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Proton impact excitation of the $1s^2 2s^2 2p^2\ ^3P$ fine-structure transitions in carbon-like ions

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Abstract. We present new cross sections and thermally averaged excitation rate coefficients for proton impact excitation of the $1s^2 2s^2 2p^2\ ^3P$ fine-structure transitions for ions in the carbon isoelectronic sequence. These data have been calculated using a close-coupled impact parameter method that incorporates the effects of higher lying levels of the triplet $2s2p^3$ configuration. We find that the inclusion of these additional states leads to significant reductions in excitation rates for high-Z ions.

Key words: Sun: chromosphere – atomic data

1. Introduction

A number of emission lines arising from collisionally induced transitions within the fine-structure levels of the ground state of carbon-like ions are observed in astronomical plasmas. Many N II, O III, Ne V, Mg VII, Ca XV and Fe XXI features are used as diagnostics in H II regions, planetary nebulae, and solar-type stars (see, for example, Keenan et al. 1992, 1996; Espey et al. 1996). In many cases line ratios for collisionally induced transitions are dominated by electron impacts. However, Seaton (1964) demonstrated that proton collisions can be important in the excitation of fine-structure levels, where the energy of the impacting proton exceeds the excitation energy.

The importance of proton impact excitation effects in the analysis of data from the ESA/NASA SOHO (Solar and Heliospheric Observatory) mission was noted by the SOHO Spectroscopic Diagnostics Working Group in November 1993, and led to the Copeland et al. (1997) review of the available atomic data. In response to this perceived need for reliable proton excitation data, we have previously examined the importance of including the effects of higher lying terms in ground state fine-structure calculations for F-, B-, and Be-like ions (Foster et al. 1994, 1996, 1997; Ryans et al. 1998). The inclusion of these higher terms via a polarization potential can significantly affect collisional excitation cross sections and rate coefficients. In this paper we report on our extension of this technique to ions in the C-like isoelectronic sequence, and compare these results to the calculations of Faucher (1977, hereafter F77) and Faucher et al. (1980, hereafter FMP80).

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2. Calculation of cross sections and excitation rate coefficients

We adopt the following notation to refer to the transitions under consideration:

- 0→1: $1s^2 2s^2 2p^2\ ^3P_0^o \rightarrow 1s^2 2s^2 2p^2\ ^3P_1^o$
- 0→2: $1s^2 2s^2 2p^2\ ^3P_0^o \rightarrow 1s^2 2s^2 2p^2\ ^3P_2^o$
- 1→2: $1s^2 2s^2 2p^2\ ^3P_1^o \rightarrow 1s^2 2s^2 2p^2\ ^3P_2^o$

Cross sections for these transitions were calculated by the symmetrized, close-coupled, semi-classical method that we have used previously (Foster et al. 1994, 1996, 1997; Ryans et al. 1998). This method is essentially the same as that described by Alder & Winther (1975) for Coulomb excitation of nuclei, except for two modifications to the interaction matrix elements. Firstly, we allow for the short-range forms of the matrix elements (rather than using the asymptotic forms for all values of the proton-ion separation, R), and secondly we allow for electric-dipole ($\mathcal{E}1$) coupling between the ground term and higher terms by a polarization potential.

We determine each required R-dependent matrix element as follows. Firstly, noting that if the coupling is by the $\mathcal{E}\lambda$ component of the interaction then the asymptotic form of the matrix element is $AR^{-\lambda-1}$, we derive the magnitude of A from the best available line strength, and take the sign of A to be that of the *LS*-coupled form with a hydrogenic radial-integral $\langle n\ell|r^\lambda|n'\ell'\rangle$. Secondly, the R-dependent factor by which the asymptotic form is multiplied to give the general form is taken to be that arising in the hydrogenic radial-integral $\langle n\ell|\ \min(r,R)^\lambda/\max(r,R)^{\lambda+1}|n'\ell'\rangle$, with the effective charge chosen to reproduce the asymptotic coefficient A (c.f. Doyle et al. 1980).

For the matrix elements between the states of the $2s^2 2p^2\ ^3P$ term, the $\mathcal{E}2$ line strength data that we have used for O III are those given by Wiese et al. (1996), while for the other ions we have used the results of Cheng et al. (1979). The *LS*-coupling expressions for the $^3P_0$–$^3P_2$ and the $^3P_1$–$^3P_2$ line strengths are

Table 1. Effective $\langle 2p|r^2|2p\rangle$ calculated from the $\mathcal{E}2$ line strength for the J–J' transitions in the $2s^2 2p^2\ ^3P$ term. Polarization coefficients $C_{JJ'}$ in the factor $(1 + C_{JJ'}/R)$ in the J–J' coupling within the $2s^2 2p^2\ ^3P$ term. Approx. A and B refer to the sets of excited terms included in the polarization potential (see text for details).

Ion	Effective $\langle 2p\|r^2\|2p\rangle$		Polarization Coefficient $C_{JJ'}$ Approx. A		Approx. B	
	0–2	1–2	0–2	1–2	0–2	1–2
O III	1.147	1.164	–0.229	–0.229	–0.135	–0.135
Ne V	0.581	0.580	–0.154	–0.154	–0.117	–0.117
Mg VII	0.351	0.350	–0.131	–0.131	–0.108	–0.108
Ca XV	0.103	0.096	–0.068	–0.074	–	–
Fe XXI	0.062	0.047	–0.045	–0.061	–0.041	–0.057

$\frac{2}{5}\langle 2p|r^2|2p\rangle^2$ and $\frac{9}{10}\langle 2p|r^2|2p\rangle^2$, respectively. The 'effective $\langle 2p|r^2|2p\rangle$' values deduced from the 0→2 and the 1→2 line strength data using these expressions are shown in Table 1. The closeness of the 0→2 and the 1→2 values for the light ions shows that *LS*-coupling is a good approximation for these ions. For the diagonal matrix elements $^3P_1$ – $^3P_1$ and $^3P_2$ – $^3P_2$, we used the *LS*-coupling expression with a mean value for $\langle 2p|r^2|2p\rangle$. For each element the short range factor is determined from the effective $\langle 2p|r^2|2p\rangle$ value.

The importance of modifying the interaction matrix elements to allow for polarization was noted by Heil et al. (1982, 1983). We incorporate these effects by a polarization potential calculated using the method given in Sect. II.6 of Alder & Winther (1975). The advantage of this method is its simplicity. We select a set of excited terms which are coupled to the ground term by the $\mathcal{E}1$ component of the interaction; the required data are the $\mathcal{E}1$ line strengths (to determine the matrix elements) and the excitation energies. The disadvantages are that it may be difficult to include sufficient excited terms in this way, and that charge-transfer contributions are excluded (c.f. Heil et al. 1983). In the present case of a $^3P^e$ ground term, the terms that can contribute to the polarization have symmetry $^3S^o$, $^3P^o$, or $^3D^o$. We have adopted two approximations:

– *Approx. A*: include only $2s2p^3\ ^3D^o$, $^3P^o$, $^3S^o$
– *Approx. B*: as Approx. A, plus $2p3s\ ^3P^o$ and $2p3d\ ^3D^o$, $^3P^o$

The purpose of Approx. B is to test Approx. A. There is no other justification for including the 2p3*l* (*l* = s,d) terms while excluding the $2s2p^2 3p$ terms. Also, we simplified the present calculation by using the multiplet strength for each excited term, then deducing the level-to-level line strengths on the basis of *LS*-coupling.

The effect of introducing the polarization potential is to replace the factor R^{-3} in the asymptotic form of the $2p^2\ ^3P_{JM}$ – $2p^2\ ^3P_{J'M'}$ matrix elements by $R^{-3}(1 + C_{JJ'}/R)$. In pure *LS*-coupling, $C_{JJ'}$ is independent of J and J'. The values of $C_{JJ'}$ resulting from the two approximations are shown in Table 1. The $\mathcal{E}1$ line strength data and the excitation energy data (including those for the $2s^2 2p^2\ ^3P$ terms) that we used were taken from the following sources: O III – Wiese et al. (1996); Ca XV – Cheng et al. (1979); Ne V, Mg VII, Fe XXI – CHIANTI database (Dere et al. 1997).

It is clear from Table 1 that, for the lighter ions, the polarization coefficients have not converged. This is not surprising, since for O III the excitation energies of the $2s^2 2p3l$ and the $2s2p^2 3l$ terms are only about twice those of the $2s2p^3$ terms. In contrast, for Fe XXI this ratio of excitation energies is about eight, and this is reflected in the improved convergence of the $C_{JJ'}$ values. However, the values of $C_{JJ'}$ are sufficiently small for the light ions that polarization has little effect, except at very high impact energies. In contrast, for Fe XXI the effect of polarization is important for all significant impact energies, and for this species the results from the two polarization approximations are very close. Therefore, when the polarization has not converged (i.e. for the lighter ions) its effects are negligible, whereas when polarization is important (i.e. for the heaver ions) its representation by Approx. A is sufficient. This leads us to conclude that our representation of polarization effects is entirely adequate for the calculation of the $2s^2 2p^2\ ^3P_J \rightarrow 2s^2 2p^2\ ^3P_{J'}$ cross sections.

We derived the rate coefficients from the corresponding calculated cross sections by the usual Maxwellian averaging. In the low energy tail of the cross sections, where close-coupling calculations become difficult, first order cross sections, modified to take account of polarization (Foster 1994), were used.

The estimated accuracy of our cross sections depends both on the impact energy and the ion. For impact energies in the region of the cross section maximae, the uncertainties in the O III cross sections are largely due to the collision treatment and to the uncertainties in the $\mathcal{E}2$ line strengths, and we would place them at about 10%. For Fe XXI, again near the cross section maximae, our error estimate rises to about 20% because polarization has such a significant effect. For all the ions, the uncertainties in the cross sections increase with impact energy due to our approximate treatment of the short-range forms of the matrix elements, perhaps rising by a further 10% at the largest impact energies. Similar estimates apply to our calculated rate coefficients, namely 10% for O III rising to 20% for Fe XXI at temperatures where the rates are increasing, but rising by a further 10% at temperatures where the rate coefficients are maximum.

3. Results

In Fig. 1 we compare our cross sections for O III, Ne V, Mg VII, Ca XV, and Fe XXI to the quantal results of F77 / FMP80. We have used Approx. B to calculate each of these, with the exception of Ca XV, for which Approx. A only was used due to a lack of reliable atomic data. In Fig. 2 we compare the corresponding thermally averaged excitation rate coefficients for the same ions, and these are also listed in Table 2.

As discussed in Sect. 2, we found that polarization had little effect on the cross sections for the lighter ions. Thus for O III, Ne V, and Mg VII the difference between our cross sections and those of FMP80 are not great, and are due to differences in the adopted values of $\langle 2p|r^2|2p\rangle$ and to our use of matrix elements that are modified at short range.

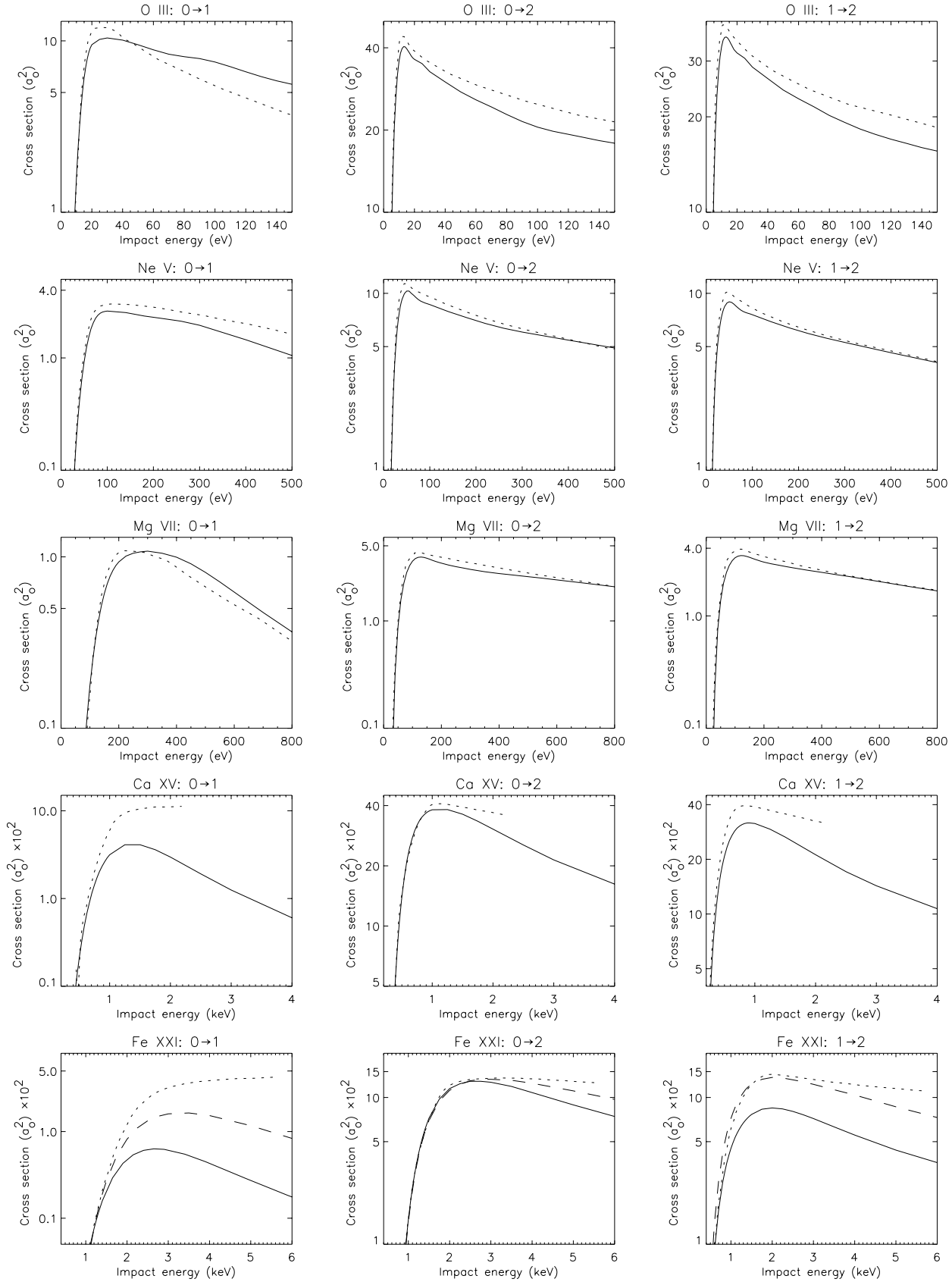

Fig. 1. Comparison of new proton collision impact cross sections to those of FMP80 (O III, Ne V, Mg VII) and F77 (Ca XV, Fe XXI). Dotted lines represent results from F77 / FMP80, solid lines represent the present calculation including the polarization potential. Dashed lines for Fe XXI represent the present calculation without polarization using data from F77, see text.

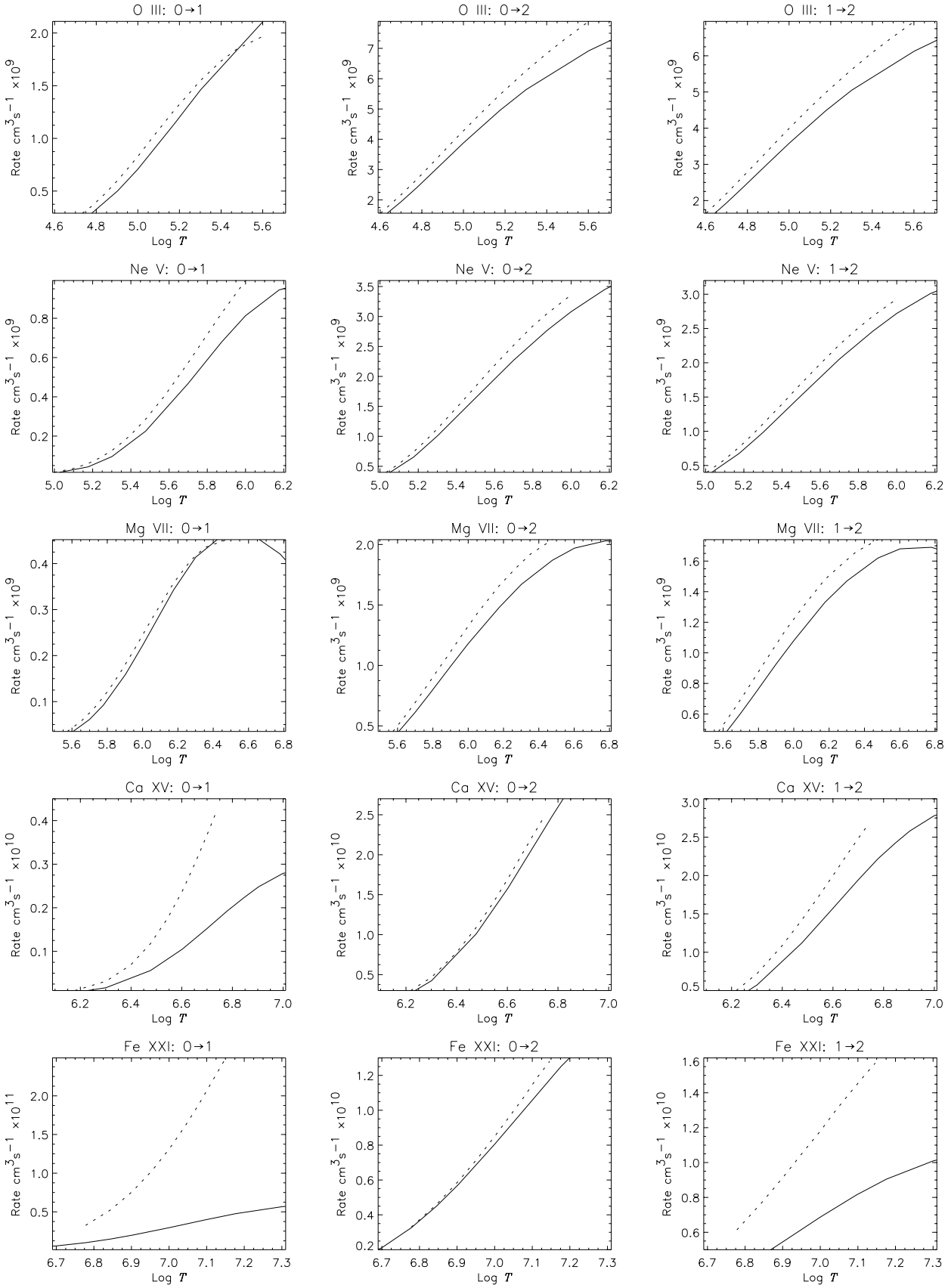

Fig. 2. Comparison of new proton impact rate coefficients to those of FMP80 (O III, Ne V, Mg VII) and F77 (Ca XV, Fe XXI). Dotted lines represent results from F77 / FMP80, solid lines represent the present calculation including the polarization potential.

Table 2. Excitation rate coefficients for $1s^2 2s^2 2p^2\ {}^3P^o_J \rightarrow 1s^2 2s^2 2p^2\ {}^3P^o_{J'}$ by proton impact.

T (K)	Rate coefficient ($cm^3\ s^{-1}$)			T (K)	Rate coefficient ($cm^3\ s^{-1}$)			T (K)	Rate coefficient ($cm^3\ s^{-1}$)		
	0→1	0→2	1→2		0→1	0→2	1→2		0→1	0→2	1→2
	O III				Ne V				Mg VII		
1.00E+04	1.79E-13	2.13E-11	4.45E-11	4.00E+04	1.05E-13	1.36E-11	2.59E-11	7.50E+04	1.12E-14	1.95E-12	5.25E-12
1.50E+04	1.83E-12	1.14E-10	1.76E-10	5.00E+04	3.86E-13	3.47E-11	5.64E-11	1.00E+05	7.27E-14	8.29E-12	1.68E-11
2.00E+04	7.48E-12	2.89E-10	3.82E-10	6.00E+04	1.02E-12	6.74E-11	9.83E-11	1.50E+05	6.96E-13	4.15E-11	6.27E-11
3.00E+04	3.90E-11	7.94E-10	8.96E-10	8.00E+04	4.08E-12	1.64E-10	2.08E-10	2.00E+05	2.72E-12	1.01E-10	1.31E-10
4.00E+04	1.00E-10	1.36E-09	1.42E-09	1.00E+05	1.04E-11	2.91E-10	3.37E-10	2.50E+05	6.86E-12	1.79E-10	2.11E-10
5.00E+04	1.84E-10	1.90E-09	1.91E-09	1.50E+05	4.32E-11	6.54E-10	6.77E-10	3.00E+05	1.34E-11	2.65E-10	2.96E-10
6.00E+04	2.81E-10	2.39E-09	2.33E-09	2.00E+05	9.56E-11	1.00E-09	9.85E-10	4.00E+05	3.36E-11	4.43E-10	4.59E-10
8.00E+04	4.90E-10	3.20E-09	3.02E-09	3.00E+05	2.25E-10	1.56E-09	1.46E-09	5.00E+05	6.08E-11	6.10E-10	6.05E-10
1.00E+05	6.94E-10	3.83E-09	3.54E-09	5.00E+05	4.67E-10	2.27E-09	2.05E-09	6.00E+05	9.23E-11	7.57E-10	7.32E-10
1.50E+05	1.12E-09	4.90E-09	4.43E-09	7.50E+05	6.79E-10	2.77E-09	2.47E-09	8.00E+05	1.59E-10	9.96E-10	9.34E-10
2.00E+05	1.43E-09	5.56E-09	4.99E-09	1.00E+06	8.13E-10	3.08E-09	2.72E-09	1.00E+06	2.22E-10	1.18E-09	1.09E-09
4.00E+05	2.07E-09	6.83E-09	6.06E-09	1.50E+06	9.44E-10	3.44E-09	3.01E-09	1.50E+06	3.43E-10	1.48E-09	1.33E-09
6.00E+05	2.31E-09	7.41E-09	6.53E-09	2.00E+06	9.79E-10	3.64E-09	3.16E-09	2.00E+06	4.14E-10	1.66E-09	1.48E-09
8.00E+05	2.40E-09	7.76E-09	6.81E-09	4.00E+06	8.72E-10	3.89E-09	3.27E-09	3.00E+06	4.69E-10	1.87E-09	1.62E-09
1.00E+06	2.42E-09	8.01E-09	7.00E-09	6.00E+06	7.27E-10	3.85E-09	3.17E-09	4.00E+06	4.68E-10	1.96E-09	1.68E-09
1.50E+06	2.37E-09	8.37E-09	7.23E-09	8.00E+06	6.13E-10	3.74E-09	3.05E-09	6.00E+06	4.21E-10	2.02E-09	1.69E-09
2.00E+06	2.25E-09	8.54E-09	7.31E-09	1.00E+07	5.27E-10	3.62E-09	2.92E-09	8.00E+06	3.68E-10	2.01E-09	1.65E-09
4.00E+06	1.76E-09	8.53E-09	7.10E-09	2.00E+07	2.99E-10	3.12E-09	2.44E-09	1.00E+07	3.22E-10	1.98E-09	1.60E-09
6.00E+06	1.42E-09	8.21E-09	6.73E-09	3.00E+07	2.04E-10	2.78E-09	2.14E-09	1.50E+07	2.40E-10	1.86E-09	1.48E-09
8.00E+06	1.18E-09	7.86E-09	6.37E-09	4.00E+07	1.53E-10	2.54E-09	1.93E-09	2.00E+07	1.88E-10	1.75E-09	1.38E-09
	Ca XV				Fe XXI						
6.00E+05	2.89E-15	2.81E-13	1.45E-12	1.50E+06	1.23E-15	9.00E-14	1.17E-12				
7.00E+05	8.47E-15	6.86E-13	2.84E-12	2.00E+06	8.82E-15	4.85E-13	3.53E-12				
8.00E+05	2.01E-14	1.38E-12	4.82E-12	3.00E+06	8.25E-14	3.14E-12	1.21E-11				
1.00E+06	7.47E-14	3.90E-12	1.05E-11	5.00E+06	6.24E-13	1.67E-11	3.67E-11				
1.50E+06	5.46E-13	1.75E-11	3.29E-11	6.00E+06	1.07E-12	2.60E-11	4.93E-11				
2.00E+06	1.68E-12	3.97E-11	6.15E-11	7.00E+06	1.57E-12	3.60E-11	6.09E-11				
3.00E+06	5.63E-12	9.47E-11	1.20E-10	8.00E+06	2.10E-12	4.61E-11	7.14E-11				
4.00E+06	1.05E-11	1.49E-10	1.68E-10	1.00E+07	3.11E-12	6.51E-11	8.88E-11				
5.00E+06	1.52E-11	1.96E-10	2.06E-10	1.25E+07	4.19E-12	8.55E-11	1.05E-10				
6.00E+06	1.92E-11	2.34E-10	2.35E-10	1.50E+07	5.00E-12	1.02E-10	1.16E-10				
7.00E+06	2.24E-11	2.65E-10	2.57E-10	2.00E+07	5.98E-12	1.25E-10	1.28E-10				
8.00E+06	2.49E-11	2.90E-10	2.73E-10	2.50E+07	6.36E-12	1.38E-10	1.33E-10				
1.00E+07	2.80E-11	3.25E-10	2.94E-10	3.00E+07	6.43E-12	1.46E-10	1.35E-10				
1.50E+07	2.98E-11	3.66E-10	3.12E-10	4.00E+07	6.12E-12	1.53E-10	1.33E-10				
2.00E+07	2.83E-11	3.76E-10	3.10E-10	5.00E+07	5.63E-12	1.54E-10	1.29E-10				
3.00E+07	2.37E-11	3.67E-10	2.92E-10	6.00E+07	5.13E-12	1.52E-10	1.24E-10				
4.00E+07	1.96E-11	3.50E-10	2.73E-10	7.00E+07	4.67E-12	1.48E-10	1.19E-10				
5.00E+07	1.65E-11	3.32E-10	2.56E-10	8.00E+07	4.25E-12	1.45E-10	1.15E-10				
6.00E+07	1.41E-11	3.15E-10	2.41E-10	1.00E+08	3.58E-12	1.38E-10	1.07E-10				
7.00E+07	1.23E-11	3.01E-10	2.29E-10	1.50E+08	2.50E-12	1.22E-10	9.25E-11				

For Ca XV and Fe XXI the differences between our results and those of F77 are more pronounced. This is because polarization, which was not included by F77 or FMP80, has a significant effect on our results. This is particularly noticeable in the 0→1 transitions, because they are more dependent on the closer collisions.

As a final comparison with the earlier work, we have also performed a calculation for Fe XXI without any polarization, and using the atomic data adopted by F77. Our calculation differs from F77 only in two respects: firstly, in the collision treatment, our semi-classical *versus* his quantal; secondly, in the interaction between matrix elements, our short-range modified forms *versus* his purely asymptotic forms. Our results are shown by the dashed lines in Fig. 1. For the 0→2 and 1→2 transitions, our results are very close to those of F77 up to 3 keV, confirming the observation by Faucher & Landman (1977) that the use of the semi-classical collision treatment does not *per se* introduce significant errors compared with the quantal treatment. For higher energies the progressive divergence in the two calculations is due to our short-range modification to the matrix elements. For

the $0 \rightarrow 1$ transition, the discrepancy between the calculations is more pronounced, because this strictly second-order process is more sensitive to the short-range forms of the matrix elements.

Our results show that including the effects of higher-lying states via the polarization potential significantly reduces proton impact fine-structure cross-sections and excitation rate coefficients for carbon-like ions. It is therefore important that these new results are incorporated in the analysis of emission diagnostics (from, for example, the SOHO CDS and SUMER instruments) especially for ions such as Ca XV and Fe XXI.

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References

Alder K., Winther A., 1975, In: Electromagnetic Excitation: Theory of Coulomb Excitation with Heavy Ions. North-Holland, Oxford

Cheng K.T., Kim Y.K., Desclaux J.P., 1979, At. Data Nuc. Data Tables 24, 111

Copeland F., Reid R.H.G., Keenan F.P., 1997, At. Data Nuc. Data Tables 67, 179

Dere K.P., Landi E., Mason H.E., Monsignori Fossi B.C., Young P.R., 1997, A&AS 125, 149

Doyle J.G., Kingston A.E., Reid R.H.G., 1980, A&A 90, 97

Espey B., Keenan F.P., McKenna F.C., Feibelman W.A., Aggarawal K.M., 1996, ApJ 465, 965

Faucher P., 1977, A&A 54, 589

Faucher P., Landman D.A., 1977, A&A 54, 159

Faucher P., Masnou-Seeuws F., Prudhomme M., 1980, A&A 81, 137

Foster V.J., 1994, Ph.D. Thesis, The Queen's University of Belfast

Foster V.J., Keenan F.P., Reid R.H.G., 1994, Phys. Rev. A49, 3092

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

Keenan F.P., Conlon E.S., Foster V.J., Aggarwal K.M., Widing K.G., 1992, ApJ 401, 411

Keenan F.P., Foster V.J., Aggarwal K.M., Widing K.G., 1996, Sol. Phys. 169, 47

Ryans R.S.I., Foster-Woods V.J., Copeland F., Reid R.H.G., Keenan F.P., 1998, A&A, in 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