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Proton impact excitation of the ground state fine-structure transition in C II, N III and O IV

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Abstract. Cross sections and thermally averaged excitation rate coefficients are presented for proton impact excitation of the ground $1s^2 2s^2 2p\ ^2P_{1/2} - 1s^2 2s^2 2p\ ^2P_{3/2}$ transition, in C II, N III and O IV. Cross sections were calculated using the close-coupled impact parameter method which has been modified to include the higher lying levels of the doublet states of the $2s2p^2$ configuration by means of a polarization potential. Excitation rate coefficients, calculated over a wide range of temperatures, are also presented and compared with previous results.

Key words: atomic data – Sun: chromosphere – plasmas

1. Introduction

The atomic and ionic emission lines which are observed from astronomical objects may be used to deduce the electron temperatures and densities of the emitting plasma. In order to deduce these parameters, it is essential that accurate atomic data be used in theoretical models of their spectra (Dufton and Kingston, 1981). This paper presents new atomic data for proton impact excitation of astrophysically important ions in the B-like isoelectronic sequence.

Emission lines from B-like ions have been identified in the IR throug h X-ray spectral region of astrophysical and laboratory plasmas, including for example transitions within the ground configuration $2s^2 2p$ ($^2P^o_{1/2}$ – $^2P^o_{3/2}$) and the intercombination lines $2s^2 2p\ ^2P^o_J - 2s2p^2\ ^4P_{J'}$ (Pwa et al., 1984; Stencel et al., 1981). Doschek and Feldman (1976) discussed the possibility of using forbidden lines in emission line diagnostics, such as those in the ground configuration of the B-like isoelectronic sequence, and lines from ions such as O IV and Mg VIII have proven to be extremely useful as spectral diagnostics of electron densities in certain astrophysical plasmas (Doschek and Feldman, 1976; Feldman and Doschek, 1979). These include low density ($N_e \leq 10^{12}$ cm^{-3}) plasmas at temperatures between 5000 K and 2×10^5 K, regimes which are typical of stellar chromospheres and transition regions. The intensity ratios of allowed and intercombination lines in B-like ions can also be used as electron density diagnostics (for example Flower and Nussbaumer, 1975), as the population of the upper level in the ground configuration ($2s^2 2p\ ^2P^o_{3/2}$) increases with increasing electron density.

The reliable determination of theoretical line ratios is dependent on the adopted electron impact excitation rates and oscillator strengths, and for certain transitions excitation by proton collisions is also important. Seaton (1964) showed the importance of proton excitation in fine-structure transitions, where $\Delta E_{ij} \ll kT_e$ at high temperatures. In the present context, ΔE_{ij} is the energy of the ground fine-structure transition $2s^2 2p$ ($^2P^o_{1/2}$ – $^2P^o_{3/2}$).

Reid et al. (1993) showed the effect of including higher lying states in the calculation of the excitation of the fine-structure $2s^2 2p^5$ ($^2P^o_{3/2} - {}^2P^o_{1/2}$) ground term transition in F-like ions. For the present case of B-like ions, the next configuration to the ground state is $2s2p^2$, which is split into eight levels, $^4P_{1/2,3/2,5/2}$, $^2D_{3/2,5/2}$, $^2S_{1/2}$, $^2P_{1/2,3/2}$. For heavy particle excitations there is no spin change so only the 5 doublet levels of the $2s2p^2$ configuration need to be included.

2. Calculation of cross sections and excitation rate coefficients

The aim is to calculate the quadrupole fine-structure ground state transition $2s^2 2p\ ^2P_{1/2} - 2s^2 2p\ ^2P_{3/2}$ for proton impact excitations, including the virtual dipole transitions to the $2s2p^2$ doublet states by means of the polarization potential (Alder et al., 1956). Reid et al. (1993) showed that such modifications to the close-coupled impact parameter method for the F-like isoelectronic sequence decreased cross sections by up to 60%, thus showing the need for including higher lying states. For the B-like isoelectronic sequence, the calculation that includes close-coupling with the $2s2p^2$ states is a 24-state calculation (including fine-structure splitting). This simplifies to 6 close-coupled states when the polarization potential is used to take

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Table 1. Cross Sections for excitation of $^2P_{1/2}$–$^2P_{3/2}$ in C II by proton impact

C.M Impact Energy (eV)	Cross Sections (a.u.)
7.000E–01	2.2344E+00
8.000E–01	6.4045E+00
9.000E–01	1.3578E+01
1.000E+00	2.3632E+01
1.200E+00	4.9977E+01
1.400E+00	7.9677E+01
1.600E+00	1.0833E+02
1.800E+00	1.3377E+02
2.000E+00	1.5450E+02
2.200E+00	1.7092E+02
2.400E+00	1.8303E+02
2.600E+00	1.9100E+02
2.800E+00	1.9553E+02
3.000E+00	1.9773E+02
3.200E+00	1.9732E+02
3.400E+00	1.9517E+02
3.600E+00	1.9206E+02
3.800E+00	1.8769E+02
4.000E+00	1.8282E+02
4.200E+00	1.7801E+02
4.400E+00	1.7308E+02
4.600E+00	1.6784E+02
4.800E+00	1.6395E+02
5.000E+00	1.5972E+02
6.000E+00	1.4449E+02
7.000E+00	1.3579E+02
8.000E+00	1.2948E+02
1.000E+01	1.1761E+02
2.000E+01	8.4168E+01
3.000E+01	6.8274E+01

Table 2. Cross Sections for excitation of $^2P_{1/2}$–$^2P_{3/2}$ in N III by proton impact.

C.M Impact Energy (eV)	Cross Sections (a.u.)
3.000E+00	5.3503E+00
4.000E+00	1.7369E+01
4.500E+00	2.4376E+01
5.000E+00	3.1321E+01
5.500E+00	3.7868E+01
6.000E+00	4.3848E+01
6.500E+00	4.9187E+01
7.000E+00	5.3825E+01
7.500E+00	5.7733E+01
8.000E+00	6.0905E+01
8.500E+00	6.3377E+01
9.000E+00	6.5189E+01
9.500E+00	6.6394E+01
1.000E+01	6.7030E+01
1.200E+01	6.5184E+01
1.400E+01	5.9968E+01
1.600E+01	5.5686E+01
1.800E+01	5.3648E+01
2.000E+01	5.2526E+01
2.500E+01	4.8429E+01
3.000E+01	4.5781E+01
3.500E+01	4.3661E+01
4.000E+01	4.1723E+01
4.500E+01	4.0067E+01
5.000E+01	3.8551E+01
6.000E+01	3.5567E+01
7.000E+01	3.3340E+01
8.000E+01	3.1862E+01
9.000E+01	3.0672E+01
1.000E+02	2.9572E+01

account of the $2s2p^2$ states. The reason that only the $2s2p^2$ configuration is included in the calculation is that the next states that would contribute to the polarization potential (i.e., states with configuration $2s^23s$ and $2s^23p$) have much larger excitation energies than those of $2s2p^2$. For example, in C II the excitation energies from the ground configuration to the $2s^23s$ or $2s^23p$ configurations are more than three times the excitation energy from the ground configuration to the $2s2p^2$ configuration.

The collision is described by a set of coupled differential equations which depend on the classical trajectory, the excitation energies and the matrix element of the interaction. Matrix elements, therefore, need to be derived from accurate available data. Using Racah algebra and the Wigner-Ekart Theorem (Edmonds, 1975) and adopting the LS coupling scheme, we are able to relate the matrix elements to the reduced matrix elements of the electric dipole and quadrupole operators, which in turn are related to the dipole and quadrupole line strengths. When calculating the reduced matrix elements in terms of one-electron reduced matrix elements, the program TENSOR (Robb, 1973) is used, where configurations with more than one open shell can be considered, and the initial and final configurations may differ.

The matrix elements are thus related to spectroscopic quantities, and enable us to use accurate values of the dipole and quadrupole operators. The quadrupole operator gives the intramultiplet matrix elements. There is a similarity between the B-like $2s^22p\ ^2P$ case and the F-like $2s^22p^5\ ^2P$ case, as they differ only in sign, while the B-like $2s2p^2\ ^2P$ case is the same as the F-like $2p^5\ ^2P$ case. The dipole operator gives the coupling matrix elements between configurations.

Excitation energies for C II were taken from Blum and Pradhan (1992) and line strengths were from Frose Fischer (1994). The atomic data needed for the calculation of the remaining ions were taken from Bashkin and Stoner (1978), and electric dipole line strengths were obtained from Cheng, Kim and Desclaux (1979).

Excitation rate coefficients were obtained by averaging the cross sections over a Maxwellian distribution for a range of temperatures. The calculated cross sections are supplemented at lower energies by cross sections calculated by a first order

Table 3. Cross Sections for excitation of $^2P_{1/2}$–$^2P_{3/2}$ in O IV by proton impact.

C.M Impact Energy (eV)	Cross Sections (a.u.)
5.000E+00	3.2354E–01
6.000E+00	1.2159E+00
7.000E+00	2.8331E+00
8.000E+00	5.0293E+00
8.500E+00	6.2708E+00
9.000E+00	7.5711E+00
1.000E+01	1.0248E+01
1.200E+01	1.5451E+01
1.400E+01	1.9961E+01
1.600E+01	2.3573E+01
1.800E+01	2.6203E+01
2.000E+01	2.7910E+01
2.200E+01	2.8790E+01
2.400E+01	2.8960E+01
2.600E+01	2.8564E+01
2.800E+01	2.7777E+01
3.000E+01	2.6789E+01
3.200E+01	2.5775E+01
3.400E+01	2.4861E+01
3.600E+01	2.4129E+01
3.800E+01	2.3598E+01
4.000E+01	2.3231E+01
5.000E+01	2.2146E+01
6.000E+01	2.0815E+01
7.000E+01	1.9712E+01
8.000E+01	1.8858E+01
1.000E+02	1.7655E+01
1.500E+02	1.5524E+01
2.000E+02	1.4033E+01
3.000E+02	1.1668E+01

theory, modified to take account of the polarization potential (Foster and Reid, 1995).

3. Results

In Tables 1-3 we present the cross sections for the fine structure ground transition $2s^22p\ ^2P_{1/2} - 2s^22p\ ^2P_{3/2}$ for C II, N III and O IV, respectively.

Tables 4-6 contain the thermally-averaged excitation rate coefficients for the three ions.

An interesting point is that for the low ionized species, the polarization potential was found to decrease the ^2P cross sections, whereas for the highly ionized ones the polarization potential increased the cross sections. The effect of the polarization potential is to replace $1/R^3$ in the intramultiplet coupling matrix-elements by $1/R^3 + c/R^4$. The parameter c involves a sum of contributions from the nine $2s2p^2$ states. We found that the sign of the c parameter was negative for the low ionized ions and positive for the highly ionized ions, which explains the change, with increasing Z, of the effect of polarization. However, only

Table 4. Excitation Rate Coefficients for $^2P_{1/2} - {}^2P_{3/2}$ in C II by proton impact

Temperature (K)	Rates ($cm^3\ s^{-1}$) p
1.00E+03	3.38595E–13
1.50E+03	6.17953E–12
2.00E+03	3.10831E–11
3.00E+03	1.86742E–10
5.00E+03	9.55999E–10
7.00E+03	2.07787E–09
1.00E+04	3.84479E–09
1.50E+04	6.28700E–09
2.00E+04	8.03312E–09
3.00E+04	1.02052E–08
4.00E+04	1.14531E–08
5.00E+04	1.22459E–08
6.00E+04	1.27870E–08
7.00E+04	1.31746E–08
8.00E+04	1.34621E–08
1.00E+05	1.38481E–08
1.50E+05	1.42650E–08
2.00E+05	1.43416E–08
3.00E+05	1.41334E–08
4.00E+05	1.37643E–08

Table 5. Excitation Rate Coefficients for $^2P_{1/2} - {}^2P_{3/2}$ in N III by proton impact

Temperature (K)	Rates ($cm^3\ s^{-1}$) p
3.00E+03	1.28570E–13
3.50E+03	4.29849E–13
4.00E+03	1.11279E–12
4.50E+03	2.40890E–12
5.00E+03	4.57648E–12
6.00E+03	1.25675E–11
7.00E+03	2.69766E–11
8.00E+03	4.92159E–11
1.00E+04	1.20102E–10
1.50E+04	4.45180E–10
2.00E+04	9.17806E–10
2.50E+04	1.45450E–09
3.00E+04	1.99954E–09
4.00E+04	3.01176E–09
5.00E+04	3.87148E–09
6.00E+04	4.58552E–09
7.00E+04	5.17964E–09
8.00E+04	5.67879E–09
1.00E+05	6.46847E–09
1.50E+05	7.73543E–09

Table 6. Excitation Rate Coefficients for $^2P_{1/2} - {}^2P_{3/2}$ in N III by proton impact

Temperature (K)	Rates (cm^3 s^{-1}) p
6.50E+03	6.36294E–14
7.00E+03	1.16660E–13
7.50E+03	1.99915E–13
8.00E+03	3.23837E–13
9.00E+03	7.42264E–13
1.00E+04	1.47930E–12
1.50E+04	1.40284E–11
2.00E+04	4.97923E–11
2.50E+04	1.13873E–10
3.00E+04	2.05023E–10
4.00E+04	4.50044E–10
5.00E+04	7.44767E–10
6.00E+04	1.05724E–09
8.00E+04	1.66481E–09
1.00E+05	2.20323E–09
1.50E+05	3.22641E–09
2.00E+05	3.92058E–09
2.50E+05	4.41942E–09
3.00E+05	4.79835E–09
3.50E+05	5.09915E–09

low ionised ions of astrophysical importance are considered in this paper.

The present calculations may be compared with the work of Hayes and Nussbaumer (1984) for C II, Nussbaumer and Storey (1979) for N III and Flower and Nussbaumer (1975) for O IV. These are shown in Table 7 for a few temperatures. An inspection of the table reveals that the present calculations for N III are up to a factor of ~3 different from those of Nussbaumer and Storey (1979), with discrepancies for the C II and O IV results ranging up to ~40%.

It is hoped that the present work will compliment the calculations of electron impact excitations for Boron-like ions, for example the work of Blum and Pradhan (1992), and Lennon et al. (1985). The work of O'Shea et al. (1995) shows the use of the rates presented here in diagnostic research.

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Table 7. Comparison of present excitation rate calculations for the $^2P_{1/2} - {}^2P_{3/2}$ transition with those of previous authors

T_e/K	C II Present	HN[a]	N III Present	NS[b]	O IV Present	FN[c]
5E+03	9.55E–10	1.03E–09				
1E+04	3.84E–09	4.39E–09	1.20E–10	1.41E–10		
2E+04	8.03E–09	9.87E–09	9.17E–10	1.18E–09		
5E+04					7.44E–10	5.58E–10
6E+04	1.27E–08	1.80E–08	4.58E–09	1.08E–08		
1E+05			6.46E–09	2.06E–08	2.20E–09	1.83E–09
2E+05					3.92E–09	3.55E–09

[a] Hayes and Nussbaumer (1984)
[b] Nussbaumer and Storey (1979)
[c] Flower and Nussbaumer (1975)

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