

# Effective collision strengths for transitions in Fe XI<sup>\*</sup>

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**Abstract.** Collision strengths for transitions among the lowest 48 fine-structure levels belonging to the  $(1s^22s^22p^6) 3s^23p^4$ ,  $3s3p^5$ ,  $3s^23p^33d$  and  $3p^6$  configurations of Fe XI have been calculated using the Dirac Atomic  $R$ -matrix Code (DARC) of Norrington & Grant (2003). Results are tabulated at energies above thresholds in the range  $10 \leq E \leq 100$  Ry, although resonances have been resolved in a fine energy mesh in the thresholds region. Effective collision strengths, obtained after integrating the collision strengths over a Maxwellian distribution of electron velocities, are also tabulated over a wide electron temperature range below  $5 \times 10^6$  K. Comparisons with other available results are made, and the accuracy of the present data is assessed.

**Key words.** atomic data – atomic processes

## 1. Introduction

Electron impact excitation of iron ions has been a subject of intense research over the last few years. This is primarily because iron is an abundant element, particularly in solar and fusion plasmas, and its lines are observed in almost all ionization stages. Emission lines of Fe XI have been observed in the ultraviolet (UV) and extreme ultraviolet (EUV) range of the solar spectrum, as well as in late-type stars – see Gupta & Tayal (1999a) and references therein. Most of the observed lines of Fe XI lie in the 170–400 Å wavelength range, and arise from transitions among the fine-structure levels of the  $(1s^22s^22p^6) 3s^23p^4$ ,  $3s3p^5$ ,  $3s^23p^33d$  and  $3p^6$  configurations. Additionally, many forbidden transitions of Fe XI lie in the 1000–3000 Å spectral range, and are observed in the spectra of solar-type stars and other astrophysical objects – see Bhatia & Doschek (1996) and references therein. Of particular interest among the Fe XI transitions is the  $^3P_1-^1S_0$  solar line at 1467.08 Å (Feldman 2001). The interpretation of the vast amount of observational data requires theoretical data for atomic parameters, such as energy levels, radiative rates, collision strengths and rate coefficients, because experimental results for these are generally not available. Therefore, in this paper we report the values of collision strengths and effective collision strengths. Results for energy levels and radiative rates have already been reported in our earlier work (Aggarwal & Keenan 2003).

Earlier calculations for Fe XI have been performed by many workers. The most notable among these are the *distorted-wave* (DW) calculations of Bhatia & Doschek (1996) and the recent  $R$ -matrix calculations of Gupta & Tayal (1999a,b). Bhatia & Doschek have reported values of energy levels, radiative rates and collision strengths ( $\Omega$ ) for transitions among the 48 fine-structure levels belonging to the above noted configurations of Fe XI. On the other hand, Gupta & Tayal have also reported the values of effective collision strengths ( $\Upsilon$ ), from which the corresponding values of excitation and de-excitation rate coefficients can easily be obtained. However, their calculations for  $\Omega$  and  $\Upsilon$  have been performed for transitions among a subset (38 levels) of the above levels, but energy levels and radiative rates have been computed among the lowest 47 fine-structure levels. Since the remaining 9 levels ( $^5D_{0,1,2,3,4}^o$ ,  $^3G_{3,4,5}^o$  and  $^1G_4^o$ ) lie *below* the highest threshold of their calculations, there is scope to extend as well as to improve upon their results.

Furthermore, for generating wavefunctions, Bhatia & Doschek (1996) have included configuration interaction (CI) among the basic configurations only, and this affects the accuracy as CI is quite important for Fe XI. This has already been discussed and demonstrated by Deb & Tayal (1998). Additionally, they have calculated values of  $\Omega$  at only three energies above thresholds, which are not sufficient for the accurate determination of excitation rates, as resonances in the thresholds region have not been accounted for. Therefore, Gupta & Tayal (1999a,b) have taken care of both of these deficiencies by including additional CI in the generation of wavefunctions, and resonances in the thresholds region. They have computed  $\Omega$  at energies below 40 Ry and have reported values of  $\Upsilon$  in a wide electron temperature range below  $5 \times 10^6$  K.

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\* Tables 2 and 3 are only available in electronic form at  
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**Table 1.** State definitions and energy levels (in Ry) for S-like Fe XI.

Index	Configuration	Level	Expt. <sup>a</sup>	GRASP <sup>b</sup>
1	3s <sup>2</sup> 3p <sub>1/2</sub> <sup>2</sup> 3p <sub>3/2</sub> <sup>2</sup>	<sup>3</sup> P <sub>2</sub> <sup>e</sup>	0.0000	0.0000
2	3s <sup>2</sup> 3p <sub>1/2</sub> <sup>2</sup> 3p <sub>3/2</sub> <sup>3</sup>	<sup>3</sup> P <sub>1</sub> <sup>e</sup>	0.1154	0.1147
3	3s <sup>2</sup> 3p <sub>1/2</sub> <sup>2</sup> 3p <sub>3/2</sub> <sup>2</sup>	<sup>3</sup> P <sub>0</sub> <sup>e</sup>	0.1304	0.1218
4	3s <sup>2</sup> 3p <sub>1/2</sub> <sup>2</sup> 3p <sub>3/2</sub> <sup>3</sup>	<sup>1</sup> D <sub>2</sub>	0.3439	0.3782
5	3s <sup>2</sup> 3p <sub>3/2</sub> <sup>4</sup>	<sup>1</sup> S <sub>0</sub> <sup>e</sup>	0.7364	0.6307
6	3s3p <sub>1/2</sub> <sup>2</sup> 3p <sub>3/2</sub> <sup>3</sup>	<sup>3</sup> P <sub>2</sub> <sup>o</sup>	2.5840	2.6601
7	3s3p <sub>1/2</sub> <sup>2</sup> 3p <sub>3/2</sub> <sup>4</sup>	<sup>3</sup> P <sub>1</sub> <sup>o</sup>	2.6715	2.7483
8	3s3p <sub>1/2</sub> <sup>2</sup> 3p <sub>3/2</sub> <sup>4</sup>	<sup>3</sup> P <sub>0</sub> <sup>o</sup>	2.7262	2.8027
9	3s3p <sub>1/2</sub> <sup>2</sup> 3p <sub>3/2</sub> <sup>3</sup>	<sup>1</sup> P <sub>1</sub> <sup>o</sup>	3.2973	3.4074
10	3s <sup>2</sup> 3p <sub>1/2</sub> <sup>2</sup> 3p <sub>3/2</sub> <sup>2</sup> 3d <sub>3/2</sub>	<sup>5</sup> D <sub>0</sub> <sup>o</sup>	.....	3.6008
11	3s <sup>2</sup> 3p <sub>1/2</sub> <sup>2</sup> 3p <sub>3/2</sub> <sup>2</sup> 3d <sub>3/2</sub>	<sup>5</sup> D <sub>1</sub> <sup>o</sup>	.....	3.6025
12	3s <sup>2</sup> 3p <sub>1/2</sub> <sup>2</sup> 3p <sub>3/2</sub> <sup>2</sup> 3d <sub>3/2</sub>	<sup>5</sup> D <sub>2</sub> <sup>o</sup>	.....	3.6048
13	3s <sup>2</sup> 3p <sub>1/2</sub> <sup>2</sup> 3p <sub>3/2</sub> <sup>2</sup> 3d <sub>5/2</sub>	<sup>5</sup> D <sub>3</sub> <sup>o</sup>	.....	3.6082
14	3s <sup>2</sup> 3p <sub>1/2</sub> <sup>2</sup> 3p <sub>3/2</sub> <sup>2</sup> 3d <sub>5/2</sub>	<sup>5</sup> D <sub>4</sub> <sup>o</sup>	.....	3.6165
15	3s <sup>2</sup> 3p <sub>1/2</sub> <sup>2</sup> 3p <sub>3/2</sub> <sup>2</sup> 3d <sub>5/2</sub>	<sup>3</sup> D <sub>2</sub> <sup>o</sup>	.....	3.8950
16	3s <sup>2</sup> 3p <sub>1/2</sub> <sup>2</sup> 3p <sub>3/2</sub> <sup>2</sup> 3d <sub>5/2</sub>	<sup>3</sup> D <sub>3</sub> <sup>o</sup>	.....	3.9161
17	3s <sup>2</sup> 3p <sub>1/2</sub> <sup>2</sup> 3p <sub>3/2</sub> <sup>2</sup> 3d <sub>5/2</sub>	<sup>3</sup> D <sub>1</sub> <sup>o</sup>	.....	3.9327
18	3s <sup>2</sup> 3p <sub>1/2</sub> <sup>2</sup> 3p <sub>3/2</sub> <sup>2</sup> 3d <sub>3/2</sub>	<sup>3</sup> F <sub>2</sub> <sup>o</sup>	.....	3.9843
19	3s <sup>2</sup> 3p <sub>1/2</sub> <sup>2</sup> 3p <sub>3/2</sub> <sup>2</sup> 3d <sub>3/2</sub>	<sup>3</sup> F <sub>3</sub> <sup>o</sup>	.....	4.0130
20	3s <sup>2</sup> 3p <sub>1/2</sub> <sup>2</sup> 3p <sub>3/2</sub> <sup>2</sup> 3d <sub>5/2</sub>	<sup>3</sup> F <sub>4</sub> <sup>o</sup>	.....	4.0524
21	3s <sup>2</sup> 3p <sub>1/2</sub> <sup>2</sup> 3p <sub>3/2</sub> <sup>2</sup> 3d <sub>5/2</sub>	<sup>1</sup> S <sub>0</sub> <sup>o</sup>	.....	4.0639
22	3s <sup>2</sup> 3p <sub>1/2</sub> <sup>2</sup> 3p <sub>3/2</sub> <sup>2</sup> 3d <sub>3/2</sub>	<sup>3</sup> G <sub>3</sub> <sup>o</sup>	.....	4.2177
23	3s <sup>2</sup> 3p <sub>1/2</sub> <sup>2</sup> 3p <sub>3/2</sub> <sup>2</sup> 3d <sub>5/2</sub>	<sup>3</sup> G <sub>4</sub> <sup>o</sup>	.....	4.2321
24	3s <sup>2</sup> 3p <sub>1/2</sub> <sup>2</sup> 3p <sub>3/2</sub> <sup>2</sup> 3d <sub>5/2</sub>	<sup>3</sup> G <sub>5</sub> <sup>o</sup>	.....	4.2501
25	3s <sup>2</sup> 3p <sub>1/2</sub> <sup>2</sup> 3p <sub>3/2</sub> <sup>2</sup> 3d <sub>3/2</sub>	<sup>1</sup> G <sub>4</sub> <sup>o</sup>	.....	4.3388
26	3s <sup>2</sup> 3p <sub>1/2</sub> <sup>2</sup> 3p <sub>3/2</sub> <sup>2</sup> 3d <sub>5/2</sub>	<sup>1</sup> D <sub>0</sub> <sup>o</sup>	.....	4.4206
27	3s <sup>2</sup> 3p <sub>1/2</sub> <sup>2</sup> 3p <sub>3/2</sub> <sup>2</sup> 3d <sub>5/2</sub>	<sup>3</sup> D <sub>0</sub> <sup>o</sup>	.....	4.5703
28	3s <sup>2</sup> 3p <sub>1/2</sub> <sup>2</sup> 3p <sub>3/2</sub> <sup>2</sup> 3d <sub>5/2</sub>	<sup>3</sup> P <sub>0</sub> <sup>o</sup>	.....	4.5990
29	3s <sup>2</sup> 3p <sub>1/2</sub> <sup>2</sup> 3p <sub>3/2</sub> <sup>2</sup> 3d <sub>5/2</sub>	<sup>3</sup> F <sub>3</sub> <sup>o</sup>	.....	4.6047
30	3s <sup>2</sup> 3p <sub>1/2</sub> <sup>2</sup> 3p <sub>3/2</sub> <sup>2</sup> 3d <sub>3/2</sub>	<sup>3</sup> F <sub>2</sub> <sup>o</sup>	.....	4.6144
31	3s <sup>2</sup> 3p <sub>3/2</sub> <sup>3</sup> 3d <sub>5/2</sub>	<sup>3</sup> F <sub>4</sub> <sup>o</sup>	.....	4.6153
32	3s <sup>2</sup> 3p <sub>1/2</sub> <sup>2</sup> 3p <sub>3/2</sub> <sup>2</sup> 3d <sub>5/2</sub>	<sup>3</sup> P <sub>1</sub> <sup>o</sup>	.....	4.6220
33	3s <sup>2</sup> 3p <sub>3/2</sub> <sup>3</sup> 3d <sub>3/2</sub>	<sup>3</sup> D <sub>0</sub> <sup>o</sup>	.....	4.6428
34	3s <sup>2</sup> 3p <sub>3/2</sub> <sup>3</sup> 3d <sub>5/2</sub>	<sup>3</sup> P <sub>2</sub> <sup>o</sup>	.....	4.7084
35	3s <sup>2</sup> 3p <sub>1/2</sub> <sup>2</sup> 3p <sub>3/2</sub> <sup>2</sup> 3d <sub>3/2</sub>	<sup>3</sup> D <sub>3</sub> <sup>o</sup>	4.5207	4.7163
36	3s <sup>2</sup> 3p <sub>3/2</sub> <sup>3</sup> 3d <sub>5/2</sub>	<sup>1</sup> F <sub>3</sub> <sup>o</sup>	.....	5.0117
37	3s <sup>2</sup> 3p <sub>1/2</sub> <sup>2</sup> 3p <sub>3/2</sub> <sup>2</sup> 3d <sub>3/2</sub>	<sup>3</sup> S <sub>1</sub> <sup>o</sup>	4.8612	5.0301
38	3s <sup>2</sup> 3p <sub>1/2</sub> <sup>2</sup> 3p <sub>3/2</sub> <sup>2</sup> 3d <sub>3/2</sub>	<sup>3</sup> P <sub>2</sub> <sup>o</sup>	4.8415	5.2142
39	3s <sup>2</sup> 3p <sub>1/2</sub> <sup>2</sup> 3p <sub>3/2</sub> <sup>2</sup> 3d <sub>3/2</sub>	<sup>3</sup> P <sub>1</sub> <sup>o</sup>	4.9335	5.2613
40	3s <sup>2</sup> 3p <sub>3/2</sub> <sup>3</sup> 3d <sub>3/2</sub>	<sup>3</sup> P <sub>0</sub> <sup>o</sup>	4.9365	5.3176
41	3s <sup>2</sup> 3p <sub>1/2</sub> <sup>2</sup> 3p <sub>3/2</sub> <sup>2</sup> 3d <sub>5/2</sub>	<sup>1</sup> P <sub>1</sub> <sup>o</sup>	.....	5.3454
42	3s <sup>2</sup> 3p <sub>1/2</sub> <sup>2</sup> 3p <sub>3/2</sub> <sup>2</sup> 3d <sub>5/2</sub>	<sup>3</sup> D <sub>3</sub> <sup>o</sup>	5.0512	5.3682
43	3s <sup>2</sup> 3p <sub>1/2</sub> <sup>2</sup> 3p <sub>3/2</sub> <sup>2</sup> 3d <sub>5/2</sub>	<sup>3</sup> D <sub>2</sub> <sup>o</sup>	5.1178	5.4332
44	3s <sup>2</sup> 3p <sub>3/2</sub> <sup>3</sup> 3d <sub>3/2</sub>	<sup>3</sup> D <sub>1</sub> <sup>o</sup>	5.1612	5.4853
45	3s <sup>2</sup> 3p <sub>1/2</sub> <sup>2</sup> 3p <sub>3/2</sub> <sup>2</sup> 3d <sub>5/2</sub>	<sup>1</sup> D <sub>2</sub> <sup>o</sup>	5.2750	5.5673
46	3s <sup>2</sup> 3p <sub>3/2</sub> <sup>3</sup> 3d <sub>3/2</sub>	<sup>1</sup> F <sub>3</sub> <sup>o</sup>	5.4132	5.7961
47	3s <sup>2</sup> 3p <sub>3/2</sub> <sup>3</sup> 3d <sub>5/2</sub>	<sup>1</sup> P <sub>1</sub> <sup>o</sup>	5.6779	6.0818
48	3p <sub>1/2</sub> <sup>2</sup> 3p <sub>3/2</sub> <sup>4</sup>	<sup>1</sup> S <sub>0</sub> <sup>e</sup>	.....	7.1606

a. Shirai et al. (1990).

b. Present results.

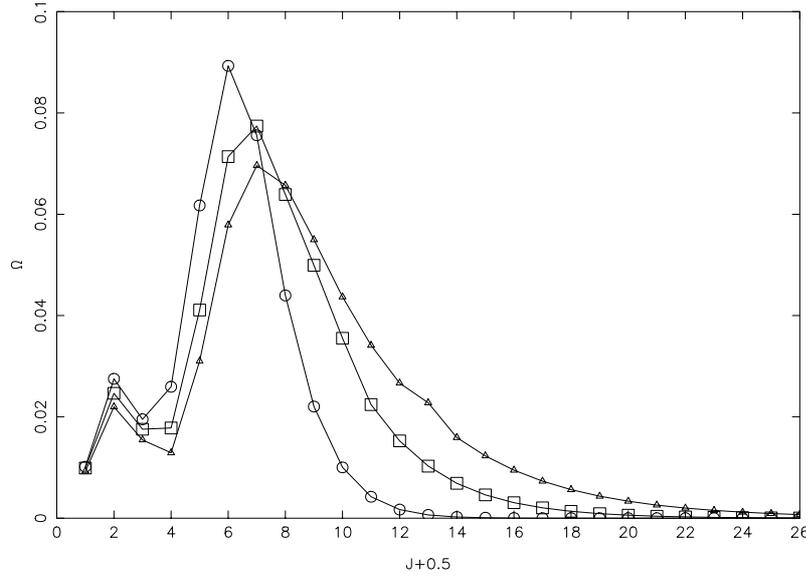
However, their energy range is not sufficient, especially towards the higher end of the temperature range, for the convergence of the integral (see Eq. (2) below) which determines the

value of  $\Upsilon$ . As a result, their reported values of  $\Upsilon$  are *underestimated* up to a factor of two, as has already been discussed and demonstrated in our earlier papers (Aggarwal & Keenan 2002, 2003) and further shown in Table 4. However, in our earlier papers we presented results of  $\Omega$  for a few selected transitions, and at a few representative energies, and of  $\Upsilon$  for only 10 transitions among the levels of the 3s<sup>2</sup>3p<sup>4</sup> configuration. In the present paper we report our results for both of these parameters for *all* transitions among the 48 fine-structure levels of Fe XI, and for a wider energy (temperature) range.

Bhatia & Doschek (1996) have employed the Super-Structure (SS) program of Eissner et al. (1974) to generate their wavefunctions and the DW code of Eissner & Seaton (1972) to compute collision strengths. Their calculations are basically in the *LS* coupling scheme, and the results in the *LSJ* coupling scheme have been obtained through the JAJOM program of Saraph (1978). One-body relativistic operators have been incorporated through *term coupling coefficients*. This approach gives reasonably satisfactory results if the fine-structure levels are not too far apart, which is the case for Fe XI (see Table 1). However, this approach can only be applied when all channels are open, and this is the main reason that Bhatia & Doschek have produced values of  $\Omega$  only at energies above thresholds. Gupta & Tayal (1999a,b) have employed the CIV3 program of Hibbert (1975) to generate the wavefunctions and the Breit-Pauli version of the *R*-matrix program (Scott & Taylor 1982) for the computations of  $\Omega$ . This approach is similar to the one described above, but allows the computation of  $\Omega$  within the threshold region also. In our calculations, the GRASP program of Dyaal et al. (1989) has been adopted for the generation of wavefunctions and the Dirac Atomic *R*-matrix Code (DARC) of Norrington & Grant (2003) for the computations of  $\Omega$ . Both of these programs are fully relativistic and are based on the *jj* coupling scheme. Thus, apart from improving the accuracy of the earlier available results, we are adopting an independent approach to report our data.

## 2. Collision strengths

The (1s<sup>2</sup>2s<sup>2</sup>2p<sup>6</sup>) 3s<sup>2</sup>3p<sup>4</sup>, 3s3p<sup>5</sup>, 3s<sup>2</sup>3p<sup>3</sup>3d and 3p<sup>6</sup> configurations of Fe XI give rise to 48 fine-structure levels, listed in Table 1. To generate our wavefunctions, we have adopted the GRASP (General purpose Relativistic Atomic Structure Program) code of Dyaal et al. (1989). Since CI is very important for this ion, we have included CI among the 3s<sup>2</sup>3p<sup>2</sup>3d<sup>2</sup>, 3s<sup>2</sup>3p<sup>3</sup>4s, 3s<sup>2</sup>3p<sup>3</sup>4p and 3s<sup>2</sup>3p<sup>3</sup>4d configurations in addition to the basic four configurations listed above. Further details about our calculations, and comparisons of energy levels and radiative rates with earlier available results, can be found in our earlier publication (Aggarwal & Keenan 2003). In Table 1, we list our calculated energy levels and include the corresponding experimentally compiled results of Shirai et al. (1990). The agreement between our theoretical and available experimental energy levels is better than 10%, except for the 3s<sup>2</sup>3p<sup>4</sup> <sup>1</sup>S<sub>0</sub> level, for which our energy is lower by 15%. The energies of the CIV3 calculations (Gupta & Tayal 1999a) are in better agreement with the measurements, but their energy order is different in a few instances, namely levels 21, 28, 32 and 41. Similarly,



**Fig. 1.** Partial collision strengths for the  $3p^4 \ ^3P_1 - 3p^3 3d \ ^1D_2^o$  (2–45) transition of Fe XI, at three energies of 8 Ry (circles), 16 Ry (squares), and 24 Ry (triangles).

the level order of the SS calculations (Bhatia & Doschek 1996) is entirely different from both theoretical as well as the experimental energy ordering. However, the differences between various theoretical calculations are within  $\sim 10\%$  as shown in Table 1 of Aggarwal & Keenan (2003).

For the computations of collision strengths, we have adopted the Dirac Atomic *R*-matrix Code (DARC) of Norrington & Grant (2003). This program includes the relativistic effects in a systematic way, in both the target description and the scattering model. It is based on the *jj* coupling scheme, and uses the Dirac-Coulomb Hamiltonian in the *R*-matrix approach. However, because of the inclusion of fine-structure in the definition of channel coupling, the matrix size of the Hamiltonian increases substantially, making the calculations computationally more expensive. The *R*-matrix radius adopted is 5.4 au, and 25 continuum orbitals have been included for each channel angular momentum for the expansion of the wavefunction. This allows us to compute  $\Omega$  up to an energy of 100 Ry. In order to obtain convergence of  $\Omega$  for all transitions and at all energies, we have included all partial waves with angular momentum  $J \leq 40.5$ , although a higher range would have been preferable for the convergence of allowed transitions, especially at higher energies. To account for the higher neglected partial waves, we have included a top-up, based on the Coulomb-Bethe approximation for allowed transitions and geometric series for forbidden transitions.

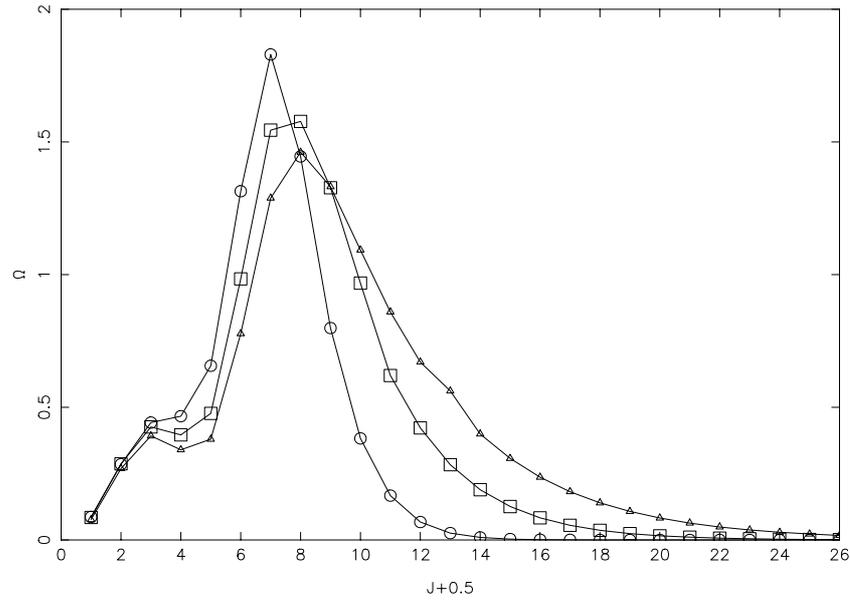
While computing  $\Omega$ , the diagonal elements of the continuum Hamiltonian have been adjusted in accordance with the Breit and QED corrected threshold energies as listed in Table 1. This is acceptable because the differences between the two sets of threshold energies (with and without Breit and QED corrections) are small ( $\leq 0.015$  Ry). However, this can only be performed if the energy ordering is the same in both sets of calculations, which is true in our case for the levels under consideration, as seen in Table 1. The procedure helps in correctly positioning the resonances in the threshold region.

The computed values of  $\Omega$  for all 1128 inelastic transitions among the lowest 48 fine-structure levels of Fe XI are presented in Table 2 at energies above thresholds in the range  $10 \leq E \leq 100$  Ry. In this energy range  $\Omega$  varies smoothly, and hence the corresponding value at any desired energy within this range can be easily interpolated. We also note here that  $\Omega$  is a dimensionless quantity, and is related to the better known parameter collision cross section by the following expression

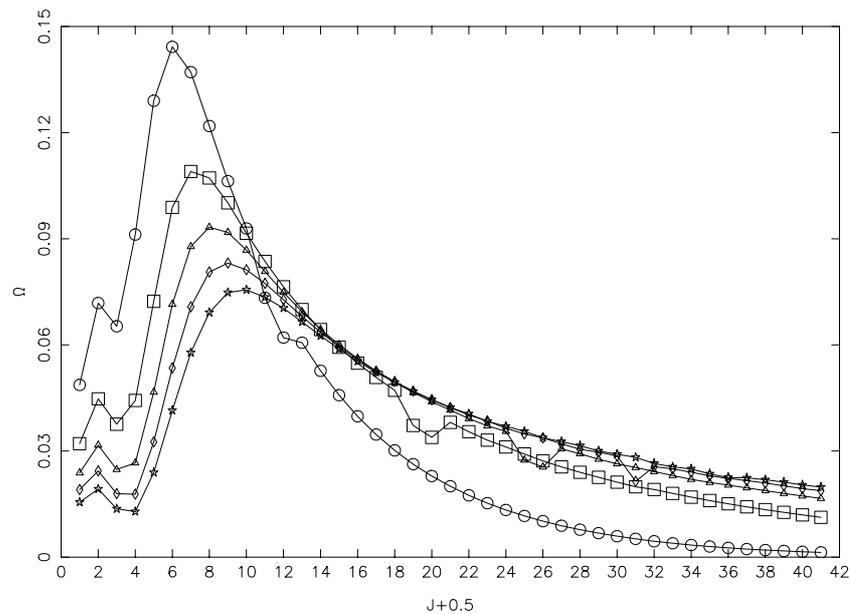
$$\Omega_{ij}(E) = k_i^2 \omega_i \sigma_{ij} (\pi a_0^2) \quad (1)$$

where  $k_i$  is the incident electron energy in rydberg,  $\omega_i$  is the statistical weight of the initial level  $i$ , and  $\sigma_{ij}$  is the collision cross section in units of  $\pi a_0^2$ .

Earlier calculations for  $\Omega$  have been performed by Bhatia & Doschek (1996: BD) and Gupta & Tayal (1999a,b: GT). BD have employed the DW code and have performed their computations of  $\Omega$  at only three energies above thresholds. On the other hand, GT have used the Breit-Pauli version of the *R*-matrix code (Scott & Taylor 1982), and have performed their computations of  $\Omega$  at a large number of energies, particularly in the threshold region, so that the contribution of resonances can be included while computing the excitation rate coefficients. Furthermore, they extended the energy range up to 40 Ry. However, both workers included the partial waves range up to  $J = 17.5$  before invoking the contribution of higher neglected partial waves from the Coulomb-Bethe approximation. This range of partial waves is sufficient for the convergence of  $\Omega$  in the energy range of their calculations for a majority of transitions. In Figs. 1 and 2 we show the variation of  $\Omega$  with angular momentum ( $J$ ) at three energies of 8, 16 and 24 Ry, for two transitions, namely 2–45 and 4–46. For both of these (and many other) transitions, values of  $\Omega$  have fully converged up to about  $J = 25.5$ . Therefore, the contribution of neglected partial waves for many transitions will almost be negligible. But for a few allowed transitions, and particularly towards the higher end of our energy range, even this large set of partial waves is



**Fig. 2.** Partial collision strengths for the  $3p^4 \ ^1D_2-3p^3 3d \ ^1F_3^o$  (4–46) transition of Fe XI, at three energies of 8 Ry (circles), 16 Ry (squares), and 24 Ry (triangles).

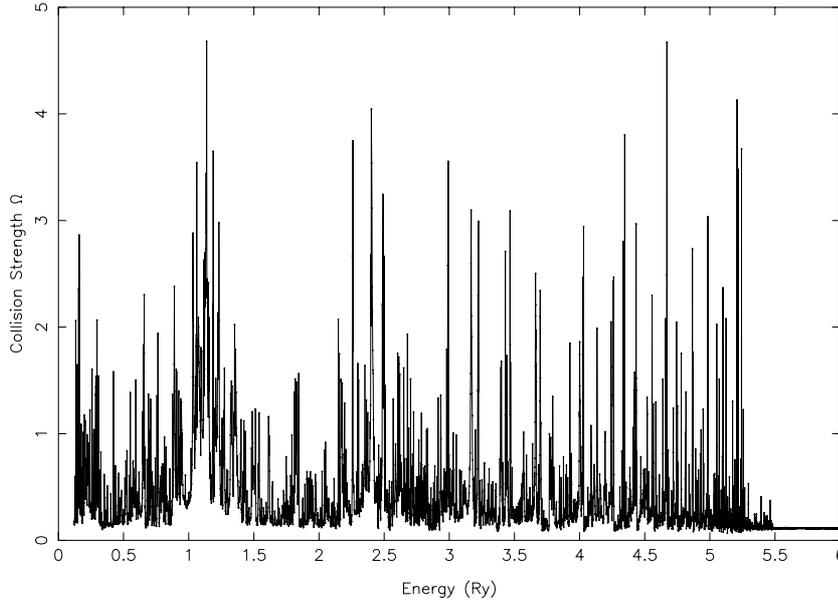


**Fig. 3.** Partial collision strengths for the  $3p^3 3d \ ^1P_1^o-3p^6 \ ^1S_1$  (41–48) transition of Fe XI, at five energies of 20 Ry (circles), 40 Ry (squares), 60 Ry (triangles), 80 Ry (diamonds), and 100 Ry (stars).

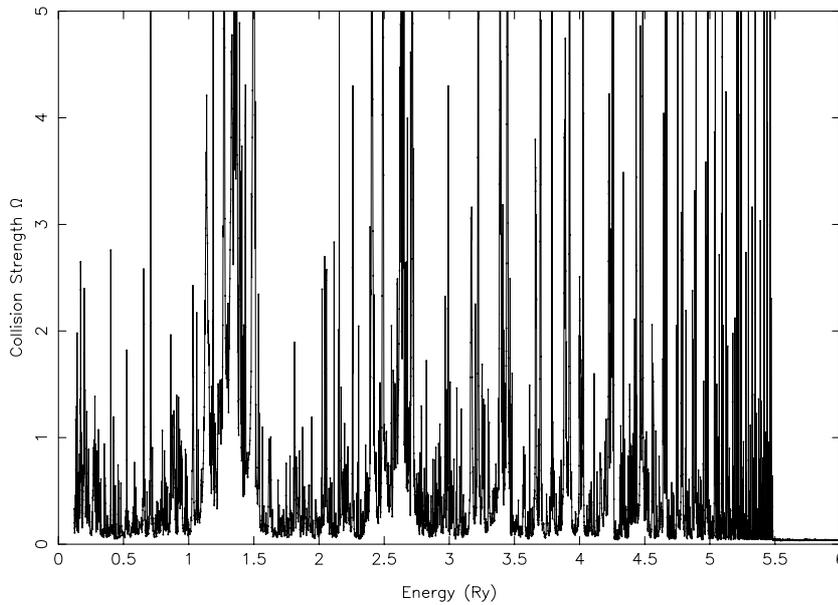
not sufficient for convergence. We demonstrate this in Fig. 3 for only one transition, namely 41–48. The values of  $\Omega$  have fully converged for all transitions up to  $E = 20$  Ry, but at higher energies a higher range of partial waves is desirable. Since there are only a few transitions ( $\sim 10\%$ ) for which a higher range of partial waves is required, we have included a top-up to account for the neglected partial waves. This may affect the accuracy of our  $\Omega$  values for a few transitions and at higher energies, but the error so introduced will be less than  $\sim 10\%$ .

A comparison of our  $\Omega$  values with those of BD and GT has already been shown in our earlier work (Aggarwal & Keenan 2003), and hence is not discussed in detail here. However to recapitulate, differences between our present  $R$ -matrix and

earlier DW calculations are within 50%, and are in accordance with the corresponding  $f$ -values, i.e. if the  $f$ -value is higher then so is the value of  $\Omega$ , and vice-versa. Since BD have included CI within the basic configurations only, their results of oscillator strengths ( $f$ -values) and collision strengths are comparatively less accurate. However, GT results differ up to a factor of 7 for some transitions, such as 1–41 and 2–41, and do not agree with any of the other two calculations for a few transitions, such as: 1–39, 2–45 and 3–5 (see Table 5 of Aggarwal & Keenan 2003). Gupta & Tayal (1999a,b) have not reported the  $f$ -values of their calculations, and therefore it is difficult to understand the source of the discrepancy. However, Deb & Tayal (1998) have reported  $f$ -values from their CIV3



**Fig. 4.** Collision strengths ( $\Omega$ ) for the  $(3s^23p^4) \ ^3P_2-^3P_0$  (1-3) transition of Fe XI.



**Fig. 5.** Collision strengths ( $\Omega$ ) for the  $(3s^23p^4) \ ^3P_1-^3P_0$  (2-3) transition of Fe XI.

calculations, but these are not compatible with the  $\Omega$  values of GT. This is because Deb & Tayal calculated the  $f$ -values using a large CI including 1523 configurations, whereas those used by GT in their computations of  $\Omega$  have been obtained from a limited set of CI including only 123 configurations. This drastic reduction in the number of configurations (by over an order of magnitude) has perhaps significantly altered the  $f$ -values, especially for those transitions for which their magnitude are comparatively smaller. Therefore, the  $\Omega$  values of GT are also comparatively less accurate, apart from differing from the DW calculations of BD and our results from DARC. A transition for which the GT values of  $\Omega$  are higher by up to a factor of 40 is  $(3s^23p^4) \ ^3P_0-^1S_0$  (3-5), which is a spin forbidden 0-0 transition of the same parity. This large difference in  $\Omega$  values is perhaps

due to errors in the (earlier) version of the  $R$ -matrix program (Scott & Taylor 1982) they adopted – see Aggarwal & Keenan (2003) for further details and comparisons.

### 3. Effective collision strengths

Effective collision strengths ( $\Upsilon$ ) are obtained after integrating the  $\Omega$  data over a Maxwellian distribution of electron velocities as follows:

$$\Upsilon(T_e) = \int_0^{\infty} \Omega(E) \exp(-E_j/kT_e) d(E_j/kT_e), \quad (2)$$

where  $k$  is Boltzmann constant,  $T_e$  is electron temperature in K, and  $E_j$  is the electron energy with respect to the final (excited) state.

**Table 4.** Comparison between our present DARC and earlier BPRM (GT: Gupta & Tayal 1999a,b) effective collision strengths ( $\Upsilon$ ) for some transitions of Fe XI. ( $a \pm b \equiv a \times 10^{\pm b}$ ).

Transition		DARC				GT			
$i$	$j$	$5 \times 10^5$	$1 \times 10^6$	$2 \times 10^6$	$5 \times 10^6$	$5 \times 10^5$	$1 \times 10^6$	$2 \times 10^6$	$5 \times 10^6$ K
1	37	1.155-0	1.245-0	1.390-0	1.646-0	1.87	1.93	1.92	1.44
1	38	4.807-0	5.236-0	5.875-0	6.926-0	4.18	4.33	4.30	3.23
1	42	7.070-0	7.728-0	8.697-0	1.032+1	7.22	7.44	7.35	5.48
1	43	8.179-1	8.892-1	9.956-1	1.175-0	1.10	1.12	1.11	0.824
2	38	1.021-0	1.106-0	1.236-0	1.450-0	1.03	1.06	1.05	0.781
2	40	1.226-0	1.336-0	1.500-0	1.797-0	1.14	1.19	1.19	0.893
2	43	3.866-0	4.226-0	4.754-0	5.609-0	4.09	4.23	4.19	3.13
2	44	1.220-0	1.332-0	1.496-0	1.759-0	1.25	1.29	1.28	0.961
3	44	1.692-0	1.849-0	2.082-0	2.529-0	1.80	1.86	1.85	1.38
4	39	6.217-1	6.665-1	7.394-1	8.668-1	1.56	1.59	1.57	1.18
4	41	3.250-0	3.528-0	3.949-0	4.653-0	1.95	2.00	1.98	1.48
4	45	3.200-0	3.488-0	3.922-0	4.701-0	4.30	4.40	4.33	3.22
4	46	8.281-0	9.055-0	1.019+1	1.208+1	7.46	7.63	7.49	5.54
5	47	2.536-0	2.773-0	3.121-0	3.715-0	2.67	2.79	2.77	2.07

Since the threshold region is dominated by numerous resonances,  $\Omega$  must be computed in a fine mesh of energy. Close to thresholds our mesh is 0.001 Ry and is 0.002 Ry in the remaining range. In total values of  $\Omega$  have been computed at 4487 energies in the threshold region below 7.16 Ry. This fine energy mesh ensures to a large extent that neither a majority of resonances are missed, nor do the exceptionally high resonances have unreasonably large width. In Figs. 4 and 5 we show resonances for only two transitions, namely  $(3s^23p^4) \ ^3P_2-^3P_0$  (1-3) and  $^3P_1-^3P_0$  (2-3). These resonances have been shown in a wide threshold region and illustrate their density, as well as importance. Additionally, resonances for these transitions have fully converged up to an energy of  $\sim 5.5$  Ry.

In Table 3 we list our values of  $\Upsilon$  for all 1128 transitions among the 48 fine-structure levels of Fe XI over a wide temperature range of  $10^4$  to  $5 \times 10^6$  K, suitable for applications in a wide variety of astrophysical, laser and fusion plasmas. This is also the temperature range in which GT (including Tayal 2000) have reported their results. An explicit comparison between our and the GT results of  $\Upsilon$  for transitions among the levels of the  $3s^23p^4$  configuration has already been shown in our earlier work (Aggarwal & Keenan 2003). Differences of a factor of two were observed for many transitions and in almost the entire temperature range. These were mainly due to our better resolution of resonances and inclusion of higher range of energy for the calculations of  $\Omega$ . In Table 4 we make a similar comparison between our and the GT results for a few representative transitions among the higher excited levels. Particularly selected are those transitions which have comparatively higher magnitude, and for which  $\Omega$  values have already been compared in Table 5 of our earlier paper (Aggarwal & Keenan 2003). Comparisons have been shown at only four temperatures ( $5 \times 10^5$ ,  $10^6$ ,  $2 \times 10^6$  and  $5 \times 10^6$  K) which cover the entire range of the calculations by GT. All of these transitions are *allowed* in the *jj* or *LSJ* coupling scheme and have comparatively large *f*-values, as shown in Table 2 of Aggarwal & Keenan (2003). As a result, the corresponding  $\Omega$  and subsequently  $\Upsilon$  values should increase with

increasing energy and temperature, respectively. This is true in our case as shown in Tables 2 and 3. The  $\Omega$  values of GT calculations also increase with energy as can be seen in Table 2 of Gupta & Tayal (1999a,b), but their values of  $\Upsilon$  decrease with increasing temperature. This is because they computed their results for  $\Omega$  up to an energy of 40 Ry only, which is not sufficient for the convergence of integral in Eq. (2), especially towards the higher end of their temperature range. As a result, their values of  $\Upsilon$  are *underestimated* by up to a factor of two, as can clearly be seen for 1-38, 2-44 and 4-46 transitions beside others.

#### 4. Conclusions

In this paper we have reported results for collision strengths and effective collision strengths in a wide energy/temperature range for transitions among the 48 fine-structure levels of Fe XI. Relativistic effects and CI have been included while generating the wavefunctions, and a large range of partial waves has been included to ensure the convergence of  $\Omega$ . Furthermore, resonances have been included in a fine energy mesh in order to determine the effective collision strengths. Differences between our present *R*-matrix and the earlier available (Bhatia & Doschek 1996) DW values of  $\Omega$  are in accordance with the differences in wavefunctions, whereas the similar results of Gupta & Tayal (1999a,b) appear to be incompatible with their (known) values of oscillator strengths.

We do not see any apparent deficiency in our calculations and estimate that the presently reported results of collision strengths are accurate to better than 10% at energies below 25 Ry (because of *convergence* of *all* transitions), but may be inaccurate up to 20% at higher energies for a few allowed transitions. This estimate is based on the presently determined values of oscillator strengths. As scope remains for improvement in our wavefunctions (by including additional CI), the present values of  $\Omega$  may easily differ by a factor of two, especially for weaker transitions. However, the corresponding values of

$\Omega$  for stronger transitions are unlikely to vary by more than 20%, as has been confirmed by our test calculations including additional CI.

The only other results for  $\Upsilon$  available in the literature are of GT (Gupta & Tayal 1999a,b), which are found to be *underestimated* by up to a factor of two, especially for the allowed transitions. This is because of the limited energy range included in their calculations of  $\Upsilon$  values. Our calculations should represent a considerable improvement over their results, because we have: (i) included CI among 235 configurations in comparison to their 123, (ii) have performed fully relativistic calculations in *jj* coupling scheme in comparison to their semi-relativistic approach in the *LSJ* coupling scheme, (iii) have included partial waves up to  $J = 40.5$  in comparison to their  $\leq 17.5$ , (iv) have computed values of  $\Omega$  up to 100 Ry in comparison to their energy below 40 Ry, (v) have included resonances among 48 levels in comparison to their 38, and finally (vi) have adopted a fine energy mesh of better than 0.002 Ry in comparison to their mesh of 0.005 Ry. Therefore, the presently reported results for both  $\Omega$  and  $\Upsilon$  are probably the most reliable available to date, and are expected to be accurate to better than 10%, especially at temperatures above  $10^5$  K. Due to the presence (or absence) of many near-threshold resonances, accuracy estimates at lower temperatures are insecure.

One way to estimate the accuracy of our calculations is to compare excitation rates with the corresponding experimental results, which are available in the literature (Wang et al 1984). Unfortunately, the experimental results were assessed to be overestimated by up to a factor of two, which is found to be true as discussed in detail in our earlier work (Aggarwal & Keenan 2003). The other way is to apply the present results in analysing the observational data for spectral emission line intensities. Adopting the earlier available  $\Upsilon$  data of GT, Pinfield et al. (2001) analysed many EUV lines of Fe XI, which is formed in the temperature range of  $6 \times 10^5$  to  $3 \times 10^6$  K. Since

the GT values of  $\Upsilon$  are *underestimated* for many of the observed lines (see Table 1 of Pinfield et al), especially at higher temperatures, the presently reported results should be of considerable significance for astrophysical applications. We hope to investigate the effect of present improved atomic data in our future work.

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