

## Stark-profile calculations for the C VI line $n = 7$ to 6 at 3434 Å from dense plasmas

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The width and the profile of the strongest line in the visible spectrum of hydrogenlike carbon broadened by electric fields from ions and electrons are calculated for plasmas with electron densities from  $10^{17}$  to  $10^{19}$   $\text{cm}^{-3}$  and temperatures near 100 eV. Most of the broadening is due to ion-produced fields whose effect is evaluated with the use of the quasistatic approximation. The electron broadening both from elastic and inelastic collisions is calculated with the use of the impact approximation. Corrections for dynamical Stark effects due to relative ion-ion motion are also discussed.

### I. INTRODUCTION

A common problem in experimental plasma physics concerns the determination of electron or ion densities. In dense plasmas observations of spectral lines broadened well beyond the usual thermal Doppler width have long served<sup>1</sup> to provide a measure of the densities of charged particles which are responsible for the major part of the observed broadening. However, this method of plasma diagnostics was almost entirely restricted to plasmas of relatively low temperature ( $kT \approx 1-10$  eV) in which most line emission was from neutral or singly ionized atoms. Only in the last few years has the Stark broadening method also been applied to plasmas approaching 1-keV temperatures, especially to compressed plasmas produced by laser irradiation of glass microballoons filled with suitable gas mixtures. To provide theoretical line profiles for such applications we had calculated profiles of Lyman-series lines of carbon, oxygen, neon, magnesium, aluminum, and silicon<sup>2</sup> and also for argon.<sup>3</sup> These calculations were based on a quantum-mechanical (distorted-wave) treatment of the full Coulomb interactions between plasma electrons and the radiating ions, whose energy levels were taken to be the (linear) Stark-shifted levels in the instantaneous and local ion-produced electric field (quasistatic approximation). These profiles were then averaged over the assumed field strengths.

The present calculations involve essentially the same approximations and procedures. However,

while perturbations of the ground state vanish in the linear Stark-effect approximation and are numerically insignificant in the electron collision broadening calculations, the perturbations of the  $n = 7$  and 6 levels, which are of interest here, are comparable in magnitude. This not only causes computational difficulties because of the large matrices to be inverted in the generalized Lorentz profiles arising from the electron broadening of the numerous Stark components, but also some theoretical uncertainty. The latter arises because of strong cancellations in the broadening caused by nearly elastic collisions, which may induce simultaneous transitions between Stark levels of both principal quantum numbers. If the differences between initial and final level positions are larger than the electron plasma frequency, such simultaneous transitions would not be consistent with overall energy conservation.<sup>4</sup> However, since for the conditions of interest here the plasma frequency is always much larger than the linewidth, this difficulty should not arise, and we may assume maximum cancellation from such simultaneous transitions. In other words, we use the correct<sup>5</sup> complex conjugate in the upper-lower-state interference term of the electron collision broadening operator.

Because of the near cancellation of broadening from electron collisions causing only  $\Delta n = 0$  transitions and the relatively small rate of  $\Delta n \neq 0$  transitions, broadening by electrons, i.e., by high-frequency field fluctuations, turns out to be less important than might have been expected. The broadening calculated here is therefore mostly due

to ions, making it more important than usual to examine any deviations from the quasistatic, linear Stark-effect approximation used in the profile calculations presented here. After describing in the next section these calculations, which closely follow our previous work,<sup>2,3</sup> we discuss therefore in the

last section which theoretical errors might be expected, especially if the present results were extrapolated from the nominal conditions of  $N_e = 10^{18} \text{ cm}^{-3}$ ,  $kT = 20 \text{ eV}$ . (Such conditions are encountered, e.g., in the blowoff from laser-irradiated surfaces.<sup>6</sup>)

## II. THEORY AND CALCULATIONS

The expression for the spectral line shape  $L(\Delta\omega)$  corresponding to the approximations described above is<sup>1,2</sup>

$$L(\Delta\omega) = -\frac{1}{\pi} \text{Re Tr} \int_0^\infty dF \mathcal{W}(F) \{ D [i\Delta\omega - i(C_7 - C_6)F + \phi]^{-1} \}. \quad (1)$$

This normalized profile function is written in terms of the angular frequency separation  $\Delta\omega$  from the unperturbed line and involves taking the real part (Re) of a trace (Tr) over the doubled states<sup>1,7</sup> of the radiating ions which contribute to the lines, namely, parabolic quantum number states with  $n=7$  multiplied with the complex-conjugate states with  $n=6$ . The operator  $D$  gives the appropriate products of dipole matrix elements which govern the various spontaneous radiative transitions. The matrix elements of  $C_7 - C_6$  are the Stark coefficients of these transitions, and  $\phi$  is the electron collision operator. Finally,  $\mathcal{W}(F)$  is the distribution function of the ion-produced electric field strength.<sup>8</sup>

Generalizing our result for Lyman-series lines,<sup>2</sup> the collision operator describing nearly elastic collisions can be written as

$$\phi_{\text{el}} = -(4\pi/3v)N_e(\hbar/m)^2 \sum_i (\vec{\mathbf{R}}_7 | i \rangle \cdot \langle i | \vec{\mathbf{R}}_7 - 2\vec{\mathbf{R}}_7 \cdot \vec{\mathbf{R}}_6^* + \vec{\mathbf{R}}_6^* | i \rangle \cdot \langle i | \vec{\mathbf{R}}_6^* ) [ \frac{2}{5} + \ln(\rho_{\text{max}}/\rho_{\text{min}}) ]. \quad (2)$$

The  $\vec{\mathbf{R}}_7$  and  $\vec{\mathbf{R}}_6$  generate matrix elements (in atomic units) of the position vector operator for the radiating electron, and the sum over intermediate states is restricted to states with  $n=7$  and 6, respectively. The so-called strong collision constant  $\frac{2}{5}$  and the minimum impact parameter

$$\rho_{\text{min}} = \frac{n^2}{Z} a_0 \quad (3)$$

were determined such that the diagonal  $\phi$ -matrix elements for  $np$  states matched distorted-wave calculations<sup>2</sup> allowing for the full Coulomb interaction between the plasma electrons and the radiating ion, rather than only for monopole-dipole interactions. Since for the levels of interest here the orbital quantum number  $l$  ranges up to 6, and since the diagonal matrix elements of  $\vec{\mathbf{R}} | nlm | \rangle \cdot \langle nlm | \vec{\mathbf{R}}$  scale with  $l$  as  $(n^2 - l^2 - l - 1)$ , one might expect that for them  $\frac{2}{5}$  should be replaced by a larger constant. Much of this increase would come from inelastic collisions, which were in Ref. 2 included in the strong collision term. Instead, we will allow explicitly for inelastic collisions by adding to  $\phi_{\text{el}}$  two inelastic terms such as

$$\phi_{\text{in}} = -\frac{4\pi}{3v} \left( \frac{\hbar}{m} \right)^2 N \frac{n^2}{4Z^2} (n^2 + 3l^2) a(\delta_n, \xi_n). \quad (4)$$

This is essentially Eq. (468) of Ref. 1, except that the logarithmic factor there is replaced by the characteristic width function  $a(\delta, \xi)$  arising in the semiclassical impact-parameter calculations (see Ref. 1, Sec. II.3). Before discussing the determination of  $\rho_{\text{max}}$  in Eq. (2) and of the parameters  $\delta_n$  and  $\xi_n$  in Eq. (4), we note that using instead of  $(n^2 + 3l^2)$  the more accurate factor  $(n^2 + 3l^2 + 3l + 11)$  from Eq. (467) of Ref. 1 would probably not increase the overall accuracy of the electron broadening calculation, because for small  $l$  some of the inelastic contribution was already accounted for in the constant  $\frac{2}{5}$ . It must also be pointed out that Eq. (468) of Ref. 1 is for the width of the line rather than for the width of a level and that in it either the  $\int d\rho/\rho$  or  $\ln(\rho_{\text{max}}/\rho_{\text{min}})$  are redundant.

The maximum impact parameter in Eq. (2) is required not only because Debye screening of the perturbing electrons and Stark splitting between levels of a given  $n$  were neglected, but also because the basic assumption of negligibly short collision times may not be valid. To allow for all three effects we used, as in Ref. 2,

$$\rho_{\text{max}} = v(\omega_p^2 + \Delta\omega_s^2 + \Delta\omega^2)^{-1/2}. \quad (5)$$

In this way we avoid overestimating effects of collisions whose characteristic frequency  $v/\rho$  is small-

er than the electron plasma frequency  $\omega_p$ , the mean Stark splitting  $\Delta\omega_s$ , or the actual frequency displacement  $\Delta\omega$ . For the conditions considered in this paper,  $\omega_s \approx 13(\hbar/m)(n^2/Z)N_e^{2/3}$  according to Ref. 2, is always much larger than  $\Delta\omega$ , i.e., adiabaticity and Debye screening limit the effectiveness of collisions with large impact parameters. The argument of the logarithm in Eq. (2) is therefore

$$\rho_{\max}/\rho_{\min} \approx \frac{Zv}{n^2 a_0 (\omega_p^2 + \omega_s^2)^{1/2}}. \quad (6)$$

Using the Maxwell average of  $v^{-1}$ , i.e.,  $v_e = (\pi kT/2m)^{1/2} = 2.35 \times 10^8$  cm/sec for  $N_e = 10^{18}$  cm $^{-3}$ ,  $kT = 20$  eV, we find  $\rho_{\max}/\rho_{\min} \approx 40.3$ , corresponding to  $\ln(\rho_{\max}/\rho_{\min}) = 3.7$ . In other words, the elastic electron broadening is rather insensitive to  $\rho_{\max}$  and to the strong collision term, which contributes about 10% in this example. In the actual calculations the Maxwell average is done exactly, changing the estimate of the logarithm to 3.5 for this case.

As to the parameters in the characteristic function  $a(\delta, \xi)$  for the inelastic collisions,  $\xi$  is in the semiclassical limit given by

$$\xi = \frac{(Z-1)e^2}{\hbar v} \frac{\Delta E}{mv^2}, \quad (7)$$

while  $\delta$  is in terms of the eccentricity corresponding to the minimum impact parameter and  $\xi$ ,

$$\delta = (\epsilon - 1)\xi. \quad (8)$$

Since typically  $\frac{2}{3}$  of the matrix element in Eq. (4) corresponds to collision-induced transitions to levels with principal quantum number  $n+1$ , we used the corresponding energy difference, obtaining  $\xi_7 \approx 0.344$  for  $v = 2.35 \times 10^8$  cm/sec. Substitution of  $\rho_{\min}$  from Eq. (3) into the relation for  $\epsilon$  gives

$$\begin{aligned} \epsilon_{\min} &= \left[ 1 + \left[ \frac{mn^2 a_0 v^2}{Z(Z-1)e^2} \right]^2 \right]^{1/2} \\ &\approx \left[ 1 + \left[ \frac{\pi n^2 kT}{4Z(Z-1)E_H} \right]^2 \right]^{1/2}, \end{aligned} \quad (9a)$$

i.e.,  $\epsilon_{\min} \approx 2.14$  for  $kT = 20$  eV, or  $\delta_7 \approx 0.39$ . Since we have no consistent strong collision term for large  $l$ , one might argue that it would be better to determine  $\epsilon_{\min}$  such that the perihelion becomes  $n^2 a_0/Z$ , rather than the impact parameter. This condition gives

$$\begin{aligned} \epsilon'_{\min} &= 1 + \left[ \frac{\hbar v}{e^2} \right]^2 \frac{n^2}{Z(Z-1)} \\ &\approx 1 + \frac{\pi n^2 kT}{4Z(Z-1)E_H}, \end{aligned} \quad (9b)$$

i.e.,  $\epsilon'_{\min} \approx 2.89$ , or  $\delta'_7 \approx 0.65$ . The corresponding values of the characteristic function  $a(\delta, \xi)$  are according to Table IIIc of Ref. 1  $a \approx 1.13$  and  $a' \approx 0.68$ , respectively. The difference is about equal to the  $np$  strong collision term and we therefore used the first determination of  $\epsilon_{\min}$  to perform the Maxwell average, which gives  $a(\delta, \xi) = 1.19$  in this case.

The profile calculations using Eqs. (1)–(9a) required the inversion of the matrix representing  $[i\Delta\omega - i(C_7 - C_6)F + \phi]$  in Eq. (1) which, depending on magnetic quantum numbers of the  $n=7$  and 6 levels, has dimensions as high as 176 for  $\Delta m = \pm 1$  radiative transitions and 182 for  $\Delta m = 0$ . The matrix inversions are facilitated by the block tri-diagonal structure of the matrices.

### III. RESULTS AND DISCUSSION

A calculated profile, in the usual  $\alpha = \Delta\lambda/F_0$  units, for  $N_e = 10^{18}$  cm $^{-3}$  and  $kT = 20$  eV, is shown on Fig. 1. Such reduced profiles are rather insensitive to changes in plasma parameters. For  $kT = 100$  eV, the  $S(\alpha)$  profile is  $\sim 10\%$  narrower. Increasing the electron density to  $N_e = 10^{19}$  cm $^{-3}$  gives a profile which is  $\sim 25\%$  wider, while increasing both density and temperature to  $N_e = 10^{19}$  cm $^{-3}$  and  $kT = 100$  eV results in only  $\sim 5\%$  larger width. All these calculations were for CH $_2$ , assuming the perturbing carbon ions to be C $^{4+}$ . The Holtmark field due to ions is therefore a factor  $[(\frac{1}{3}) + 4^{3/2}(\frac{1}{6})]^{2/3} = 1.41$  larger than that due to electrons. For a pure carbon plasma, this factor would be  $4(\frac{1}{4})^{2/3} = 1.59$ , suggesting  $\sim 10\%$  differences between the corresponding field-strength distribution functions. Because of ion-ion interactions, calculated distribution functions $^8$  for various ion mixtures actually show somewhat smaller variations.

Before estimating theoretical uncertainties, which are larger than the sensitivity of  $S(\alpha)$  to most of the variations in plasma conditions just discussed, we note (see Fig. 1) that our calculated profiles are closely approximated by a (normalized) Lorentz profile of (half) halfwidth  $\alpha_{1/2} = 3.1 \times 10^{-3}$  Å/cgs field-strength units. This near-Lorentzian shape, to

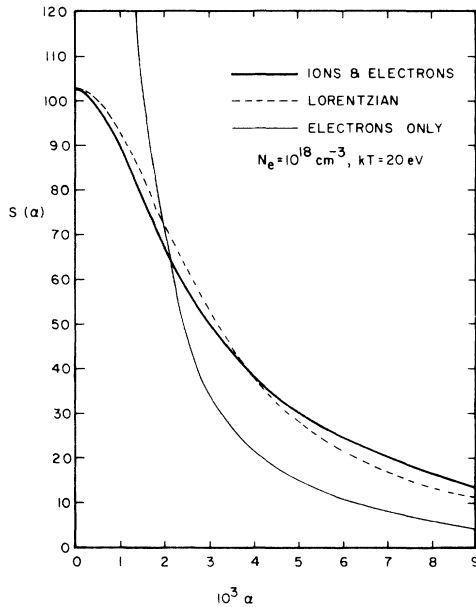


FIG. 1. Calculated Stark profile of the C VI 3434-Å line in reduced wavelength units  $\alpha = \Delta\lambda/F_0$ . Only  $\frac{1}{2}$  of the profile is shown, because the profile is symmetric around  $\Delta\lambda = (\lambda - 3434)$  Å in the approximation used. Also shown are a Lorentzian fit to the calculated Stark profile and a profile accounting only for broadening by electron collisions.

about  $\pm 10\%$ , is somewhat surprising for quasistatic broadening. On the other hand, the broadening by electrons alone is expected to be near Lorentzian, with (half) halfwidths due to elastic and inelastic collisions, respectively, of

$$W_{el} \approx \frac{4\pi}{3\nu} \left[ \frac{\hbar}{m} \right]^2 N \frac{9\bar{n}^2}{4Z^2} \left[ \frac{3}{2} + \frac{2}{e^2} \ln\left(\frac{2}{3}\bar{n}\right) \right] \times \left[ \frac{2}{5} + \ln(\rho_{\max}/\rho_{\min}) \right], \quad (10)$$

$$W_{in} \approx \frac{4\pi}{3\nu} \left[ \frac{\hbar}{m} \right]^2 N \frac{5}{4Z^2} \bar{n}^4 a(\delta_n, \xi_n). \quad (11)$$

The former relation was derived<sup>9</sup> to calculate the broadening of radio-frequency  $n$ - $\alpha$  lines by ion collisions [see also Eq. (466) of Ref. 1]. Only the strong collision constant  $\frac{2}{5}$  and the expression for  $\rho_{\max}/\rho_{\min}$ , i.e., Eq. (6) are different here. The second relation, also first derived in Ref. 9, corresponds to the sum of  $\phi_{in}$  from Eq. (4), averaged over  $l$ .

The Maxwell averages of Eqs. (10) and (11) are for our standard conditions, after transforming to the  $\alpha$  scale,  $\alpha_{el} = 0.24 \times 10^{-3}$  and  $\alpha_{in} = 0.9 \times 10^{-3}$ .

These values are considerably smaller than the halfwidth  $\alpha_{1/2}$  of the computed Stark profile which is therefore mostly determined by ion broadening. This conclusion was checked by replacing the ion field-strength distribution function by  $\delta(F)$  in the code. Considering in turn elastic and inelastic electron collisions only, we obtained narrow, near-Lorentzian profiles with  $\alpha_{1/2} \approx 0.25 \times 10^{-3}$  and  $0.85 \times 10^{-3}$ , respectively. The total electron broadening therefore amounts to  $\alpha_e \approx 1.1 \times 10^{-3}$  at  $N_e = 10^{18} \text{ cm}^{-3}$ ,  $kT = 20 \text{ eV}$ . The corresponding profile (see Fig. 1) obtained using the code is Lorentzian within  $\sim 2\%$  out to points with  $\sim 10\%$  of its peak intensity  $S_e(0) \approx 282$ . The best fit is obtained by changing the width from 1.10 to  $1.13 \times 10^{-3}$ .

The near-Lorentzian behavior of both the total Stark profile and the electron collision profile implies that quasistatic broadening by ions per se also gives near-Lorentzian profiles, with  $\alpha_{qs} \approx 2.0 \times 10^{-3}$  for CH<sub>2</sub> plasmas or  $\alpha_{qs} \approx 2.2 \times 10^{-3}$  for C plasmas. In other words, for our standard conditions almost  $\frac{2}{3}$  of the calculated broadening in the line core is due to ions. As a corollary, inelastic and elastic electron collisions are responsible for only a correspondingly small fraction of the wing intensities, namely,  $\sim \frac{1}{3}$  (see Fig. 1). As can be seen from Table I, relative contributions from the various broadening mechanisms do vary with plasma conditions, quasistatic broadening by ions contributing  $\geq \frac{2}{3}$  in most cases of experimental interest. (Note that significant emission at the highest density and lowest temperature is rather unlikely.)

Estimated errors in the broadening from elastic ( $\Delta n = 0$ ) electron collisions are of the order of the strong collision term,<sup>1,2</sup> i.e.,  $\leq 15\%$ . The inelastic collision contribution may be overestimated in our calculations, because it was calculated as if it was entirely due to  $n = 7 \rightarrow 8$  collisions and as if the entire  $\Delta n \neq 0$  dipole strength was in  $\Delta n = 1$  transitions, while actually only  $\sim \frac{2}{3}$  of this strength is in  $\Delta n = 1$  matrix elements. On the other hand, other multipole contributions (than dipole) to  $\Delta n \neq 0$  transitions were neglected, although their contribution is also of the order of the strong collision term, i.e.,  $\sim \frac{1}{3}$  of the inelastic collision broadening calculated here. We shall therefore assume an error of  $\sim 15\%$  in the calculated broadening from inelastic collisions as well. The calculations of quasistatic broadening by ions as such should be more accurate, even though the Lorentzian fit causes some additional errors. This suggests an overall error of  $\sim 10\%$  of most of the resultant widths  $\alpha_{1/2}$  present-

TABLE I. (Half) halfwidths  $\alpha_{1/2}$  of Lorentzian fits to total Stark profiles, inferred widths  $\alpha_{qs}$  (see text) due to quasistatic broadening by ions for CH<sub>2</sub> plasmas (values for C plasmas in parentheses), and contributions to the halfwidth from inelastic ( $\alpha_{in}$ ) and elastic ( $\alpha_{el}$ ) electron collisions. All widths are in reduced wavelength units  $\alpha = \Delta\lambda/F_0$  with  $\Delta\lambda$  in Å and  $F_0 = 1.25 \times 10^{-9} N_e^{2/3}$ ,  $N_e$  in cm<sup>-3</sup>. The last column gives values of the characteristic parameter for ion-dynamical corrections.

$N_e$ (cm <sup>-3</sup> )	$kT$ (eV)	$10^3\alpha_{1/2}$	$10^3\alpha_{qs}$	$10^3\alpha_{in}$	$10^3\alpha_{el}$	$\bar{\epsilon}$
$10^{17}$	20	3.0(3.1)	2.43(2.61)	0.39	0.14	0.03
$10^{18}$	20	3.1(3.3)	2.03(2.18)	0.85	0.25	0.03
$10^{18}$	100	2.8(3.0)	2.27(2.48)	0.41	0.14	0.16
$10^{19}$	20	3.9(3.9)	1.71(1.78)	1.83	0.33	0.01
$10^{19}$	100	3.2(3.3)	2.12(2.23)	0.88	0.20	0.04
$10^{19}$	200	3.2(3.4)	2.25(2.46)	0.82	0.16	0.07

ed in Table I.

While the plasma conditions and linewidths are well within the validity range of the basic (impact) approximation used to calculate the broadening caused by electrons, the validity of the quasistatic approximation for the broadening by ions, especially by protons, must be questioned. According to a systematic correction procedure<sup>10,11</sup> the dimensionless parameter characterizing the additional broadening is

$$\epsilon = \left[ \frac{v_i/r_i}{\omega_F} \right]^2, \quad (12)$$

where  $v_i$  is the relative velocity of radiating and perturbing ions and  $r_i$  their mean separation,  $r_i = (4\pi N_i/3)^{-1/3}$  in terms of the ion density  $N_i$ . The ratio of the typical frequency  $v_i/r_i$  of ion-produced field fluctuations to a typical splitting  $\omega_F$  caused by ion-produced fields enters quadratically, because first-order corrections for the time dependence of these fields cancel. In Ref. 11,  $\omega_F$  was taken as  $\sim \frac{1}{4}$  of the halfwidth. We therefore set  $\omega_F \approx 0.8 \times 10^{-3} F_0 2\pi c/\lambda^2$  in order to estimate ion-dynamical corrections in analogy to these calculations for the Lyman- $\beta$  line of hydrogen.

For mixtures, it seems reasonable to take a weighted mean of  $(v_i/r_i)^2$  for the various ions. Using the squares of the relative contributions of H<sup>+</sup> and C<sup>4+</sup> to the ionic Holtsmark field (see the beginning of this section) as weight factors, the effective mean value of  $(v_i/r_i)^2$  is then

$$\overline{(v_i/r_i)^2} \approx \frac{3kT}{M_H} \left( \frac{4}{3} \pi N_e \right)^{2/3} \frac{\left(\frac{1}{3}\right)^2 + \left(\frac{1}{6}\right)4^2\left(\frac{1}{6}\right)^2}{\left(\frac{1}{3}\right)^{4/3} + 4^2\left(\frac{1}{6}\right)^{4/3}}, \quad (13)$$

if we also take the Maxwell average and use a reduced mass of  $6M_H$  for the carbon ions ( $M_H$  is the proton mass). Corresponding mean values  $\bar{\epsilon}$  for the small parameter for dynamical corrections are listed in the last column of Table I. (For pure carbon plasmas,  $\bar{\epsilon}$  values are  $\sim 60\%$  of those listed.)

Relative corrections to Lyman- $\beta$  profiles were found to be of the order  $\sim \bar{\epsilon}/2$ . This suggests that the additional broadening is  $\leq 10\%$  for the conditions covered by Table I. However, at  $N_e = 10^{17}$  cm<sup>-3</sup>,  $kT = 100$  eV, we would have  $\bar{\epsilon} \approx 0.8$  and therefore very substantial corrections.

It is interesting to note that (small) ion-dynamical corrections would tend to further reduce the variation of  $\alpha_{1/2}$  with plasma conditions. For example, if we tentatively accept  $\bar{\epsilon}/2$  as relative correction to the halfwidth, then  $\alpha_{1/2} = 3.2 \times 10^{-3}$  (and  $3.3 \times 10^{-3}$  for pure carbon plasmas) represents corrected widths within  $\sim 5\%$  for all conditions in Table I except  $N_e = 10^{19}$  cm<sup>-3</sup>,  $kT = 20$  eV.

Pending actual calculations of broadening with allowance for the time dependence of the ion-produced field, we propose to adopt these values, with an estimated theoretical error of  $\sim 20\%$ . For density determinations from measured full width at half maximum (FWHM) widths  $\Delta\lambda$  (in Å units and corrected for Doppler broadening if necessary) one should accordingly use

$$N_e = \left[ \frac{\Delta\lambda}{8.0} \right]^{3/2} 10^{18} \quad (14)$$

in units of cm<sup>-3</sup>, for CH<sub>2</sub> plasmas, with a theoretical uncertainty of  $\lesssim 30\%$  for almost all conditions in the range of Table I. For C plasmas, 8.0 should be replaced by 8.25. Ion densities can then be calculated from the appropriate quasineutrality relations. This can usually be done without significant error,

although some corrections would be in order if most perturbing carbon ions were  $C^{5+}$  rather than  $C^{4+}$ . These corrections can be estimated by realizing that for fixed electron density quasistatic broadening scales as the cube root of the charge of the perturbing ions and that this broadening amounts to  $\sim \frac{2}{3}$  of the total broadening. In this way one obtains total widths for use in Eq. (14) which are 8.25 and 8.5 Å, respectively. Allowance for Coulomb interac-

tions and Debye screening would result in even smaller corrections.<sup>8</sup>

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