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Atomic data from the IRON Project

XLII. Electron impact excitation of Fe XXI⋆

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Abstract. Collision strengths and collisional rate parameters are provided for transitions among the $n = 2$ and $2p3\ell$ levels of C-like Fe XXI. The data have been computed in a 52-state Breit-Pauli approximation thus accounting for the most prominent relativistic effects. An R-matrix close-coupling calculation comprising partial wave contributions up to $J = 59/2$ and of order 8000 energy points in the range up to 260 Ryd gave cross sections expected to be accurate to better than 20% for transitions among the $n = 2$ levels.

Key words: atomic data — atomic processes

1. Introduction

The Iron Project (IP) is an international collaboration that aims primarily to generate accurate atomic data for ions of iron group elements. The project has produced more than 40 papers to this date. A list is to be found on the project WWW home page at http://www.am.qub.ac.uk/projects/iron.

The overall aims and methods of the project were summarized in the first paper of the IP series (Hummer et al. 1993). The current paper is the first in a short IP subseries presenting collisional data for C, N and O-like iron using essentially similar techniques and approximations.

In this connection, C-like iron Fe XXI is of particular interest from both the theoretical and observational point of view. On the observational side, lines of Fe XXI have been seen in both solar flares (e.g. Mason et al. 1979; Cheng & Pallavicini 1988; Cheng et al. 1979) and the coronae of cool stars, particularly that of Capella (Linsky et al. 1998). In their analysis, Linsky et al. report on discrepant results obtained from the λ1354 line as compared with the Fe XXI EUV lines. They suggest four possible explanations for the discrepancy, one of which, inaccurate or incomplete atomic data, they rule out on the grounds that the available data (Aggarwal 1991; Aggarwal et al. 1997) are good to 10%. As we shall see, this error estimate is too optimistic due to the omission of high energy resonant contributions to the collisional data. In addition, the oscillator strengths provided by Aggarwal et al. (1997) differ markedly (up to six orders of magnitude) from the earlier work of Bhatia et al. (1987). Aggarwal et al. in fact indicate that their results are accurate to 20% for the *stronger* transitions and state that it would be desirable to have collisional data of comparable accuracy for the higher lying levels. Our oscillator strengths are in good agreement with those of Aggarwal et al. and we hope to go some way to fulfilling the latter need in the current paper. Very recently Aggarwal & Keenan (1999) have published new results for this iron ion on the basis of an extended Dirac R-matrix calculation but only for the region where all channels are open. Their collision strengths are in good agreement with the earlier work for the strong transitions but there are discrepancies for the weaker transitions. Since they do not, as yet, include resonance effects a detailed comparison is not made here.

On the other hand, Zhang & Sampson (1996, 1997) provide extensive tables of collision and oscillator strengths for C-like ions including Fe XXI. They present results for *all* $n = 2 - 3$ transitions calculated in a relativistic distorted wave approximation. Since these represent a complete set of data they complement the present calculations and those of Aggarwal (1991). We compare with these data at high energy to provide some further indication as to the accuracy of the available collisional data.

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⋆ Detailed tables of the present data are available in electronic form at the CDS via anonymous ftp to 130.79.128.5 or via http://cdsweb.u-strasbg.fr/Abstract.html. Table 3 is only available in electronic form at the CDS.

The first distorted wave calculation was performed by Mason et al. (1979). Their calculation was extended to higher levels by Bhatia et al. (1987) although, as noted earlier, their oscillator strengths are discrepant in many cases. They tabulate the collision strength at a single energy. The distorted wave approximation is well suited to this highly ionized system although it does omit resonance effects thus underestimating collision rates. With this proviso the Mason et al. data for the background cross sections are in fact reasonably accurate as has been shown by Aggarwal (1991). On the other hand, the distorted wave collision rates can be in error by up to an order of magnitude because of this omission of resonances. The original Mason et al. (1979) work does suffer from lack of convergence in J for some forbidden transitions at high energies/temperatures. Also the use of an algebraic transformation from LS to intermediate coupling means that the data for the transitions which are not allowed in LS coupling but which are permitted in intermediate coupling are inaccurate. The former point has been corrected by a further distorted wave calculation undertaken by Phillips et al. (1996) who extended the calculation further to include some $n = 4$ levels. They seem to have been unaware of the earlier work of Aggarwal (1991) who obtained accurate collision strengths for the $n = 2$ levels in a fully-relativistic Dirac formulation using the R-matrix code of Wijesundera et al. (1991). This calculation includes resonance effects and the paper includes a detailed discussion and comparison with the work of Mason et al. (1979).

A comparison of our own and Aggarwal's (1991) data will thus allow us to investigate the two different approaches to the relativistic problem, the Dirac and Breit-Pauli approximations. Aggarwal (1991) has made a detailed comparison with the distorted wave results of Mason et al. (1979) and has already emphasized the importance of the resonance contributions and the correct treatment of intermediate coupling. The current work also demonstrates the necessity of including resonant contributions from higher-lying configurations, a point made by Aggarwal et al. (1997).

In the next section, we give a short description of the present calculation which is followed by a discussion of the results. Here we concentrate on a comparison with the work of Aggarwal (1991) since he has provided an excellent commentary on the earlier distorted wave results and with the newer, comprehensive relativistic distorted wave data of Zhang & Sampson (1996, 1997).

2. Method

The method is described in detail in the first paper in the series (Hummer et al. 1993). A brief summary is provided here together with data relevant to the assessment of the accuracy of the present calculation.

The electron + target scattering problem was solved using the close-coupling method in a Breit-Pauli approximation. The configuration interaction target wavefunctions were obtained using the program SUPERSTRUCTURE (Eissner et al. 1974) in a version due to Nussbaumer & Storey (1978). The latter provides for more flexibility in the wavefunctions through the possible use of Coulomb functions and individual free parameters for the one-electron orbitals. The present target incorporated the following configurations:

$2s^22p^2$	$2s2p^3$	$2p^4$
$2s^22p3s$	$2s^22p3p$	$2s^22p3d$
$2s2p^23s$	$2s2p^23p$	$2s2p^23d$
$2p^33s$	$2p^33p$	$2p^33d$

although only the first six configurations and a few of the $2s2p^23s$ states that are energetically lower than the higher lying $2s^22p3d$ levels appear explicitly in the current computation. This leads to a 28-term LS-coupling and a 52-level intermediate coupling target. Of course, the neglect of the other configurations has consequences for the accuracy to be expected.

All orbitals have been made spectroscopic to avoid possible problems with pseudoresonances. The free parameters in the Thomas-Fermi-Dirac-Amaldi potential, $\lambda_{n\ell}$, obtained on minimizing the weighted sum of all the target energies are given in Table 1 while the calculated energies are compared with those observed (Corliss & Sugar 1982) in Table 2. The energies are in some cases not as accurate as those obtained by Mason et al. (1979) or Aggarwal (1991) as no correlation configurations have been included while many more spectroscopic states have been incorporated.

Table 1. The λ parameters for Fe XXI

$n\ell$	$\lambda_{n\ell}$	$n\ell$	$\lambda_{n\ell}$
1s	1.43161	3s	1.28949
2s	1.43035	3p	1.23930
2p	1.34480	3d	1.37441

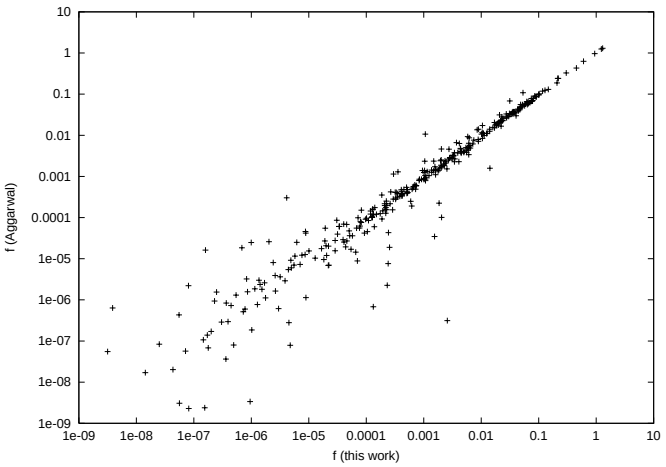

Fig. 1. Comparison of the f-values obtained in the present Fe XXI target calculation with those of Aggarwal et al. (1997)

Table 2. Calculated versus observed (Corliss & Sugar 1982) target energies (cm^{-1})

Index	Term		E_{calc}	E_{obs}
1	$2s^22p^2$	$^3P^e_0$	0	0.0
2	$2s^22p^2$	$^3P^e_1$	82342	73850
3	$2s^22p^2$	$^3P^e_2$	131240	117353
4	$2s^22p^2$	$^1D^e_2$	266159	244560
5	$2s^22p^2$	$^1P^e_0$	392420	371900
6	$2s2p^3$	$^5S^o_2$	492100	486950
7	$2s2p^3$	$^3D^o_1$	788117	776780
8	$2s2p^3$	$^3D^o_2$	790592	777350
9	$2s2p^3$	$^3D^o_3$	824580	803930
10	$2s2p^3$	$^3P^o_0$	933542	916380
11	$2s2p^3$	$^3P^o_1$	945013	924880
12	$2s2p^3$	$^3P^o_2$	966608	942320
13	$2s2p^3$	$^3S^o_1$	1115277	1095600
14	$2s2p^3$	$^1D^o_2$	1156183	1126800
15	$2s2p^3$	$^1P^o_1$	1293363	1261000
16	$2p^4$	$^3P^e_2$	1667455	1646300
17	$2p^4$	$^3P^e_0$	1761165	1735700
18	$2p^4$	$^3P^e_1$	1770134	1740500
19	$2p^4$	$^1D^e_2$	1853211	1817300
20	$2p^4$	$^1S^e_0$	2091087	2048200
21	$2s^22p3s$	$^3P^o_0$	7687260	
22	$2s^22p3s$	$^3P^o_1$	7696818	
23	$2s^22p3s$	$^3P^o_2$	7811152	
24	$2s^22p3s$	$^1P^o_1$	7836056	
25	$2s^22p3p$	$^3D^e_1$	7864901	
26	$2s^22p3p$	$^3P^e_1$	7922276	
27	$2s^22p3p$	$^3D^e_2$	7926976	
28	$2s^22p3p$	$^3P^e_0$	7937875	
29	$2s^22p3p$	$^1P^e_1$	8012716	
30	$2s^22p3p$	$^3D^e_3$	8025472	
31	$2s^22p3p$	$^3S^e_1$	8034786	
32	$2s^22p3p$	$^1D^e_2$	8037228	
33	$2s2p^23s$	$^5P^e_1$	8094750	
34	$2s^22p3p$	$^3P^e_2$	8101009	
35	$2s^22p3d$	$^3F^o_2$	8103486	
36	$2s^22p3d$	$^3F^o_3$	8143904	8101400
37	$2s^22p3d$	$^1D^o_2$	8149622	8098000
38	$2s2p^23s$	$^5P^e_2$	8150261	
39	$2s^22p3p$	$^1S^e_0$	8157038	
40	$2s^22p3d$	$^3D^o_1$	8166771	
41	$2s2p^23s$	$^3P^e_0$	8204657	
42	$2s2p^23s$	$^5P^e_3$	8205472	
43	$2s^22p3d$	$^3F^o_4$	8235261	
44	$2s^22p3d$	$^3D^o_2$	8241715	8187400
45	$2s2p^23s$	$^3P^e_1$	8244042	
46	$2s^22p3d$	$^3D^o_3$	8264769	8195000
47	$2s^22p3d$	$^3P^o_1$	8275594	
48	$2s^22p3d$	$^3P^o_2$	8279138	8230900
49	$2s^22p3d$	$^3P^o_0$	8284450	
50	$2s2p^23s$	$^3P^e_2$	8302380	
51	$2s^22p3d$	$^1F^o_3$	8338459	8313600
52	$2s^22p3d$	$^1P^o_1$	8339760	8293900

The calculated oscillator strengths may also indicate the quality of the target wavefunctions. In Fig. 1 we compare oscillator strengths in the length approximation with those of Aggarwal et al. (1997) who used the CIV3 configuration-interaction program of Hibbert (1975). The figure clearly demonstrates that there are no major inconsistencies between the two datasets and that the overall agreement is excellent. This is in sharp contrast to the earlier f-values of Bhatia et al. (1987) who also used SUPERSTRUCTURE.

Table 4. Transition probabilities for $2s^22p^2 - 2s2p^3$ lines from this work and that of Froese Fischer & Saha (1985)

Upper	Lower	This work	FFS
$^5S^o_2$	$^3P^e_1$	4.210E+07	3.560E+07
$^5S^o_2$	$^3P^e_2$	3.625E+07	3.272E+07
$^5S^o_2$	$^1D^e_2$	1.343E+06	8.548E+05
$^3D^o_1$	$^3P^e_0$	1.257E+10	1.191E+10
$^3D^o_1$	$^3P^e_1$	6.485E+08	7.490E+08
$^3D^o_1$	$^3P^e_2$	1.027E+08	6.727E+07
$^3D^o_1$	$^1D^e_2$	2.000E+08	1.869E+08
$^3D^o_1$	$^1P^e_0$	4.293E+07	4.191E+07
$^3D^o_2$	$^3P^e_1$	9.636E+09	9.498E+09
$^3D^o_2$	$^3P^e_2$	2.035E+07	5.570E+06
$^3D^o_2$	$^1D^e_2$	3.841E+07	3.612E+07
$^3D^o_3$	$^3P^e_2$	6.275E+09	6.472E+09
$^3D^o_3$	$^1D^e_2$	1.060E+09	7.912E+08
$^3P^o_0$	$^3P^e_1$	2.309E+10	2.254E+10
$^3P^o_1$	$^3P^e_0$	4.301E+09	4.248E+09
$^3P^o_1$	$^3P^e_1$	1.770E+10	1.642E+10
$^3P^o_1$	$^3P^e_2$	2.515E+09	2.838E+09
$^3P^o_1$	$^1D^e_2$	2.316E+08	1.959E+08
$^3P^o_1$	$^1P^e_0$	1.640E+08	1.509E+08
$^3P^o_2$	$^3P^e_1$	2.968E+08	3.791E+08
$^3P^o_2$	$^3P^e_2$	2.177E+10	2.078E+10
$^3P^o_2$	$^1D^e_2$	1.335E+08	5.708E+07
$^3S^o_1$	$^3P^e_0$	9.560E+09	9.311E+09
$^3S^o_1$	$^3P^e_1$	2.547E+10	2.538E+10
$^3S^o_1$	$^3P^e_2$	6.306E+10	5.799E+10
$^3S^o_1$	$^1D^e_2$	4.072E+08	9.426E+07
$^3S^o_1$	$^1P^e_0$	7.092E+08	6.489E+08
$^1D^o_2$	$^3P^e_1$	4.658E+08	3.953E+08
$^1D^o_2$	$^3P^e_2$	8.651E+09	6.413E+09
$^1D^o_2$	$^1D^e_2$	4.602E+10	4.626E+10
$^1P^o_1$	$^3P^e_0$	2.943E+07	3.573E+07
$^1P^o_1$	$^3P^e_1$	5.294E+09	5.963E+09
$^1P^o_1$	$^1D^e_2$	6.888E+10	6.641E+10
$^1P^o_1$	$^1P^e_0$	1.799E+10	1.753E+10

Froese Fischer & Saha (1985) performed detailed MCHF (Froese Fischer & Saha 1983) calculations of the $2s^22p^2 - 2s2p^3$ transition probabilities for C-like ions. We compare these results with ours in Table 4. Again the overall agreement is excellent. It should be borne in mind that our energy levels are worst for these configurations so that the target as a whole is better than this comparison would indicate. The data on which Fig. 1 is based are tabulated in Table 3 which is only available in electronic form.

These target wavefunctions were then used to perform an R-matrix close-coupling calculation to determine the scattering states of the $N+1$ electron system. An R-matrix package due to Eissner (unpublished) was used for this purpose. The asymptotic solutions, in particular the scattering matrices and consequently the collision strengths, were then obtained using the standard program suite described by Hummer et al. (1993). The use of 18 continuum orbitals in the scattering problem for each ℓ value leads to matrices of order 4500 and approximately 220 channels for each $J\pi$ combination.

To ensure convergence in the total angular momentum values of J up to 59/2 were obtained. This is more than sufficient for the majority of transitions but for the

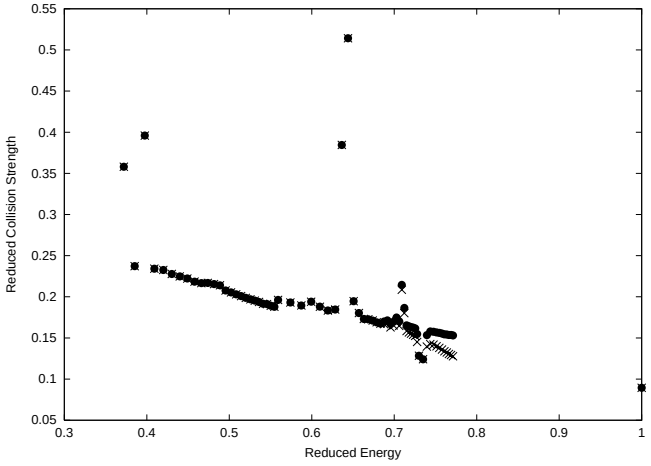

Fig. 2. The $2s^2 2p^2\ {}^3P_2^e - 2s2p^3\ {}^3D_3^\circ$ collision strength with (filled circles) and without (x) top-up. Note that the data with top-up converge to the correct limit

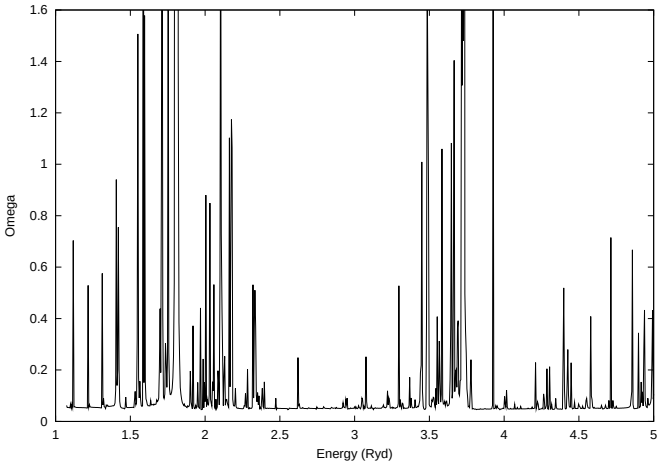

Fig. 3. The $2s^2 2p^2\ {}^3P_1^e - {}^3P_2^e$ collision strength at low energies. Comparison with Aggarwal's (1991) Fig. 1 shows good agreement with a cross section obtained in a Dirac approximation

allowed transitions and a few $J \rightarrow J$ among the $n = 2$ levels the values so obtained had to be "topped-up" to account for the infinity of J values omitted from the summation. For the allowed transitions an implementation of the Coulomb-Bethe approximation due to Eissner (Eissner et al. 1999) and based on the top-up procedure of Burke & Seaton (1986) for LS-coupling was available. For the slowly converging forbidden transitions a simple geometric progression was assumed but see the following section for further discussion of this point. The collision rates or effective collision strengths were obtained by integrating the collision strengths in the manner suggested by Burgess & Tully (1992) to ensure the proper behaviour at low temperatures.

Finally, the maximum total energy of 260 Ryd was insufficient to provide converged results at the highest temperatures so that the present results had to be extrapolated to higher energies. Here we have simply assumed the collision strength to be constant. Of course, this is not a good approximation but at 10^7 K this high-energy correction is never more than 10% of the total for any given cross section and hence the error is well within the bounds of other systematic errors. It does, however, mean that the present results should *not be extrapolated* to higher temperatures without paying careful attention to this point. Since the present results cover the maximum of the Fe^{20+} ionization balance determined by Arnaud & Rothenflug (1985), this should not be necessary.

3. Results and discussion

The full set of results (Table 5) are to be found on the ftp server of the CDS (Centre de Données astronomiques de Strasbourg) in computer readable form. Here we show a small selection to illustrate some of the more important points.

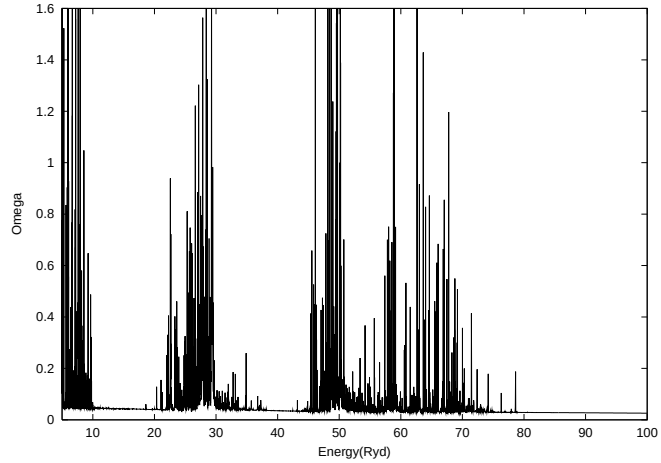

Fig. 4. The $2s^2 2p^2\ {}^3P_1^e - {}^3P_2^e$ collision strength at high energies. These resonances do not appear in the Aggarwal (1991) calculation

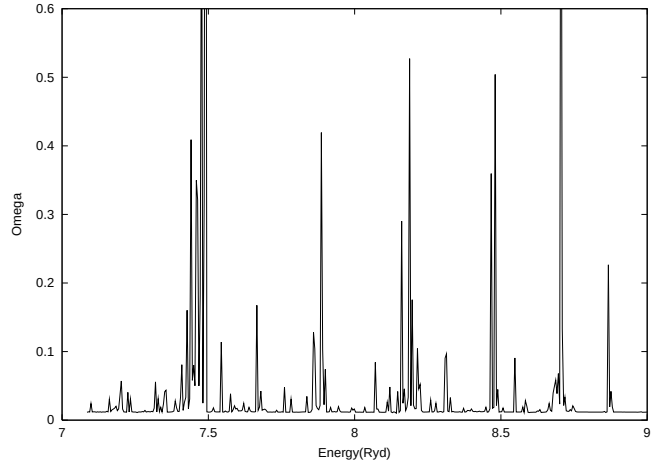

Fig. 5. The $2s^2 2p^2\ {}^1D_2^e - 2s2p^3\ {}^3D_2^\circ$ collision strength at low energies. Comparison with Aggarwal's (1991) Fig. 2 shows good agreement with a cross section obtained in a Dirac approximation

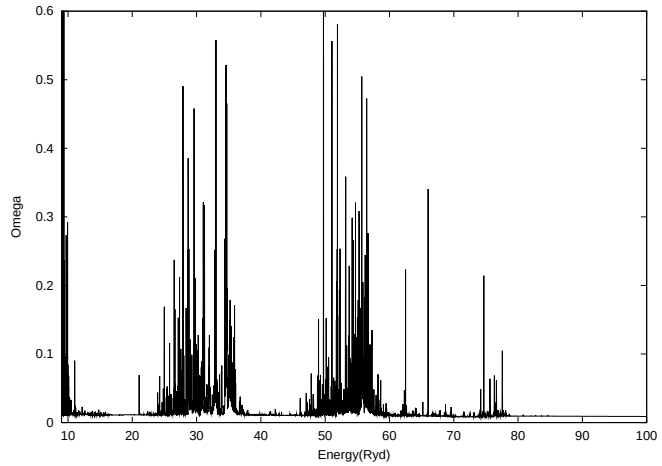

Fig. 6. The $2s^2 2p^2\ {}^1D^e_2 - 2s2p^3\ {}^3D^\circ_2$ collision strength at high energies. These resonances have been omitted from the Aggarwal (1991) calculation

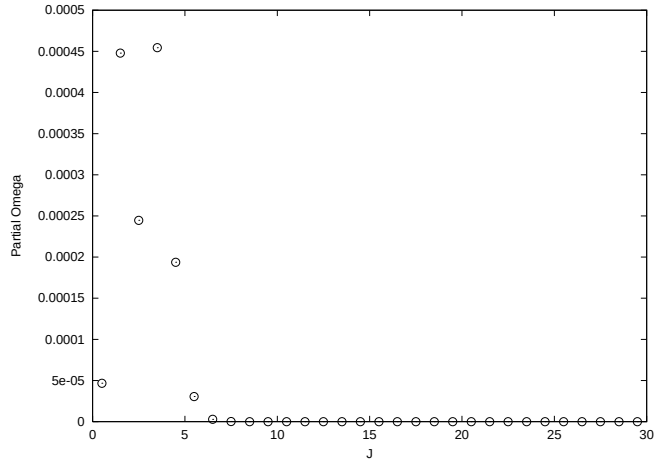

Fig. 7. The individual J contributions to the $2s^2 2p^2\ {}^3P^e_0 - 2s2p^3\ {}^5S^\circ_2$ forbidden transition at an energy of 118 Ryd. The convergence is rapid

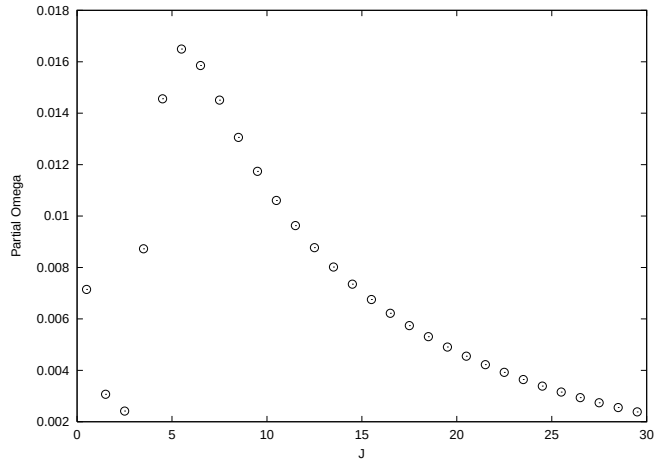

Fig. 8. The individual J contributions to the $2s^2 2p^2\ {}^3P^e_0 - 2s2p^3\ {}^3D^\circ_1$ allowed transition at an energy of 118 Ryd. Note the long tail and corresponding slow convergence

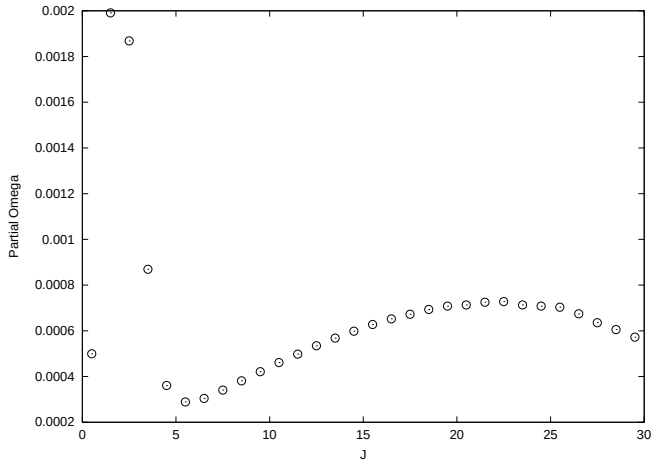

Fig. 9. The individual J contributions to the $2s2p^3\ {}^5S^\circ_2 - 2s2p^3\ {}^3P^\circ_2$ forbidden transition at an energy of 118 Ryd. The convergence is slow (compare with Fig. 7)

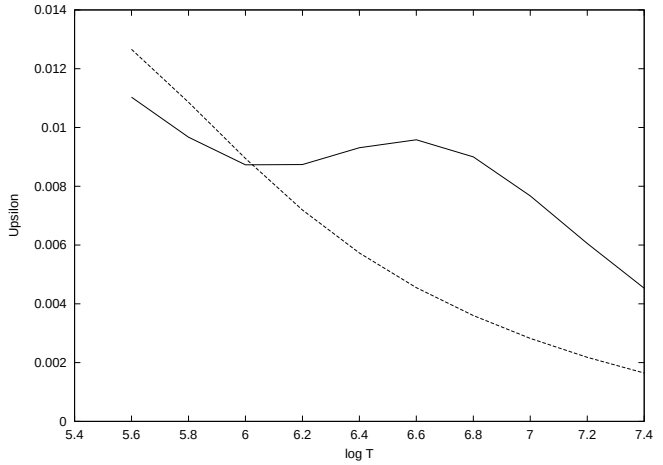

Fig. 10. The effective collision strength plotted as a function of temperature for the $2s^2 2p^2\ {}^3P^e_0 - 2s^2\ 2p^2\ {}^1D^e_2$ forbidden transition. The solid curve are the present results, dashed are from Aggarwal (1991). The contribution of the higher lying resonances is apparent

One of the more interesting aspects for this ion is that an earlier calculation based on the Dirac formulation exists. We have plotted the collision strength for the $2s^2 2p^2\ {}^3P^e_1$ – $\ {}^3P^e_2$ transition in Fig. 3 and for the $2s^2 2p^2\ {}^1D^e_2 - 2s2p^3\ {}^3D^\circ_2$ transition in Fig. 5. The scales have been chosen to allow a direct comparison with the Dirac results obtained by Aggarwal (1991) (see Figs. 1 and 2 on pa. 681 of that paper). It is obvious that the agreement is excellent. It should be noted, however, that the inclusion of the $n = 3$ states has a pronounced effect on the overall results as the resonances at higher energies to be seen in Figs. 4 and 6 for the same cross sections are not present in the earlier calculation. In the same way, resonances converging to the $2s^2 2p4\ell$ and higher thresholds are lacking in the current work. This could be remedied by extending the calculation to include these higher thresholds but

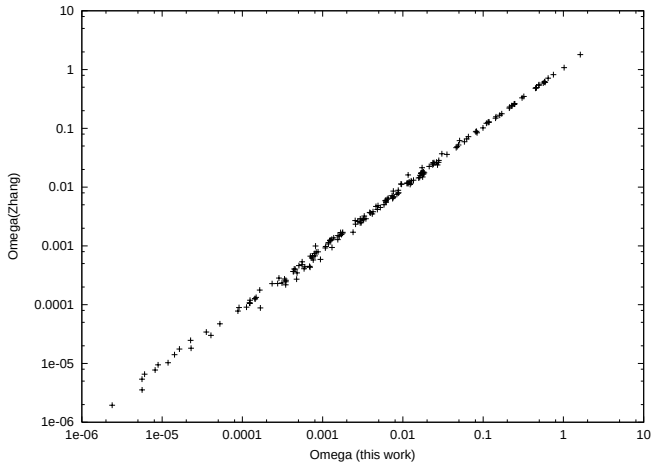

Fig. 11. Collision strengths from the present work compared with those of Zhang & Sampson (1996) at an ejected electron energy of 95.3 Ryd

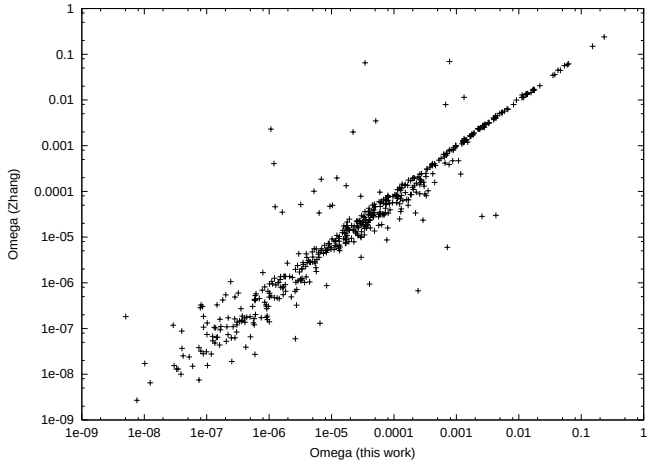

Fig. 12. Collision strengths from the present work compared with those of Zhang & Sampson (1997) at an ejected electron energy of 57.2 Ryd

the cost is prohibitive. In any case, the effect on the $n = 2$ transitions would be small at the temperatures of interest.

There are two different sorts of top-up involved in the provision of the final data, a top-up in J, the total angular momentum and a top-up in energy. For the most part, the collision strengths for the maximum J value (59/2) calculated explicitly are sufficient to ensure convergence. In Figs. 7–9 we show the convergence in J for three different types of transition at an energy of 118 Ryd. For the $2s^22p^2\ {}^3P^e_0 - 2s2p^3\ {}^5S^o_2$ forbidden transition in Fig. 7, convergence is rapid even at this high energy. The $2s^22p^2\ {}^3P^e_0 - 2s2p^3\ {}^3D^o_1$ allowed transition in Fig. 8 on the other hand varies very slowly but as can be seen in the next paragraph good results may be obtained using the Coulomb-Bethe approximation. Transitions of the type $J \rightarrow J$ as illustrated in Fig. 9 for the $2s^22p^2\ {}^3P^e_0 - 2s^22p^2\ {}^1D^e_2$ are a real problem since they show a peak at relatively high J and a rather slow decline. This implies that the fraction of the cross section coming from the top-up is relatively large. In the present case, we have simply calculated partial wave contributions from a $J_{\max}$ high enough so that a geometric progression may be used. This phenomenon was also observed and commented on by Aggarwal (1991) and more recently by Eissner et al. (1999). Aggarwal set $J_{\max}$ to 29/2 which is just sufficient for an energy of 100 Ryd. At higher energies, as shown in the figure, his cross sections are not converged so that his top-up has a larger error for these few cases.

The top-up in energy has been made small by extending the calculation to large total energies. The error in this contribution is perhaps relatively large but since it only comprises a small correction at the temperatures of interest this is unimportant.

The allowed transitions have been "topped-up" using a scheme similar to that devised by Burke and Seaton for LS-coupling, based on Coulomb-Bethe recursion laws for the collision strengths (Eissner et al. 1999). It is accurate as long as it is carried out for values of J that are not too small or too large. For small values of J the Coulomb-Bethe approximation is not applicable while at large J values the recursion formulae become inaccurate. The collision strength displayed in Fig. 2 shows how effective this method is. Plotted is the reduced collision strength $(\Omega(E)/\ln(E/\Delta E + e))$ versus the reduced energy $(1 - \ln(c)/\ln(E/\Delta E + c))$ as suggested by Burgess & Tully (1992). Here ΔE is the transition energy, E is the electron energy with respect to the reaction threshold and c is an adjustable scaling parameter. The change in scale compresses the range in energy from $0 \rightarrow \infty$ to $0 \rightarrow 1$. The correct cross section should, on this scale, converge to the value $4gf/\Delta E$ at $x = 1$ where gf is the weighted oscillator strength for the transition, which indeed it does.

The relativistic distorted wave calculations of Zhang & Sampson (1996, 1997) are also available for comparison. Overall the agreement for transitions among the $n = 2$ states is excellent as is evidenced by Fig. 11. Here we compare all the $n = 2$ data at an *ejected* electron energy of 95.3 Ryd. The same comparison for the $n = 2-3$ common to the two calculations is made in Fig. 12. Here the agreement is poorer but there are no systematic differences. The few transitions where the discrepancies are larger are due to a few energy levels, for example the level number 36 in the present calculation, labelled j3 by Zhang & Sampson (1997). Here the level is strongly mixed with the $2p^33p\ {}^3F^\circ$ state. Presumably the mixture is different in the Zhang and Sampson calculation. Such differences are bound to arise when configuration mixing is large. The question as to which value is more accurate can only be decided, if at all, by even more extensive calculations. Fortunately only a few of the more than 1300 transitions are affected so the problem should not be serious.

In summary we may say that the present results provide cross sections that are accurate to better than 20%

for transitions involving only the $n = 2$ states. Collisional data for the 2p3ℓ are also tabulated but will be much less accurate, chiefly due to the absence of resonances converging to higher thresholds. A more complete set of data for the $n = 3$ levels is provided by the work of Zhang & Sampson (1996, 1997) while data including the $n = 4$ levels are to be found in the paper by Phillips et al. (1996). But note that the resonance contribution is lacking in both. Lastly, although oscillator strengths have been tabulated in Table 3 the values to be found in Froese Fischer & Saha (1985) are to be preferred since they have considered configuration interaction effects in much more detail.

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