Astron. Astrophys. 336, 393–396 (1998)

ASTRONOMY AND ASTROPHYSICS

Proton impact excitation of the $1s^2 2s2p\ ^3P$ fine-structure transitions in the Be-like ions C III, N IV, and O V

R.S.I. Ryans[1,⋆], V.J. Foster-Woods[1], R.H.G. Reid[2,⋆⋆], F.P. Keenan[1,⋆⋆⋆], and F. Copeland[1]

[1] Department of Pure and Applied Physics, Queen's University, Belfast, BT7 1NN, Northern Ireland, UK
[2] Department of Applied Mathematics and Theoretical Physics, Queen's University, Belfast, BT7 1NN, Northern Ireland, UK

Received 10 February 1998 / Accepted 6 May 1998

Abstract. Cross sections and thermally averaged excitation rate coefficients are presented for proton impact excitations of the $1s^2 2s2p\ ^3P$ fine-structure transitions in the Be-like ions C III, N IV, and O V. The cross sections were calculated using a close-coupled impact parameter method that has been modified to include the higher lying levels of the triplet states of the $2p^2$, 2s3s, and 2s3d configurations. Excitation rate coefficients have been calculated using these cross-sections for a wide range of temperatures.

Key words: atomic data – Sun: chromosphere

1. Introduction

A number of important solar and stellar diagnostic lines arise from transitions in Be-like atoms, their ratios being used to obtain information on parameters such as electron density or temperature structure (e.g. Jordan 1974, Keenan et al. 1995, Keenan & Warren 1993). In most cases line ratios for collisionally induced transitions are dominated by electron impacts (Mason & Monsignori Fossi 1994). However, Seaton (1964) showed that proton collisions can be significant in fine-structure transitions, where the energy of the impacting proton exceeds the excitation energy. For example, Doyle et al. (1980) found that in solar-type plasmas the predicted strength of the electron density sensitive line ratio $I(2s2p\ ^3P \rightarrow 2p^2\ ^3P)/I(2s^2\ ^1S \rightarrow 2s2p\ ^1P)$ in Be-like ions is decreased by up to 25 percent when proton rates are included for the $2s2p\ ^3P_J \rightarrow 2s2p\ ^3P_{J'}$ fine-structure transitions.

In November 1993 the Spectroscopic Diagnostics Working Group for the ESA/NASA SOHO (Solar and Heliospheric Observatory) mission noted the importance of proton excitation effects in the analysis of data from both the CDS (Coronal Diagnostic Spectrometer) and SUMER (Solar UV Measurements of Emitted Radiation) instruments. They called for the accuracy of the available proton excitation data to be assessed, in a manner similar to that performed for electron impact excitation rates (Lang 1994). Copeland et al. (1997) compiled and assessed proton impact fine-structure excitation data for Be- to Cl-like ions, and found that the best available data for Be-like ions (Doyle 1987 [hereafter D87], Malinovsky 1975, Masnou-Seeuws & McCarroll 1972, Bhatia et al. 1980, Feldman et al. 1980) was accurate to within 25 percent.

However, Reid et al. (1993) and Foster et al. (1996, 1997) demonstrated the importance of including the effects of higher lying states in the calculation of ground term fine-structure transitions in F-like and B-like ions. We have therefore extended this work to Be-like ions, and calculated proton excitation cross sections and rate coefficients for transitions among the $1s^2 2s2p\ ^3P^o_J$ fine-structure levels of several ions of importance in solar physics, namely C III, N IV, and O V. We compare these results with the work of D87.

2. Calculation of cross sections and excitation rate coefficients

The cross sections for transitions between the $1s^2 2s2p\ ^3P^o_J$ fine-structure levels were calculated using the technique we previously applied to F-like and B-like ions (cf Foster et al. 1996, 1997). The collision is treated by the symmetrized close-coupled semi-classical method, with the proton following a hyperbolic Coulomb trajectory, as described by Alder & Winther (1975) for the case of Coulomb excitation of nuclei. However, we modify the interaction matrix elements so that they are not simply the long-range forms, but rather allow for the possibility that the proton can penetrate the ion's electron cloud. This is achieved by multiplying the long-range forms by a 'penetration factor' which ensures that the matrix elements have the correct short-range forms. The penetration factor is estimated by using appropriately scaled hydrogenic radial integrals (cf Doyle et al. 1980).

We also modify the interaction matrix elements to include the effects of dipole coupling to nearby terms by means of a polarization potential. This modification is especially significant in the current calculation. The importance of allowing for polarization in the interaction was first noted by Heil et al. (1982, 1983). We incorporate it using the method of Alder & Winther (1975). The effect of polarization is to replace the factor R^{-3} that appears in the asymptotic forms of all the quadrupole-coupling

Send offprint requests to: R.S.I. Ryans
⋆ e-mail: R.Ryans@qub.ac.uk
⋆⋆ e-mail: R.Reid@qub.ac.uk
⋆⋆⋆ e-mail: F.Keenan@qub.ac.uk

matrix elements by the factor $R^{-3}(1 + C_{\rm pol}/R)$, where R is the proton-ion separation. For LS-coupling $C_{\rm pol}$ is the same for all matrix elements. In the present case of excitation within the 2s2p ^{3}P^o multiplet, we have included dipole coupling to the 2p^2 ^{3}P, 2s3s ^{3}S, and 2s3d ^{3}D terms in the polarization potential. The resulting values of $C_{\rm pol}$ were large: –0.898 for C III; –0.750 for N IV, and –0.654 for O V. The major contribution to these values of $C_{\rm pol}$ comes from the 2p^2 ^{3}P term. The effect of these large negative values of $C_{\rm pol}$ is to reduce the cross sections significantly, especially at higher impact energies where smaller values of R can occur on the classical trajectories.

The magnitudes of the interaction matrix elements, including those involved in the polarization potential, are determined from the best available line-strengths, while their signs are taken to be those that would arise from LS-coupled hydrogenic orbitals. The atomic data required for the present calculation, namely the dipole and quadrupole line strengths together with the excitation energies, were taken from Wiese et al. (1996).

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 first order theory, modified to take account of the polarization potential (Foster 1994).

In our previous work on F-like and B-like ions (Foster et al. 1996, 1997), we estimated the accuracy of our calculated cross sections and rates to be about 10 percent. This figure was based on our experience of: the reliability of using the symmetrized semi-classical (rather than the fully quantal) treatment of the proton-ion relative motion; the numerical accuracy of the solution of the close-coupled differential equations; and the sensitivity of the cross sections to the physical features, such as the cloud-penetration and the polarization potential, that we treat only approximately. The same considerations apply to the current calculation, but in view of the large reductions caused by the introduction of the polarization potential, we incline to place the accuracy at about 20 percent.

3. Results

For simplicity, we use the following notation to refer to the transitions we consider:

- 0→1 : 1s^{2}2s2p ^{3}P$^o_0$ → 1s^{2}2s2p ^{3}P$^o_1$
- 0→2 : 1s^{2}2s2p ^{3}P$^o_0$ → 1s^{2}2s2p ^{3}P$^o_2$
- 1→2 : 1s^{2}2s2p ^{3}P$^o_1$ → 1s^{2}2s2p ^{3}P$^o_2$

In Fig. 1 we compare our cross sections for C III, N IV, and O V to those of D87 for the above transitions. Table 1 lists the corresponding thermally-averaged excitation rate coefficients, and in Fig. 2 we compare these results to the excitation rates reported in D87.

Fig. 1 illustrates the good agreement between the D87 cross sections and the values produced by our models when the effects of the polarization potential are excluded. However, inclusion of the polarization potential term clearly leads to a significant reduction in both cross sections, and excitation rate coefficients (Fig. 2). For example, the 0→1 cross sections in O V are reduced by up to a factor of 4, and the corresponding excitation

Table 1. Excitation rate coefficients for 1s^{2}2s2p ^{3}P^o_J → 1s^{2}2s2p ^{3}P$^o_{J'}$ by proton impact. The temperature of maximum fractional abundance in ionization equilibrium (Arnaud & Rothenflug 1985) is underlined for each ion.

T (K)	Rate coefficient (cm^3 s^{-1})		
	0→1	0→2	1→2
C III			
3.0E+03	4.96E–15	4.64E–12	8.25E–12
4.0E+03	3.57E–14	2.11E–11	3.07E–11
6.0E+03	4.04E–13	1.17E–10	1.35E–10
1.0E+04	5.37E–12	5.80E–10	5.51E–10
2.0E+04	8.58E–11	2.46E–09	2.03E–09
3.0E+04	2.87E–10	4.25E–09	3.41E–09
4.0E+04	5.60E–10	5.63E–09	4.51E–09
6.0E+04	1.15E–09	7.46E–09	6.08E–09
<u>8.0E+04</u>	1.67E–09	8.59E–09	7.11E–09
1.0E+05	2.09E–09	9.35E–09	7.85E–09
1.5E+05	2.82E–09	1.05E–08	9.02E–09
2.0E+05	3.24E–09	1.12E–08	9.73E–09
4.0E+05	3.77E–09	1.26E–08	1.11E–08
8.0E+05	3.55E–09	1.36E–08	1.17E–08
1.5E+06	2.84E–09	1.36E–08	1.14E–08
N IV			
4.00E+03	1.99E–17	3.77E–14	1.33E–13
6.00E+03	8.03E–16	8.35E–13	1.89E–12
8.00E+03	7.09E–15	4.82E–12	8.48E–12
1.00E+04	3.18E–14	1.52E–11	2.27E–11
2.00E+04	1.56E–12	2.18E–10	2.26E–10
3.00E+04	9.84E–12	6.37E–10	5.78E–10
6.00E+04	1.14E–10	2.17E–09	1.77E–09
1.00E+05	3.91E–10	3.70E–09	2.98E–09
<u>1.50E+05</u>	7.71E–10	4.83E–09	3.95E–09
2.00E+05	1.10E–09	5.50E–09	4.58E–09
3.00E+05	1.56E–09	6.29E–09	5.35E–09
4.00E+05	1.83E–09	6.75E–09	5.81E–09
6.00E+05	2.07E–09	7.27E–09	6.31E–09
1.00E+06	2.07E–09	7.71E–09	6.66E–09
2.00E+06	1.63E–09	7.79E–09	6.55E–09
O V			
8.00E+03	1.61E–17	2.63E–14	9.36E–14
1.00E+04	1.37E–16	1.60E–13	4.41E–13
1.50E+04	3.62E–15	2.35E–12	4.40E–12
2.00E+04	2.57E–14	1.08E–11	1.61E–11
3.00E+04	2.80E–13	5.89E–11	6.99E–11
5.00E+04	3.44E–12	2.87E–10	2.76E–10
7.00E+04	1.37E–11	6.20E–10	5.47E–10
1.00E+05	4.72E–11	1.16E–09	9.66E–10
1.50E+05	1.45E–10	1.94E–09	1.57E–09
<u>2.00E+05</u>	2.71E–10	2.51E–09	2.03E–09
4.00E+05	7.42E–10	3.65E–09	3.05E–09
8.00E+05	1.15E–09	4.36E–09	3.75E–09
1.00E+06	1.20E–09	4.51E–09	3.89E–09
1.50E+06	1.17E–09	4.68E–09	4.01E–09
3.00E+06	8.78E–10	4.63E–09	3.86E–09

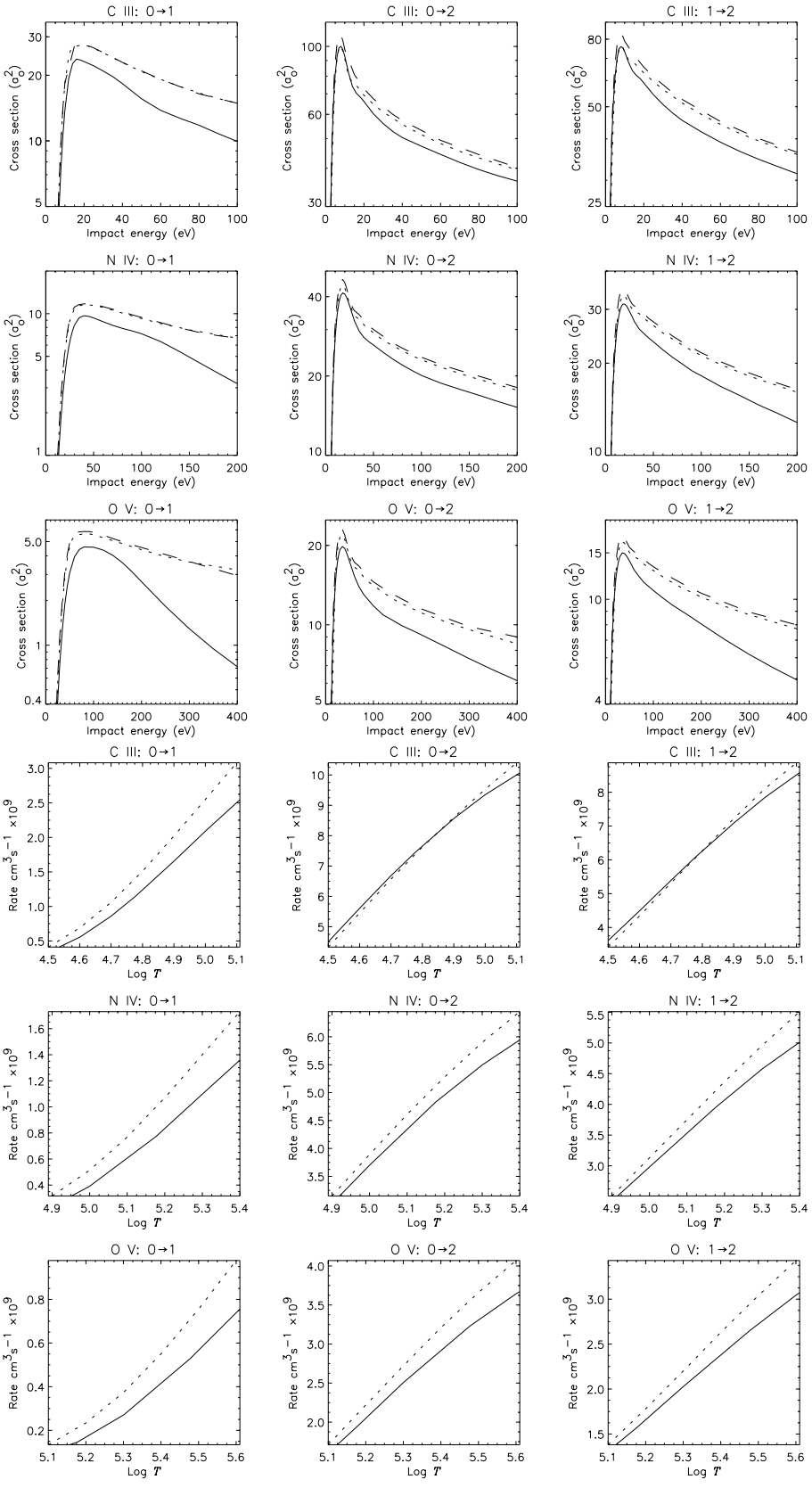

Fig. 1. Comparison of new proton impact cross sections to those of D87. Dotted lines represent results from D87, dashed lines represent new calculations *without* the polarization potential, solid lines represent cross sections *including* the polarization potential.

Fig. 2. Comparison of new proton impact excitation rates to those of D87. Dotted lines represent results from D87, solid lines represent new rates including the polarization potential.

rate coefficients are reduced by up to 25 percent. The effect is even greater for more heavily ionised atoms in the Be-like isoelectronic sequence, but many of these ions are of little astrophysical significance, and so lie outside the scope of this discussion. However, cross sections and excitation rate coefficients for these ions may be obtained electronically from the authors.

Clearly, including the effects of higher-lying states via the polarization potential can cause significant changes to proton impact fine-structure cross-sections and excitation rate coefficients. It is therefore important that these results are included in the analysis of emission line diagnostics (e.g. Keenan et al. 1993, 1995). We intend to continue this work to examine the effect of the polarization potential on other isoelectronic sequences whose species can be observed in the CDS and SUMER wavelength ranges .

Acknowledgements. RSIR, VJFW, and FC acknowledge financial support from the United Kingdom Particle Physics and Astronomy Research Council.

References

Arnaud M., Rothenflug R., 1985, A&AS 60, 425
Alder K., Winther A., 1975, in Electromagnetic Excitation: Theory of Coulomb Excitation with Heavy Ions. North-Holland, Oxford
Bhatia A.K., Feldman U., Doschek G.A., 1980, A&A 51, 1464
Copeland F., Reid R.H.G., Keenan F.P., 1997, At. Data Nuc. Data Tables 67, 179
Doyle J.G., 1987, At. Data Nuc. Data Tables 37, 441
Doyle J.G., Kingston A.E., Reid R.H.G., 1980, A&A 90, 97
Feldman U., Doschek G.A., Cheng C., 1980, J. Appl. Phys. 51, 190
Foster V.J., 1994, Ph.D. Thesis, The Queen's University of Belfast
Foster V.J., Keenan F.P., Reid R.H.G., 1996, A&A 308, 1009
Foster V.J., Reid R.H.G., Keenan F.P., 1997, MNRAS 288, 973
Heil T.G., Green S., Dalgarno A., 1982, Phys. Rev. A26, 3293
Heil T.G., Kirby K., Dalgarno A., 1983, Phys. Rev. A27, 2826
Jordan C., 1974, A&A 34, 69
Keenan F.P., Warren G.A., 1993, Sol. Phys. 146, 19
Keenan F.P., Brekke P., Byrne P.B., Greer C.J., 1995, MNRAS 276, 915
Lang J., 1994, At. Data Nuc. Data Tables 57, 1
Malinovsky M., 1975, A&A 43, 101
Masnou-Seeuws F., McCarroll R., 1972, A&A 17, 441
Mason H.E., Monsignori Fossi B.C., 1994, A&A Rev 6, 123
Reid R.H.G., Foster V.J., Keenan F.P., 1993, UV and X-ray Spectroscopy of Laboratory and Astrophysical Plasmas, p. 154, Cambridge University Press
Seaton M.J., 1964, MNRAS 127, 191
Wiese W.L., Fuhr J.R., Deters T.M., 1996, J. Phys. Chem. Ref. Data Monograph 7