ground-state ionization of lithiumlike and berylliumlike ions, one might have to account for contributions from the filled 1s shell (see Ref. 11). For large Z, these contributions are reasonably well approximated by the rate coefficient for ionization of the corresponding heliumlike ion; this can be shown by comparing Eq. (2) for a heliumlike ion with the rates for K-shell ionization of the neutral atom as deduced from measured cross sections.[14] One obtains thus contributions from in-

ner shells smaller than 20%. They can therefore be neglected, at least for most applications where $kT \le 10 E_i$.

## III. PRINCIPLE OF MEASUREMENTS

The principle of the measurements is identical to that used by Hinnov.[4] The atoms of interest are introduced into a plasma which is heated and compressed to desired temperatures and densities. The ions then go successively through the various ionization stages, the degree of ionization lagging behind the corresponding quasistationary corona equilibrium. During that time they emit line radiation, the time history of which can be interpreted in terms of desired ionization-rate coefficients.

The concentration $N_j$ of the $j$th ionization stage is determined by the following rate equation:

$$\frac{dN_j}{dt} = NN_{j-1} I_{j-1} - NN_j I_j + NN_{j+1} \alpha_{j+1} - NN_j \alpha_j$$

$$+ \frac{1}{N} \frac{dN}{dt} N_j , \tag{3}$$

where $N$ is the electron density and $\alpha_j$ the recombination-rate coefficient. The last term in Eq. (3) is a source term keeping the total concentration of the ions constant during compression or expansion phases of the discharge. For the plasma conditions used in the present experiment, the recombination rates usually are so small that they can be neglected. This simplifies Eq. (3) considerably: The concentrations of the ions are then solely governed by the ionization rates. In Eq. (3), the products $N_j I_j$ represent the sum of the ionization rates from the ground state and all excited levels, among which contributions from metastable levels can be considerable. As was shown for heliumlike C V,[5] these contributions from excited metastable levels could be made small by going to low electron densities, so that the ionization occurred solely from the ground state. In this limit, it is also justified to assume nearly all ions to be in their respective ground states.

For an optically thin allowed line, whose upper level is essentially populated by electron collisions from the ground state, the emission coefficient is given by

$$\epsilon = \frac{h\nu}{4\pi} NXN_j , \tag{4}$$

$N_j$ now representing the ground-state population and $X$ the rate coefficient for excitation from the ground state. If $N$ and $X$ were constant, the time history of the line would reflect exactly the time history of the respective ion. Otherwise, the time variation of $N$ and $X$ can readily be corrected for even if the absolute value of $X$ is not known too accurately. Its time dependence should be presented sufficiently well by the effective Gaunt-factor approximation

(see, for example, Ref. 15), at least for the usually small temperature variations occurring during the emission of many of the lines investigated in our plasma. For the solution of Eqs. (3) and (4) one mostly has to know the electron density and temperature. Both were determined using the light-scattering technique.[16]

With the measured electron density and temperature as input the coupled rate equations (3) were solved using a computer program.[17,18] The ionization rates used were essentially those given by Eq. (2). However, a variable factor $R$ was introduced by

$$I_{\text{ex}} = R I_i, \tag{5}$$

which was varied until the calculated time histories obtained with Eq. (4) agreed with those of the observed lines.

One has to check whether the neglect of recombination is still justified, especially for higher ionization stages. Using recombination rates as given by Düchs and Griem,[18] this was found to be the case for our conditions.

We finally have to consider the particular ions being investigated here. Ions of the lithium isoelectronic sequence are characterized by a low-lying $2p\,^2P$ level. With increasing electron density its population will approach the Boltzmann value, and ionization from it would be stronger than from the ground state. At lower densities, the population can be obtained by equating collisional rates into that state with radiative and collisional rates out of it. Using excitation rates as given by Bely[19] and by Burke et al.,[20] and transition probabilities as given by Wiese et al.[21] one finds, e. g., for extreme conditions in our experiment ($N \sim 7.\,10^{15}$ cm$^{-3}$, $T_e \sim 100$ eV) that in this case only $\sim 60\%$ of all N v ions are in the ground state and almost $40\%$ in the excited $2p\,^2P$ level. For higher ions in the isoelectronic sequence, the population of this level will be, of course, much smaller.

In general, one will obtain an average ionization-rate coefficient (contributions from higher levels being small due to low population densities) given by

$$I_j \approx [N(2s)/N_j]\,I(2s) + [N(2p)/N_j]\,I(2p). \tag{6}$$

The ionization from the $2p$ level can be estimated from Eq. (2). In our experiment, the electron temperatures are of the order of the ionization energies of the ions investigated, and the ionization energies for the $2s$ and $2p$ levels are also of the same magnitude [$E(2p) \approx 0.\,8E(2s)$ for C IV and $E(2p) \geq 0.\,9E(2s)$ for higher ions in the isoelectronic sequence]: Ionization rates from the $2s$ and $2p$ level should agree, therefore, for our conditions to within $\sim 20\%$. This is suggested both by the theoretical calculations of Schwartz[8] for the ionization of O VI and those of Beigman and Vainshtein[13] for the ionization from the

2s and 2p levels of hydrogenic C VI. The error introduced when interpreting the observed ionization rates as solely due to ionization from the ground state should therefore be negligible for our conditions.

We further have to select appropriate spectral lines to observe. As long as the $2p$-level population is sufficiently small, most upper levels will be populated directly by collisions from the ground state, and lines will reflect the ground-state density according to Eq. (4). This does not hold any more, however, for our specific N v example. Here, the strongest channel for populating the $3p$ and $3d$ levels is via the $2p$ level.[20] It is best, therefore, to observe the $3s \rightarrow 2p$ transition, the excitation rate $2p \rightarrow 3s$ being sufficiently below the $2s \rightarrow 3s$ rate.

More complicated is the situation for beryllium-like ions, which have five low-lying $n = 2$ excited levels, the lowest one being even metastable ($2p\,^3P$). Because of the large statistical weight (9 compared to 1 of the ground state), its population will usually be much larger than that of the ground state, although it is not established that the Boltzmann value is achieved. For all our experimental conditions the ionization thus occurs mainly from the $2s2p\,^3P$ metastable level, the average ionization rate being given again by a relation similar to Eq. (6). All further considerations are analogous to those for lithiumlike ions; the ionization rates from the ground state and the $2s2p\,^3P$ level should again be practically the same for our cases. The population of the other low-lying excited levels may be estimated using semiempirical excitation rates (see, e. g., Ref. 15). However, they can also be determined experimentally by measuring the absolute intensities of the corresponding lines.[22] One can observe the $2p^2\,^3P$-$2s2p\,^3P$ transition, since it is populated primarily from the $2s2p\,^3P$ level and should thus reflect the change in its population. If lines appear to become optically thick, transitions from $n = 3$ levels are also suited; they will be populated from both the ground state and the metastable triplet level.

Finally, the time history of each ionization stage is strongly influenced by the history of the previous ionization stages. For this reason, lines from ions of the boron- and carbon-isoelectronic sequences were also observed and their time-dependent intensities matched with computed values.

## IV. EXPERIMENT

The plasma used for our measurements was produced in a theta-pinch device, which is described in Ref. 23. For the present experiments it was operated with a stored energy of 15 kJ in the main bank. Compared to the description in Ref. 23 the capacitance of the preheater was increased slightly from 0.5 to 0.7 $\mu$F; we also increased the damping
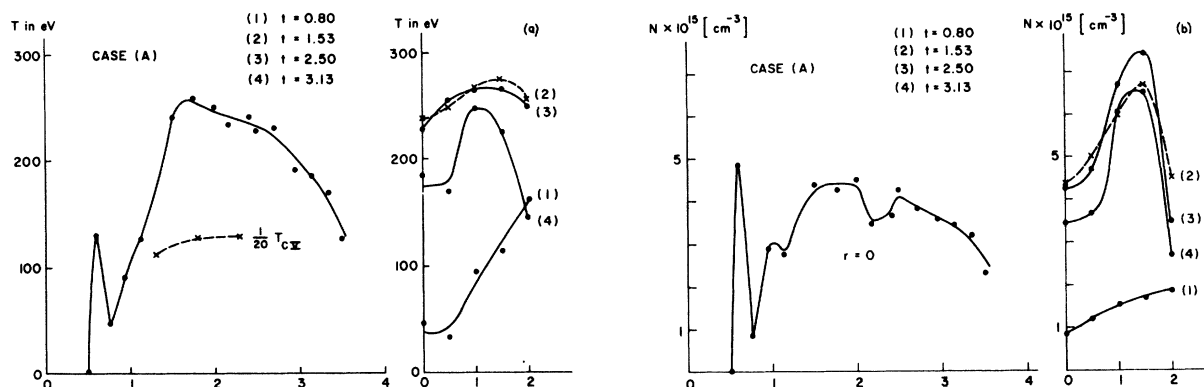
FIG. 1. Values obtained as a function of time $t$, radius $r$, from the Thomson-scattering measurements for case (A): (a) for electron temperature $T$, and (b) for electron density $N$.

of the preheater discharge by introducing a damping resistor into the discharge circuit and thus were able to fire the main discharge somewhat earlier.

Three different discharge conditions were investigated; they were obtained by varying the filling pressure, the bias magnetic field, and the time $\Delta t$ between the beginning of the preheater discharge and the ignition of the main bank. The discharge parameters are given in Table I.

Electron densities and temperatures were obtained as a function of radius and time in the midplane of the coil using the light-scattering technique. The setup is the same as used in Ref. 5. The absolute sensitivity calibration was done again using the Rayleigh scattering in $N_2$. (The cross section used was $\sigma_R = 1.73 \times 10^{-27}$ cm).[2] As an example, Fig. 1 gives the electron density and temperature as a function of time on the axis of the discharge tube ($r = 0$) for case (A) as well as the radial profiles at four different time points. Figure 1 also shows the time history of the temperature of $C_V$ ions as deduced from Doppler profiles observed side-on in the midplane of the coil. Case (A) is somewhat unfavorable for our measurements, since part of the trapped negative magnetic field exists during the whole first half-cycle of the discharge, resulting in a very stable hole in the plasma. The other cases investigated do not show such holes, the trapped negative magnetic field disappearing quite early in the discharge cycle. At early times of the discharge, the plasma column experiences also a strong axial compression, and the length of the

plasma column was measured by observing lines of various ionization stages of carbon through equidistant holes in the theta-pinch coil.

Spectroscopic observations were made end-on as well as side-on in the midplane of the coil. End-on, a vacuum-uv monochromator of the Seya-mount type and a 2-m grazing incidence instrument were used. Stops assured that only the center of the plasma column (1.25 cm in diameter) was observed. Side-on observations were made in the visible using a $\frac{1}{2}$-m monochromator. It was quite important to compare end-on and side-on observations. In general, it turned out that the time histories did not agree for the lower ionization stages, the lines observed end-on usually displaying much slower decay rates than the ones obtained side-on. However, with increasing ionization stage, the time histories became more and more alike until they agreed for the higher ones, indicating the plasma was then essentially homogeneous as assumed in our analysis.

This situation is readily explicable. The higher ionization stages will exist only in the hot plasma core whereas the lower stages will prevail for some time in cooler or low-density zones at the ends of the plasma column. Here, not only plasma is lost, but the axial compression is also not complete and will leave some low-density plasma behind. For this reason, side-on observations were preferred, when suitable visible lines could be found. Carbon, nitrogen, oxygen, and neon ions were investigated. Carbon and oxygen are natural impurities in our plasma, whereas nitrogen and neon were added in small amounts (< 1%) to the initial filling gas.

## V. RESULTS AND DISCUSSION

Table II gives the factor $R$, which is the ratio of experimental rate coefficient to the theoretical one as given by Eq. (2). Column 2 shows the temperature range over which the ions could be observed in the three cases (A), (B), and (C). Several more

TABLE I. Discharge conditions.

| | Filling pressure | Bias magnetic field | $\Delta t$ |
|---|---|---|---|
| A | 11 mTorr $H_2$ | − 600 G | 15.5 μsec |
| B | 11 mTorr $H_2$ | − 200 G | 22.5 μsec |
| C | 23 mTorr $H_2$ | − 600 G | 15.5 μsec |

TABLE II. Ratio $R$ of experimental to theoretical rate coefficients.

| Ion | $T_e$[eV] | Case (A) | Case (B) | Case (C) | Average |
|---|---|---|---|---|---|
| O VI | 140–260 | 0.7 | 0.6 | 0.6 | 0.6 |
| N V | 120–250 | 0.3 | 0.6 | 0.6 | 0.5 |
| C IV | 100–150 | (0.6) | (0.5) | (0.6) | 0.6 |
| | | | | Average | 0.6 |
| Ne VII | 130–260 | 0.5 | 0.9 | ... | 0.7 |
| O V | 130–210 | 0.4 | 0.5 | 0.6 | 0.5 |
| | | | | Average | 0.6 |

cases were investigated, but gave less reliable values.

As mentioned in Sec. III, although a constant electron density and temperature would be desirable, some variations of $N$ and $T$ can be accounted for. This, however, is possible only as long as the variations are not too strong. The time history of a line is characterized by the derivative of the intensity $P_j = \epsilon l$ ($l$ equals depth of the plasma along the line of sight), and from Eqs. (2) and (3) one obtains

$$\frac{1}{P_j}\frac{dP_j}{dt} = \frac{2}{N}\frac{dN}{dt} + \frac{1}{X}\frac{dX}{dT}\frac{dT}{dt}$$

$$+ \frac{1}{l}\frac{dl}{dt} + \frac{N_{j-1}}{N_j}NI_{j-1} - NI_j. \tag{7}$$

For a good determination of the ionization rates, the first three terms should not dominate the time history. Unfortunately, however, they tend to do so for the lower ionization stages, which occur early during the discharge, because then compression and heating of the plasma are very rapid.

For this reason, the values for C IV in Table II are not too reliable and are quoted, therefore, only in brackets. (For this case, it was also not possible to match computed and observed time histories very well.) For similar reasons, no ionization rates for higher stages like Ne VIII were obtained.

These ions occur so late during the discharge cycle that plasma losses become considerable, and it was found that the time history of Ne VIII, for example, was essentially determined by the first term of Eq. (7). In some cases the values of $R$ in Table II could not be varied by more than 20% before deviations of computed and observed time histories of lines became obvious; in other cases this limit was about 50%. The absolute values of the electron density and temperature should be accurate to ~15%. It is difficult to determine systematic errors introduced, for example, by ions in the low-density plasma outside the hot core. Possible errors due to the fact that during the early compression phases of the discharge ionization of ions occurs already in the high-density shock region, while the low-ionization stages at the center are still unaffected, have been reduced by using lower "effective" ionization rates for the lower stages. It was estimated that the over-all accuracy of our experimental rates is a factor of 2 or better.

The experimental rate coefficients obtained are only about 60% the theoretical rates given by Eq. (2). However, this is within the experimental accuracy, and these measurements thus not only are in agreement with Eq. (2) but also with the predicted rate coefficients of Lotz[11] and the theoretical calculations of Schwartz[8] for O VI. In addition, possible systematic errors in our measurements as mentioned above would tend to yield too-low values.

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# Energy and Angular Distributions of Electrons from Ionization Excitation of Helium by Proton Bombardment

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Double-differential cross sections (ddcs), relative to ejection energy and angle, have been calculated for electrons emitted from helium by proton bombardment for all excited states of the resulting helium ion through the third hydrogenic shell. Comparable calculations were made by using both a 12-term correlated wave function and a product of one-electron wave functions for the initial state of the helium atom. Results are presented for an incident proton energy of 300 keV with various ejection energies and angles. The effect of the correlated wave function was significant for cases involving excitation to the *P* states. The contribution from these states represented an appreciable percentage of the total ddcs over all states for low and intermediate ejection energies, which was not indicated by the corresponding results from the uncorrelated wave function.

## INTRODUCTION

Previous papers have presented results of the double-differential cross section (ddcs), relative to the electron momentum and ejection angle, of electrons ejected from helium by protons from the helium ion in the ground state.[1,2] These calculations used the Born approximation with both the initial- and the final-state wave function of helium approximated by products of hydrogenlike wave functions.

This paper presents the results of similar calculations made for various excited states as well as the ground state of the helium ion. In addition, a correlated wave function is used to represent the ground-state wave function of the helium atom.

### CORRELATED WAVE FUNCTION

A 45-term correlated wave function for the ground state of the helium atom, presented in a recent paper,[3] is expressed by the expansion

$$\psi_l(\vec{r}_1, \vec{r}_2) = (4\pi)^{-1} \sum_l F_l(r_1, r_2) P_l(\cos\theta_{12}) \ ,$$

$$F_l(r_1, r_2) = \sum_{m \le n} A_{mn}(l) r_1^l r_2^l (r_1^m r_2^n + r_1^n r_2^m) \tag{1}$$

$$\times e^{-\beta(r_1 + r_2)/2} \ ,$$

in which the index $l$ has the range of 0 to 2, and

indices $m$ and $n$ have ranges of 0 to 5 with $m+n \le 6$. Although the functional form of the individual terms of this expansion appeared favorable for its application to the proposed ddcs calculation, the number of terms was regarded as excessive.

Consequently, the Rayleigh-Ritz variation method was used to construct a wave function with terms of the same functional form but with fewer terms. A 12-term wave function yielding a binding energy of 2.8985 a.u. was obtained. This is in reasonable agreement with the value of 2.9020 reported for the 45-term wave function and with the accepted experimental value of 2.9037.

This 12-term wave function was adopted for application in the ddcs calculation. The wave function is expressed by Eq. (1) with index $l$ given the values

TABLE I. Coefficients of the ground-state wave function of the helium atom as given in Eq. (1).

| $(m, n)$ | $A_{mn}(0)$ | $A_{mn}(1)$ |
|---|---|---|
| (0, 0) | 8.766 14 | -7.472 92 |
| (0, 1) | 2.912 98 | 9.680 23 |
| (0, 2) | 4.261 85 | -1.022 25 |
| (0, 3) | -0.230 101 | -0.095 520 0 |
| (1, 1) | -3.802 84 | -4.146 37 |
| (1, 2) | 0.462 243 | 1.045 30 |