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Atomic data from the IRON Project

XXXVI. Electron excitation of Be-like Fe XXIII between $1s^2\,2l_1\,2l_2\,SLJ$ and $1s^2\,2l_3\,2l_4\,S'L'J'$

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Abstract. Partial collision strengths for electron induced transitions in the beryllium-like ion Fe XXIII are calculated using the Belfast R-matrix programs (Berrington et al. 1995). Our target has 98 fine structure states $1s^2\,nl\,n'l'\,SLJ$ corresponding to $n = 2$ and $n' = 2, 3, 4$. The present calculation is carried out for electron impact energies in the range 3.15 to 350 Ry. Below 115.185 Ry, corresponding to the highest excited state of our model ion, we use the Breit-Pauli version of the R-matrix code. For energies between 116 and 350 Ry we use the non-relativistic LS-coupling version of the R-matrix code together with JAJOM (Saraph 1978). When T exceeds about ten million degrees one needs to take account of contributions to the thermally averaged collision strength Υ coming from electrons with energies in excess of 350 Ry. We discuss a way of estimating these contributions. Values of Υ are computed and tabulated as functions of $\log T$ for transitions between the $2s^2\ {}^1S_0$, $2s2p\ {}^3P^o_{0,1,2}$, $2s2p\ {}^1P^o_1$, $2p^2\ {}^3P_{0,1,2}$, $2p^2\ {}^1D_2$ and $2p^2\ {}^1S_0$ states. The temperature range $6.3 \leq \log T \leq 8.1$ is centred on $\log T = 7.1$ which, according to Arnaud & Rothenflug (1985), is where Fe XXIII has maximum coronal abundance.

Key words: atomic data — Sun: corona

1. Introduction

The present calculation is a contribution to the international IRON Project (Hummer et al. 1993; Paper I) whose members are working to obtain reliable rate coefficients for collisional excitation of fine-structure transitions in positive ions induced by electron impact. Other papers in the series are given in the section References, while a complete list of IRON Project published papers and those in press is available at the Internet address http://www.am.qub.ac.uk. The present paper is devoted to the beryllium-like iron ion Fe^{+22}.

The temperature dependent rate coefficient $q(i \to j)$ for a transition between atomic levels with indices i and j and energy separation E_{ij} is given in terms of the effective, or thermally averaged, collision strength $\Upsilon(i-j)$ by

$$q(i \to j) = 2\pi^{1/2} a_0\, \hbar\, m_{\rm e}^{-1}\, ({\rm Ry}/kT)^{1/2} \exp(-E_{ij}/kT)\, \Upsilon(i-j)/(2J_i+1) \qquad (1)$$

where $2\pi^{1/2} a_0\, \hbar\, m_{\rm e}^{-1} = 3.610\ 10^{-24}\ {\rm m^3\ s^{-1}}$. For energies we use the Rydberg unit, which has the value Ry = 13.6058 eV, while the Boltzmann constant is given by $k = 8.617\ 10^{-5}$ eV deg^{-1}, the temperature T being in degrees Kelvin. The factor $(2J_i + 1)$ is the statistical weight of level i.

Following Seaton (1953) we define the effective collision strength Υ as follows:

$$\Upsilon(i-j) = \int_0^\infty \Omega(i-j) \exp(-E_j/kT)\, {\rm d}(E_j/kT) \qquad (2)$$

where E_j is the energy of the colliding electron after excitation has occurred. The energy dependent collision strength $\Omega(i-j)$ and cross section $Q(i \to j)$ are related as follows:

$$Q(i \to j) = \frac{\pi\, \Omega(i-j)}{(2J_i+1)k_i^2} \qquad (3)$$

where k_i is the wave number of the colliding electron incident on the target ion in level i.

Eighteen years ago Bhatia & Mason (1981) used W.B. Eissner's distorted wave collision code, which originated at University College London, to calculate collision strengths for many transitions in Fe^{+22}. Five years later Bhatia &

Table 1. Chronological list of work on electron excitation of Fe XXIII

1976	Davis J., Kepple P.C., Blaha M., J. Quant. Spectrosc. Radiat. Transfer 16, 1043-1055
1977	Parks A.D., Sampson D.H., Phys. Rev. A 15, 1382-1392
1980	Clark R.E.H., Sampson D.H., Parks A.D., ApJS 44, 215-222
1980	Feldman U., Doschek G.A., Cheng C.-C., Bhatia A.K., J. Appl. Phys. 51, 190-201
1980	Goett S.J., Clark R.E.H., Sampson D.H., Atomic Data Nuclear Data Tab. 25, 185-217
1980	Sampson D.H., Clark R.E.H., Golden L.B., ApJS, 44, 193-213
1980	Scott N.S., Burke P.G., J. Phys. B. 13, 4299-4314
1980	Younger S.M., J. Quant. Spectrosc. Radiat. Transfer 23, 489-498
1981	Bhatia A.K., Mason H.E., A&A 103, 324-330,
1981	Sampson D.H., Clark R.E.H., Goett S.J., Phys. Rev. A 24, 2979-2994
1983	Mann J., Atomic Data Nuclear Data Tab. 29, 407-452
1986	Bhatia A.K., Mason H.E., A&A, 155, 413-416
1987	Norrington P.H., Grant I.P., J. Phys. B 20, 4869-4881
1988	Kim Y.-K., Desclaux J.-P., Phys. Rev. A 38, 1805-1808
1989	Qian W.-J., Kim Y.-K., Desclaux J.-P., Phys. Rev. A 39, 4509-4517
1992	Safranova U.I., Vainshtein L.A., Kato T., Masai K., Phys. Scr. 46, 409-428
1992	Zhang H.L., Sampson D.H., Atomic Data Nuclear Data Tab. 52, 143-173
1998	Chen Guo-xin, Ong P.P., Phys. Rev. A 58, 1183-1194

Table 2. Exponents for the Fe^{+22} radial orbitals using analytic forms similar to that shown in (4). The coefficients are fixed by orthonormality conditions

nl	r^1	r^2	r^3	r^4
3s	15.643784	7.599631	7.775178	
3p		10.034376	7.495761	
3d			7.745244	
4s	3.304296	8.881686	5.709845	5.510196
4p		8.898516	5.698224	5.712733
4d			6.634467	5.641839
4f				5.756527

Mason (1986) extended their work to energies both below and above those they considered in 1981; they gave a comprehensive tabulation covering the interval from 15 to 350 Ry. In order to carry out thermal averaging Bhatia & Mason (1986) linearly interpolated their data and integrated the resulting function $\Omega \times \exp(-E_j/kT)$ analytically (Mason 1998, private communication) in order to obtain $\Upsilon(T)$. Corliss & Sugar (1982) estimate the ionization energy of the ground state to be 15797000 cm^{-1} (143.95 Ry), which means that three of Bhatia & Mason's (1986) energies lie above the ionization threshold while the rest are below. Since Bhatia & Mason (1981) include a thorough discussion of collision calculations devoted to Fe^{+22} up to the time of their own investigation, the reader is encouraged to consult their paper for information on this ion and we shall refrain from giving further details here except for a list of relevant papers in Table 1.

2. The calculation

Paper I in this series gives the basic atomic theory, approximations and computer codes used in the IRON Project. For electrons incident with kinetic energies relative to the ground state of the target less than or equal to 350 Ry we make use of the R-matrix method based on the close coupling approximation. This allows us to take account of channel coupling up to the $n = 4$ levels. Relativistic effects are allowed for, either by using the Breit-Pauli version of the R-matrix code, or by running the non-relativistic version and then carrying out an algebraic transformation of the appropriate collision matrix elements by means of Saraph's (1978) code JAJOM. We use the former procedure for energies below 116 Ry and the latter for energies from 116 to 350 Ry. We are able to extend our R-matrix collision strengths beyond 350 Ry with some confidence by using A. Burgess's graphics program OmeUps with the appropriate high energy limits (see Burgess & Tully 1992). For the optically allowed transitions the limits are determined by the oscillator strengths (see Table 7), while for the non-exchange optically forbidden transitions we have calculated the Born limits using the program discussed by Burgess et al. (1997) and results are given in Table 8.

The radial orbitals for the Be-like target are as follows: P_{1s}, P_{2s} are from Clementi & Roetti (1974). P_{2p} is the 2 exponent function

$$P_{2p}(r) = 544.2971\, r^2 \exp(-11.83976\, r) + 63.0511\, r^2 \exp(-20.83824\, r) \quad (4)$$

which we obtained by using Hibbert's (1975) variational program CIV3 to minimise the sum of the energies of the $1s^2\,2s2p\ ^1P^o$ and $^3P^o$ terms with trial exponents and

Table 3. Fe XXIII level energies in rydberg units relative to the ground state. Theoretical results from the Breit-Pauli R-matrix program. Observed results from Corliss & Sugar (1982) assuming 1 Ry = 109737.32 cm^{-1}. % diff is the percentage difference between the theoretical and observed energies

Index	Theoretical	% diff	Observed	Label	Index	Theoretical	% diff	Observed	Label
1	0.000000		0.000000	2s2s ^{1}S$_0$	50	109.648162			2s4p ^{3}P$^o_1$
2	3.152098	(−0.65)	3.172840	2s2p ^{3}P$^o_0$	51	109.756588			2s4p ^{3}P$^o_2$
3	3.443526	(−0.33)	3.454880	2s2p ^{3}P$^o_1$	52	109.800074	(+0.04)	109.752999	2s4p ^{1}P$^o_1$
4	4.276639	(−0.52)	4.299170	2s2p ^{3}P$^o_2$	53	110.096981	(+0.07)	110.017266	2s4d ^{3}D$_1$
5	6.893095	(+0.48)	6.860380	2s2p ^{1}P$^o_1$	54	110.112145	(+0.07)	110.035492	2s4d ^{3}D$_2$
6	8.690250	(−0.26)	8.712620	2p2p ^{3}P$_0$	55	110.139278	(+0.04)	110.090168	2p3p ^{3}D$_3$
7	9.322161	(−0.41)	9.360530	2p2p ^{3}P$_1$	56	110.320875	(+0.07)	110.245083	2s4d ^{1}D$_2$
8	9.763415	(−0.03)	9.766040	2p2p ^{3}P$_2$	57	110.355438			2s4f ^{3}F$^o_2$
9	10.978704	(+0.05)	10.973470	2p2p ^{1}D$_2$	58	110.362603			2s4f ^{3}F$^o_3$
10	12.984295	(+0.13)	12.967320	2p2p ^{1}S$_0$	59	110.376497			2s4f ^{3}F$^o_4$
11	81.272400	(+0.28)	81.048088	2s3s ^{3}S$_1$	60	110.417055			2s4f ^{1}F$^o_3$
12	81.858246			2s3s ^{1}S$_0$	61	112.757456			2p4s ^{3}P$^o_0$
13	82.758298			2s3p ^{3}P$^o_0$	62	112.800546			2p4s ^{3}P$^o_1$
14	82.762057	(+0.07)	82.706594	2s3p ^{3}P$^o_1$	63	113.187344			2p4p ^{3}D$_1$
15	83.036732	(+0.06)	82.989087	2s3p ^{1}P$^o_1$	64	113.415746			2p4p ^{3}P$_1$
16	83.066611			2s3p ^{3}P$^o_2$	65	113.431838			2p4p ^{3}D$_2$
17	83.886696	(+0.07)	83.827452	2s3d ^{3}D$_1$	66	113.452788			2p4p ^{3}P$_0$
18	83.931305	(+0.02)	83.918579	2s3d ^{3}D$_2$	67	113.638586			2p4d ^{3}F$^o_2$
19	84.002080	(+0.07)	83.945917	2s3d ^{3}D$_3$	68	113.784918			2p4d ^{3}D$^o_2$
20	84.576932	(+0.09)	84.501790	2s3d ^{1}D$_2$	69	113.823771	(+0.05)	113.762574	2p4d ^{3}F$^o_3$
21	85.247271	(+0.64)	84.702269	2p3s ^{3}P$^o_0$	70	113.874581	(+0.07)	113.799024	2p4d ^{3}D$^o_1$
22	85.404821			2p3s ^{3}P$^o_1$	71	113.923012			2p4s ^{3}P$^o_2$
23	86.261817	(+0.12)	86.160296	2p3p ^{3}D$_1$	72	113.923467			2p4f ^{3}G$_3$
24	86.365730			2p3s ^{3}P$^o_2$	73	113.950366			2p4f ^{3}F$_2$
25	86.784405	(+0.56)	86.296986	2p3s ^{1}P$^o_1$	74	113.959549			2p4f ^{3}G$_4$
26	86.840297	(+0.06)	86.789070	2p3p ^{3}D$_2$	75	113.961356			2p4s ^{1}P$^o_1$
27	86.847965			2p3p ^{1}P$_1$	76	113.985080			2p4f ^{3}F$_3$
28	87.027071			2p3p ^{3}P$_0$	77	114.395802			2p4p ^{1}P$_1$
29	87.376192			2p3d ^{3}F$^o_2$	78	114.457726			2p4p ^{3}P$_2$
30	87.661761			2p3p ^{3}P$_1$	79	114.458331	(+0.00)	114.455137	2p4p ^{3}D$_3$
31	87.725901	(+0.03)	87.700337	2s4d ^{3}D$_3$	80	114.506333			2p4p ^{3}S$_1$
32	87.767479	(+0.07)	87.709450	2p3d ^{3}F$^o_3$	81	114.680007			2p4p ^{1}D$_2$
33	87.878111	(+0.06)	87.827914	2p3d ^{1}D$^o_2$	82	114.813657			2p4d ^{3}F$^o_4$
34	87.891869			2p3p ^{3}S$_1$	83	114.814505	(+0.02)	114.792305	2p4d ^{1}D$^o_2$
35	87.907601	(+0.03)	87.882590	2p3p ^{3}P$_2$	84	114.887275	(+0.04)	114.846981	2p4d ^{3}D$^o_3$
36	88.049510			2p3d ^{3}D$^o_1$	85	114.931118			2p4p ^{1}S$_0$
37	88.474956			2p3p ^{1}D$_2$	86	114.957060	(+0.01)	114.947221	2p4d ^{3}P$^o_2$
38	88.587512			2p3d ^{3}F$^o_4$	87	114.957247	(+0.00)	114.956333	2p4d ^{3}P$^o_1$
39	88.673734			2p3d ^{3}D$^o_2$	88	114.966466			2p4d ^{3}P$^o_0$
40	88.903053	(+0.07)	88.839421	2p3d ^{3}D$^o_3$	89	115.026529			2p4f ^{1}F$_3$
41	89.082548			2p3d ^{3}P$^o_2$	90	115.050435			2p4f ^{1}G$_4$
42	89.089201			2p3d ^{3}P$^o_1$	91	115.085217			2p4f ^{3}D$_2$
43	89.111477			2p3d ^{3}P$^o_0$	92	115.091897			2p4f ^{3}G$_5$
44	89.192547	(+0.05)	89.149252	2p3p ^{1}S$_0$	93	115.106058			2p4f ^{3}D$_3$
45	89.643329	(+0.07)	89.577547	2p3d ^{1}F$^o_3$	94	115.121693			2p4f ^{3}F$_4$
46	89.732485	(+0.19)	89.559322	2p3d ^{1}P$^o_1$	95	115.139730	(+0.03)	115.102136	2p4d ^{1}F$^o_3$
47	109.064669			2s4s ^{3}S$_1$	96	115.148317			2p4f ^{3}D$_1$
48	109.261867			2s4s ^{1}S$_0$	97	115.182667			2p4d ^{1}P$^o_1$
49	109.632815			2s4p ^{3}P$^o_0$	98	115.185330			2p4f ^{1}D$_2$

Table 4. Labels chosen to identify levels dominated by the same SLJ term

Index	Label	Contribution of SLJ terms
40	2p3d $^1D^o_2$	$+0.551\,(^3P^o_2) - 0.572\,(^1D^o_2) + 0.531\,(^3D^o_2) + 0.266\,(^3F^o_2)$
42	2p3d $^3D^o_2$	$-0.309\,(^3P^o_2) - 0.652\,(^1D^o_2) - 0.568\,(^3D^o_2) + 0.391\,(^3F^o_2)$
72	2p4f $^3F_2$	$-0.534\,(^1D_2) - 0.447\,(^3D_2) - 0.753\,(^3F_2)$
90	2p4f $^3D_2$	$+0.422\,(^1D_2) + 0.591\,(^3D_2) - 0.684\,(^3F_2)$
89	2p4f $^3F_3$	$+0.698\,(^3D_3) - 0.440\,(^1F_3) + 0.559\,(^3F_3) + 0.062\,(^3G_3)$
95	2p4f $^3D_3$	$+0.713\,(^3D_3) + 0.471\,(^1F_3) - 0.518\,(^3F_3) - 0.012\,(^3G_3)$
77	2p4d $^3D^o_2$	$+0.604\,(^3P^o_2) - 0.350\,(^1D^o_2) + 0.522\,(^3D^o_2) + 0.204\,(^3F^o_2)$
83	2p4d $^3P^o_2$	$+0.713\,(^3P^o_2) + 0.255\,(^1D^o_2) - 0.643\,(^3D^o_2) + 0.088\,(^3F^o_2)$

coefficients taken from the Opacity Project. For the remaining orbitals P_{nl}, with $nl = 3s, 3p, 3d, 4s, 4p, 4d, 4f$, we used the minimum number of exponents dictated by nl and calculated their values, as given in Table 2, by minimising the sum of the energies of the $1s^2\,2snl\ ^1l$ and ^3l terms. We used the minimization routine VA04A by setting IDAVID = 0 and IVA04A = 1. (Note that the same procedure was adopted by Berrington et al. (1998) in spite of the unintentionally contradictory statements they make.) Furthermore, by setting MAXIT1 = 5 we limited the maximum number of iterations to 5. Additional work by one of us (JAT) has shown that some improvement can be obtained by using values of MAXIT1 larger than 5.

Our collision calculation makes use of theoretical target energies produced by the Breit-Pauli R-matrix code. They are given in Table 3 along with the observed energies for some of the levels taken from Corliss & Sugar (1982). Most of these observed values, with some small differences, can also be found on the Web page of the National Institute of Standards and Technology, http://physics.nist.gov. As can be seen there is very good agreement between theory and experiment, where we assume 1 Ry = 109737.32 cm^{-1}. Finally, we find that the data in Table 3 are in excellent agreement with results we have obtained using Hibbert's (1975) atomic structure code CIV3.

In order to delineate the multitude of resonance peaks we ran the Breit-Pauli code at 7704 values of the collision energy starting at 3.15210 Ry, relative to the ground state, and going up to 103.05816 Ry. Originally we meant to go as far as 115 Ry but finally abandoned this goal because of the excessive amount of computer time required. We therefore covered the interval between 103.05816 and 116 Ry by making a linear extrapolation backwards using the values of the collision strength at 116 and 127.5 Ry. In a few cases, especially for optically allowed transitions, a noticeable step up occurs in the collision strength when the energy increases beyond 103.05816 Ry, see Fig. 2.

2.1. Energy levels

The 98 energy levels given in Table 3, together with the way of indexing them, are from the Breit-Pauli branch of the R-matrix program. Using the CIV3 code we have been able to make the identifications given in the columns with the heading "Label". We use the customary procedure of letting the label be the configuration with the largest absolute mixing coefficient. However in four cases we abandoned this procedure in order to avoid the confusing situation of having the same label for more than one level. The last column in Table 4 shows SLJ terms which make a significant contribution to each of 4 pairs of levels where this problem arises. The mixing coefficients given in Table 4 are from CIV3 with ICSTAS = 1.

3. The effect of resonances

Resonances appear as spikes or dips on the graph of Ω. The spikes are sometimes isolated but more often they come as a dense forest of peaks. Resonances can have a big effect on Υ, especially when the transition is optically forbidden, and may cause Υ to be between a few per cent or several factors larger than the predictions of distorted wave approximations. For the purpose of comparison we list in Table 5 results for $\Upsilon(1-2)$ based on collision strengths from (a) the IRON Project, (b) the IRON Project (chopped) and (c) a distorted wave approximation. The collision strength in (b) was obtained by imposing an arbitrary maximum peak height of $1.25\,10^{-3}$ which effectively chops the tops off the resonance peaks. The distorted wave collision strength used in (c) is from Bhatia & Mason (1986).

As mentioned above, we use the Breit-Pauli R-matrix code for collision energies up to 103.05816 Ry after which we replace it by the simpler LS coupling code together with the algebraic code JAJOM (Saraph 1978). In this way we are able to extend the Breit-Pauli results to higher energies by running the LS code at 116, 127.5, 170, 250,

Table 5. Showing the effect on $\Upsilon(1-2)$ of chopping off the IRON Project resonances: (a), IRON; (b) IRON (chopped); (c) Bhatia & Mason (1986)

log$T$	(a)	(b)	(c)
6.3	1.97	1.22	1.34
6.5	2.17	1.18	1.27
6.7	2.18	1.12	1.17
6.9	2.01	1.02	1.04
7.1	1.71	0.90	0.89
7.3	1.36	0.75	0.74
7.5	1.04	0.61	0.60
7.7	0.77	0.47	0.46
7.9	0.55	0.36	0.34
8.1	0.39	0.26	0.24

Table 6. Showing how the high energy contribution to Υ increases with temperature for three types of transition. Intersytem (non electric dipole) transition: (a) $\Upsilon(1-2)$ with $E_{\max} = 346.8$ Ry; (b) $\Upsilon(1-2)$ with $E_{\max} = 10^5$ Ry. Intersystem (electric dipole) transition: (c) $\Upsilon(1-3)$ with $E_{\max} = 346.6$ Ry; (d) $\Upsilon(1-3)$ with $E_{\max} = 10^5$ Ry. Electric dipole transition: (e) $\Upsilon(2-7)$ with $E_{\max} = 340.7$ Ry; (f) $\Upsilon(2-7)$ with $E_{\max} = 10^5$ Ry. $E_{\max}$ is the value used for the upper limit in the integral that defines Υ and it should in theory be ∞. ($2.01^{-3} \equiv 2.01\ 10^{-3}$)

log$T$	(a)	(b)	(c)	(d)	(e)	(f)
6.9	2.01^{-3}	2.01^{-3}	1.33^{-2}	1.33^{-2}	1.61^{-1}	1.62^{-1}
7.1	1.70^{-3}	1.71^{-3}	1.33^{-2}	1.35^{-2}	1.74^{-1}	1.77^{-1}
7.3	1.35^{-3}	1.36^{-3}	1.28^{-2}	1.39^{-2}	1.78^{-1}	1.97^{-1}
7.5	1.01^{-3}	1.04^{-3}	1.14^{-2}	1.47^{-2}	1.65^{-1}	2.18^{-1}
7.7	7.25^{-4}	7.66^{-4}	9.27^{-3}	1.59^{-2}	1.38^{-1}	2.41^{-1}
7.9	5.00^{-4}	5.51^{-4}	7.00^{-3}	1.74^{-2}	1.06^{-1}	2.64^{-1}
8.1	3.34^{-4}	3.90^{-4}	4.98^{-3}	1.93^{-2}	7.62^{-2}	2.86^{-1}

350 Ry. This sparse mesh is ample for our purposes since no resonances are encountered over this energy range. It is difficult to go much beyond 350 Ry using the R-matrix codes. In order to obtain meaningful and reliable thermally averaged collision strengths at the high temperatures given in Table 9 it is necessary to know Ω at energies of one or two thousand rydbergs, i.e. well beyond 350 Ry. We are able to make reasonable extrapolations of our data by means of the computer program OmeUps (Burgess & Tully 1992).

4. Family portraits

We give pictures of the different types of collision strength encountered in the present investigation by plotting $\Omega(i-j)$ versus the final electron energy E_j in Ry.

Figures 1 and 2 show $\Omega(1-5)$. This is an optically allowed transition meaning that the collision

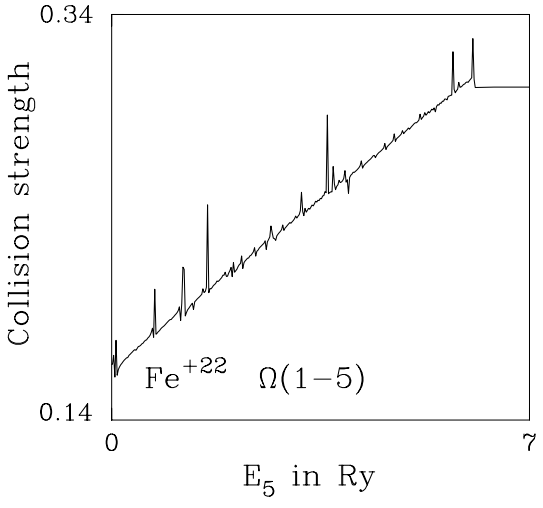

Fig. 1. An optically allowed transition

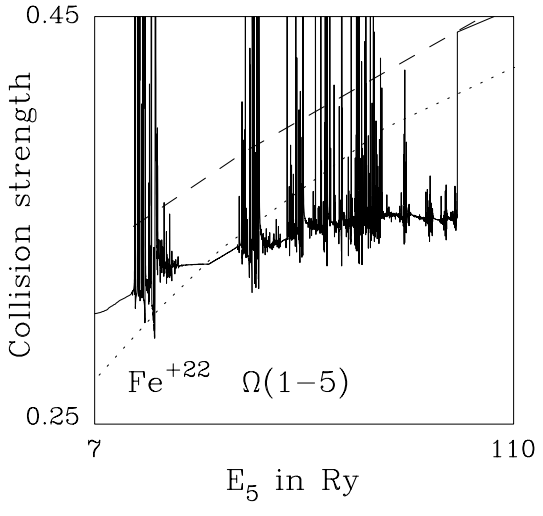

Fig. 2. Optically allowed: full, present; dotted, Bhatia & Mason (1986); dashed, Zhang & Sampson (1992)

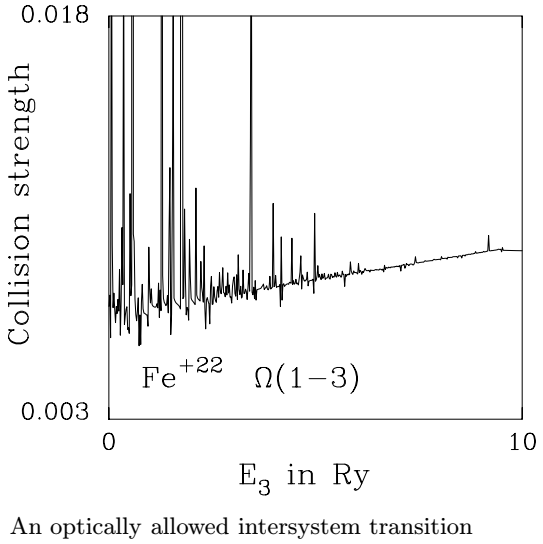

Fig. 3. An optically allowed intersystem transition

Table 7. Line and oscillator strengths, S_{ij} and f_{ij}, from CIV3; results obtained using the length gauge. ($1.310^{-3} \equiv 1.310\ 10^{-3}$)

i	S_{i2}	f_{i2}	S_{i3}	f_{i3}	S_{i4}	f_{i4}	S_{i5}	f_{i5}
1			1.310^{-3}	1.503^{-3}			6.770^{-2}	1.555^{-1}
6			3.135^{-2}	1.832^{-2}			1.311^{-3}	2.634^{-4}
7	3.080^{-2}	6.341^{-2}	2.270^{-2}	1.514^{-2}	3.811^{-2}	1.286^{-2}	4.792^{-4}	1.369^{-4}
8			3.941^{-2}	2.763^{-2}	8.615^{-2}	3.145^{-2}	2.715^{-2}	8.622^{-3}
9			1.947^{-3}	1.630^{-3}	2.895^{-2}	1.293^{-2}	1.209^{-1}	5.484^{-2}
10			7.648^{-5}	8.109^{-5}			5.141^{-2}	3.480^{-2}

Table 8. High energy Born limits. ($4.778^{-5} \equiv 4.778\ 10^{-5}$)

$i-j$	$\Omega(i-j)$
$1-6$	4.778^{-5}
$1-8$	4.904^{-4}
$1-9$	7.234^{-4}
$1-10$	3.429^{-4}
$2-4$	7.930^{-3}
$3-4$	1.784^{-2}
$3-5$	1.266^{-3}
$4-5$	4.331^{-4}
$6-8$	7.930^{-3}
$6-9$	3.950^{-5}
$6-10$	3.947^{-5}
$7-8$	1.338^{-2}
$7-9$	4.453^{-3}
$8-9$	2.338^{-2}
$8-10$	4.253^{-3}
$9-10$	2.477^{-2}

strength increases logarithmically with energy as $E_j \to \infty$. In order to delineate the low energy resonances in Fig. 1 we use a magnified energy scale there compared to the one in Fig. 2.

Figures 3 and 4 show $\Omega(1-3)$. This is an intersystem transition that behaves as though it were optically allowed owing to the breakdown of LS coupling. For this to happen the initial and final levels must have different parities and $\Delta J = 0, \pm 1$, subject to the condition that $J = 0 \not\to J' = 0$.

Figures 5 and 6 show $\Omega(1-9)$. This is a forbidden transition in which neither the parity nor the spin change. The collision strength for this type of transition tends to a finite limiting value as $E_j \to \infty$. We have used the methods discussed by Burgess et al. (1997) to calculate the Born limits for all such transitions between levels whose index does not exceed 10 (see Table 8).

Figures 7 to 12 show $\Omega(1-2)$. This is a forbidden intersystem transition for which the collision strength normally falls off like E_j^{-2} in the high energy limit.

It is well known that when a new threshold is crossed the collision strength for a transition involving two lower levels will in general decrease, or sometimes increase,

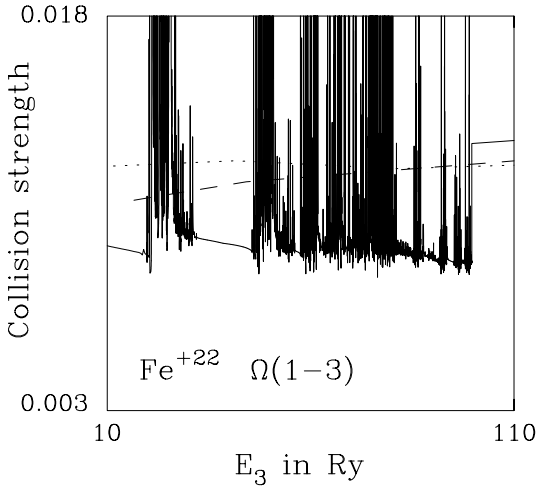

Fig. 4. Optically allowed intersystem: full, present; dotted, Bhatia & Mason (1986); dashed, Zhang & Sampson (1992)

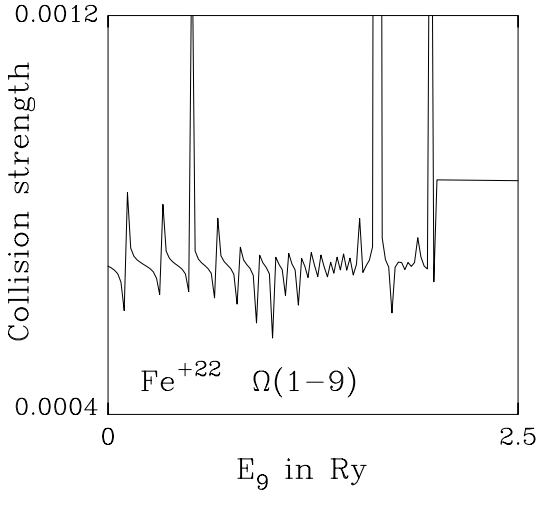

Fig. 5. An optically forbidden (electric quadrupole) transition

so that the collision strength in question behaves like a step function. This is explained by the influence of newly opened channels which cause a redistribution of the total electron flux to occur. The other thing to notice is the change in slope that occurs at the passage from the "low" to the "intermediate" energy region. This may be the result of having calculated fewer partial waves in the "low" energy region where we maintained $J \leq 5$. We did

Table 9. Fe^{+22} effective collision strengths $\Upsilon(i-j)$ for $6.3 \leq \log T \leq 8.1$. ($2.421^{-3} = 2.421\ 10^{-3}$)

$i-j$	6.3	6.5	6.7	6.9	7.1	7.3	7.5	7.7	7.9	8.1
$1-2$	2.421^{-3}	2.460^{-3}	2.371^{-3}	2.127^{-3}	1.782^{-3}	1.411^{-3}	1.069^{-3}	7.856^{-4}	5.637^{-4}	3.983^{-4}
$1-3$	1.179^{-2}	1.261^{-2}	1.314^{-2}	1.340^{-2}	1.353^{-2}	1.369^{-2}	1.395^{-2}	1.431^{-2}	1.478^{-2}	1.531^{-2}
$1-4$	1.139^{-2}	1.221^{-2}	1.215^{-2}	1.110^{-2}	9.374^{-3}	7.425^{-3}	5.609^{-3}	4.094^{-3}	2.916^{-3}	2.042^{-3}
$1-5$	2.865^{-1}	3.028^{-1}	3.210^{-1}	3.451^{-1}	3.771^{-1}	4.161^{-1}	4.600^{-1}	5.070^{-1}	5.549^{-1}	6.028^{-1}
$1-6$	2.230^{-4}	3.001^{-4}	3.770^{-4}	4.067^{-4}	3.804^{-4}	3.218^{-4}	2.564^{-4}	1.989^{-4}	1.539^{-4}	1.210^{-4}
$1-7$	3.085^{-4}	3.899^{-4}	4.467^{-4}	4.454^{-4}	3.900^{-4}	3.090^{-4}	2.282^{-4}	1.606^{-4}	1.095^{-4}	7.304^{-5}
$1-8$	7.294^{-4}	8.378^{-4}	9.140^{-4}	9.195^{-4}	8.605^{-4}	7.726^{-4}	6.871^{-4}	6.188^{-4}	5.701^{-4}	5.376^{-4}
$1-9$	1.252^{-3}	1.376^{-3}	1.440^{-3}	1.429^{-3}	1.365^{-3}	1.286^{-3}	1.216^{-3}	1.161^{-3}	1.116^{-3}	1.077^{-3}
$1-10$	8.002^{-4}	8.962^{-4}	9.713^{-4}	9.788^{-4}	9.192^{-4}	8.234^{-4}	7.205^{-4}	6.272^{-4}	5.501^{-4}	4.902^{-4}
$2-3$	2.619^{-2}	2.438^{-2}	2.222^{-2}	1.938^{-2}	1.603^{-2}	1.263^{-2}	9.569^{-3}	7.029^{-3}	5.051^{-3}	3.577^{-3}
$2-4$	1.962^{-2}	1.891^{-2}	1.796^{-2}	1.648^{-2}	1.464^{-2}	1.282^{-2}	1.129^{-2}	1.014^{-2}	9.342^{-3}	8.804^{-3}
$2-5$	6.584^{-3}	7.337^{-3}	7.388^{-3}	6.706^{-3}	5.568^{-3}	4.317^{-3}	3.185^{-3}	2.268^{-3}	1.577^{-3}	1.078^{-3}
$2-6$	1.312^{-3}	1.405^{-3}	1.427^{-3}	1.336^{-3}	1.151^{-3}	9.265^{-4}	7.088^{-4}	5.230^{-4}	3.765^{-4}	2.669^{-4}
$2-7$	1.330^{-1}	1.397^{-1}	1.479^{-1}	1.599^{-1}	1.764^{-1}	1.963^{-1}	2.184^{-1}	2.413^{-1}	2.641^{-1}	2.864^{-1}
$2-8$	4.103^{-3}	4.656^{-3}	4.778^{-3}	4.421^{-3}	3.742^{-3}	2.958^{-3}	2.225^{-3}	1.614^{-3}	1.142^{-3}	7.952^{-4}
$2-9$	1.952^{-3}	2.362^{-3}	2.442^{-3}	2.217^{-3}	1.818^{-3}	1.384^{-3}	1.001^{-3}	6.997^{-4}	4.781^{-4}	3.222^{-4}
$2-10$	4.235^{-4}	5.191^{-4}	5.492^{-4}	5.080^{-4}	4.203^{-4}	3.201^{-4}	2.301^{-4}	1.589^{-4}	1.069^{-4}	7.071^{-5}
$3-4$	8.504^{-2}	7.761^{-2}	7.070^{-2}	6.266^{-2}	5.366^{-2}	4.490^{-2}	3.736^{-2}	3.145^{-2}	2.709^{-2}	2.402^{-2}
$3-5$	2.285^{-2}	2.380^{-2}	2.329^{-2}	2.102^{-2}	1.758^{-2}	1.386^{-2}	1.051^{-2}	7.796^{-3}	5.750^{-3}	4.281^{-3}
$3-6$	1.318^{-1}	1.386^{-1}	1.474^{-1}	1.603^{-1}	1.779^{-1}	1.989^{-1}	2.219^{-1}	2.456^{-1}	2.689^{-1}	2.916^{-1}
$3-7$	1.022^{-1}	1.074^{-1}	1.135^{-1}	1.220^{-1}	1.335^{-1}	1.475^{-1}	1.629^{-1}	1.791^{-1}	1.954^{-1}	2.113^{-1}
$3-8$	1.789^{-1}	1.889^{-1}	1.997^{-1}	2.143^{-1}	2.338^{-1}	2.573^{-1}	2.834^{-1}	3.107^{-1}	3.381^{-1}	3.651^{-1}
$3-9$	1.624^{-2}	1.783^{-2}	1.849^{-2}	1.840^{-2}	1.799^{-2}	1.768^{-2}	1.768^{-2}	1.805^{-2}	1.872^{-2}	1.963^{-2}
$3-10$	1.794^{-3}	2.057^{-3}	2.106^{-3}	1.957^{-3}	1.695^{-3}	1.414^{-3}	1.174^{-3}	9.960^{-4}	8.776^{-4}	8.075^{-4}
$4-5$	4.712^{-2}	4.474^{-2}	4.132^{-2}	3.592^{-2}	2.921^{-2}	2.242^{-2}	1.646^{-2}	1.171^{-2}	8.151^{-3}	5.600^{-3}
$4-6$	1.466^{-3}	1.660^{-3}	1.742^{-3}	1.644^{-3}	1.401^{-3}	1.103^{-3}	8.205^{-4}	5.867^{-4}	4.084^{-4}	2.792^{-4}
$4-7$	1.576^{-1}	1.678^{-1}	1.800^{-1}	1.967^{-1}	2.187^{-1}	2.448^{-1}	2.731^{-1}	3.020^{-1}	3.306^{-1}	3.581^{-1}
$4-8$	3.712^{-1}	3.911^{-1}	4.154^{-1}	4.501^{-1}	4.972^{-1}	5.539^{-1}	6.161^{-1}	6.804^{-1}	7.442^{-1}	8.061^{-1}
$4-9$	1.506^{-1}	1.578^{-1}	1.646^{-1}	1.726^{-1}	1.826^{-1}	1.947^{-1}	2.081^{-1}	2.222^{-1}	2.364^{-1}	2.507^{-1}
$4-10$	3.521^{-3}	4.038^{-3}	4.170^{-3}	3.858^{-3}	3.243^{-3}	2.534^{-3}	1.878^{-3}	1.342^{-3}	9.347^{-4}	6.397^{-4}
$5-6$	6.533^{-3}	7.211^{-3}	7.917^{-3}	8.748^{-3}	9.775^{-3}	1.097^{-2}	1.224^{-2}	1.351^{-2}	1.470^{-2}	1.580^{-2}
$5-7$	9.081^{-3}	9.895^{-3}	1.026^{-2}	1.004^{-2}	9.410^{-3}	8.648^{-3}	7.970^{-3}	7.466^{-3}	7.144^{-3}	6.978^{-3}
$5-8$	1.175^{-1}	1.269^{-1}	1.384^{-1}	1.546^{-1}	1.762^{-1}	2.011^{-1}	2.272^{-1}	2.527^{-1}	2.768^{-1}	2.993^{-1}
$5-9$	5.074^{-1}	5.376^{-1}	5.772^{-1}	6.363^{-1}	7.169^{-1}	8.124^{-1}	9.149^{-1}	1.018	1.118	1.213
$5-10$	2.274^{-1}	2.341^{-1}	2.454^{-1}	2.641^{-1}	2.907^{-1}	3.232^{-1}	3.592^{-1}	3.968^{-1}	4.346^{-1}	4.717^{-1}
$6-7$	2.064^{-2}	2.256^{-2}	2.266^{-2}	2.079^{-2}	1.761^{-2}	1.401^{-2}	1.062^{-2}	7.775^{-3}	5.535^{-3}	3.863^{-3}
$6-8$	1.768^{-2}	1.885^{-2}	1.910^{-2}	1.826^{-2}	1.670^{-2}	1.494^{-2}	1.331^{-2}	1.196^{-2}	1.092^{-2}	1.013^{-2}
$6-9$	6.622^{-3}	7.835^{-3}	8.080^{-3}	7.368^{-3}	6.089^{-3}	4.679^{-3}	3.415^{-3}	2.405^{-3}	1.652^{-3}	1.117^{-3}
$6-10$	2.240^{-3}	2.714^{-3}	2.820^{-3}	2.569^{-3}	2.108^{-3}	1.600^{-3}	1.149^{-3}	7.957^{-4}	5.380^{-4}	3.596^{-4}
$7-8$	5.455^{-2}	5.915^{-2}	6.006^{-2}	5.653^{-2}	4.986^{-2}	4.212^{-2}	3.485^{-2}	2.881^{-2}	2.414^{-2}	2.073^{-2}
$7-9$	3.495^{-2}	3.859^{-2}	3.920^{-2}	3.641^{-2}	3.131^{-2}	2.548^{-2}	2.007^{-2}	1.561^{-2}	1.219^{-2}	9.711^{-3}
$7-10$	8.358^{-3}	9.568^{-3}	9.572^{-3}	8.527^{-3}	6.928^{-3}	5.257^{-3}	3.798^{-3}	2.650^{-3}	1.805^{-3}	1.208^{-3}
$8-9$	7.725^{-2}	8.478^{-2}	8.637^{-2}	8.139^{-2}	7.201^{-2}	6.127^{-2}	5.137^{-2}	4.330^{-2}	3.720^{-2}	3.281^{-2}
$8-10$	1.193^{-2}	1.318^{-2}	1.331^{-2}	1.238^{-2}	1.085^{-2}	9.211^{-3}	7.774^{-3}	6.651^{-3}	5.835^{-3}	5.270^{-3}
$9-10$	2.521^{-2}	2.718^{-2}	2.791^{-2}	2.748^{-2}	2.643^{-2}	2.534^{-2}	2.455^{-2}	2.411^{-2}	2.396^{-2}	2.398^{-2}

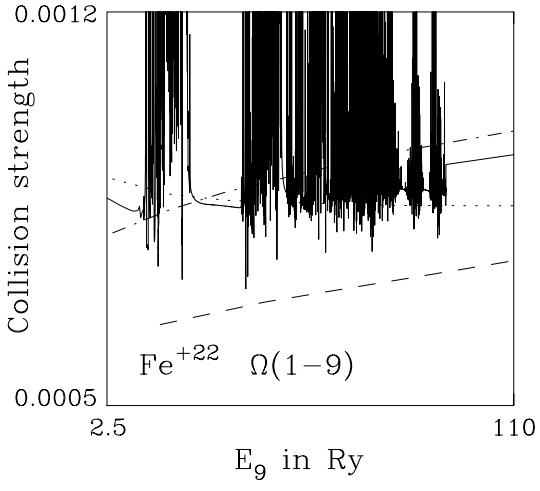

Fig. 6. Optically forbidden (electric quadrupole): full, present; dotted, Bhatia & Mason (1986); dashed, Zhang & Sampson (1992); dot-dashed, Chen & Ong (1998)

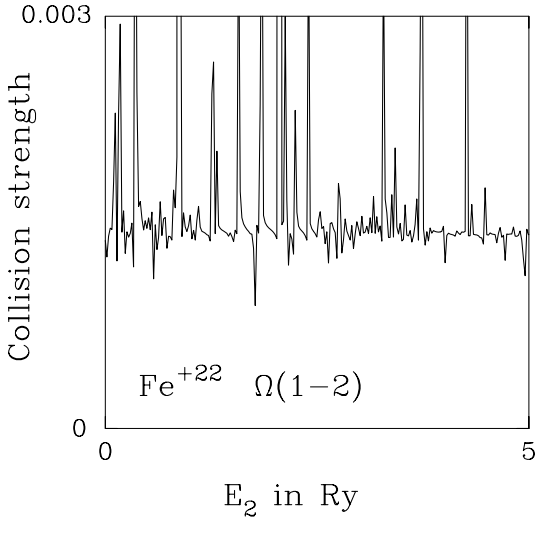

Fig. 7. An optically forbidden intersystem transition

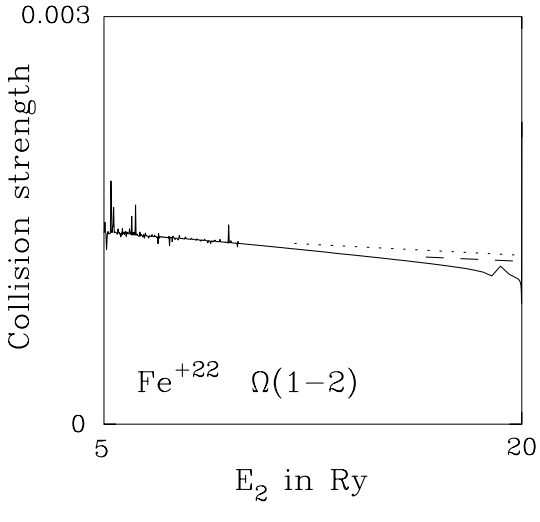

Fig. 8. Optically forbidden intersystem: full, present; dotted, Bhatia & Mason (1986); dashed, Zhang & Sampson (1992)

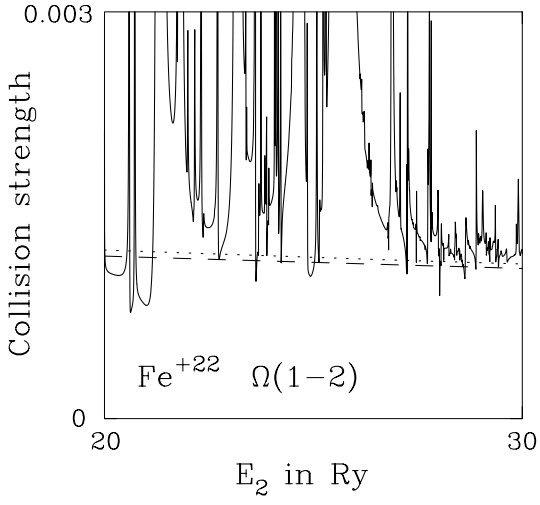

Fig. 9. Optically forbidden intersystem: full, present; dotted, Bhatia & Mason (1986); dashed, Zhang & Sampson (1992)

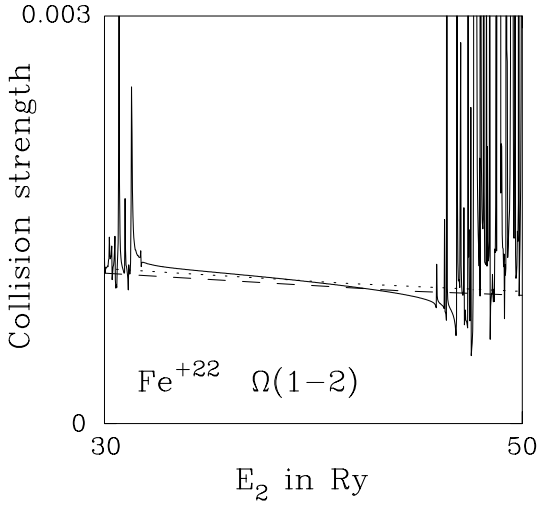

Fig. 10. Optically forbidden intersystem: full, present; dotted, Bhatia & Mason (1986); dashed, Zhang & Sampson (1992)

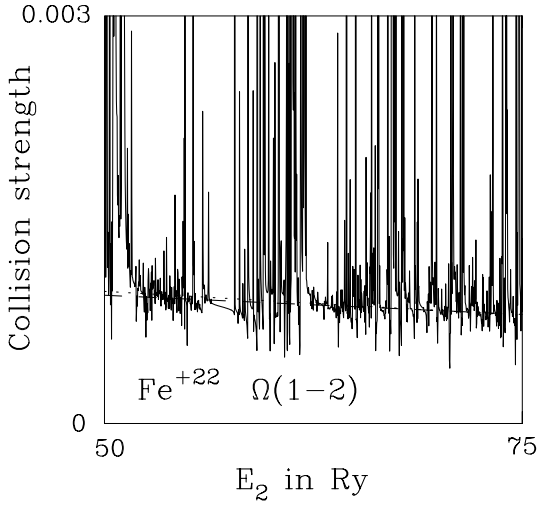

Fig. 11. Optically forbidden intersystem: full, present; dotted, Bhatia & Mason (1986); dashed, Zhang & Sampson (1992)

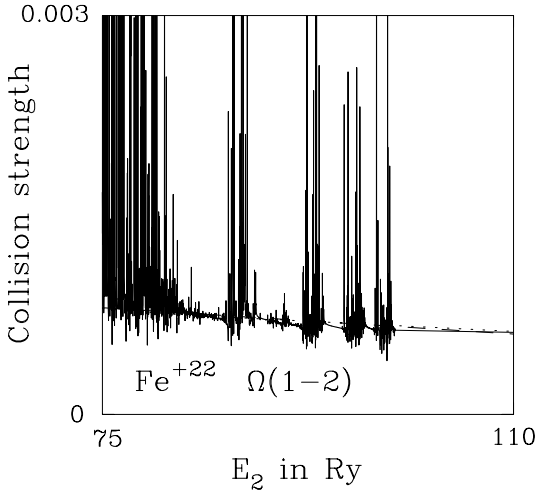

Fig. 12. Optically forbidden intersystem: full, present; dotted, Bhatia & Mason (1986); dashed, Zhang & Sampson (1992)

however carry out a top-up procedure in order to account for the higher partial waves.

5. Quality of results

The IRON Project's aim is to produce high quality collision data for a wide range of electron induced transitions in positive ions. We outline the steps taken in the present work which justify our belief that the results given here are the most reliable ones at present available to those in search of rate coefficients for Fe^{+22}. We first of all went to some trouble in order to obtain a good target model. Our confidence in it stems from the good agreement it affords between the theoretical energy levels and observational data (see Table 3). Furthermore, on comparing the length gauge oscillator strengths listed in Table 7 with those we have obtained using the velocity gauge, we find that in all cases except two, their ratio lies between 1.03 and 1.77. Only for the transitions $1-3$ and $7-5$ does the ratio exceed 2, but not by a great deal: $f_{\rm V}(1-3)/f_{\rm L}(1-3) = 2.56$ and $f_{\rm V}(7-5)/f_{\rm L}(7-5) = 3.53$. Although close agreement between the length and velocity f-values is not an absolute guarantee that the oscillator strengths are the correct ones, it is obviously desirable that the ratio $f_{\rm L}/f_{\rm V}$ should not deviate from unity a lot. As regards the collision calculation, we have made use of the R-matrix method in both the Breit-Pauli and LS-coupling modes. The Belfast-London-Meudon suite of programs has been developed over many years by a great number of scientists. The present programs, which are based on approximations that take into account much of the collision physics responsible for resonance scattering and relativistic effects, are widely considered as the most elaborate and satisfactory ones in existence for this type of calculation. With increasing energy, more and more partial waves need to be calculated. In order to ensure convergence of the expansion we let the partial wave quantum number J extend up to $J = 35.5$. This applies only to collision energies greater than 12.9843 Ry with respect to the ground state; for energies between 3.1521 and 12.9843 Ry we limited J to 5 and then did a top-up by estimating the contributions from higher partial waves. As mentioned earlier, we used OmeUps in order to estimate collision strengths at much higher energies than could be reached by the R-matrix codes. This procedure gives added reliability to the high temperature results in Table 9.

6. Comparison with the work of others

Of the papers listed in Table 1 those by Bhatia & Mason (1981, 1986); Zhang & Sampson (1992); Chen & Ong (1998) deal with the transitions in Table 9. These workers all used distorted wave approximations which do not take account of resonance effects. We give some graphical comparisons which show that there is fairly good agreement between our background collision strengths and the distorted wave results. Only for the forbidden transitions $1-9$ (electric quadrupole) and $1-10$ (electric monopole), which involve 2 electron jumps, are the differences more noticeable. Figure 6 shows that Zhang & Sampson's (1992) relativistic distorted wave collision strength $\Omega(1-9)$ is significantly lower than ours. We can see no obvious explanation for this. Chen & Ong's (1998) results, which came to our attention as the present investigation was drawing to a close, are in better agreement with our data for this transition (see Fig. 6).

7. Effective collision strengths

Thermal averaging of the collision strengths is done using the linear interpolation method described by Burgess & Tully (1992). The resulting effective collision strengths Υ are given in Table 9 for the temperature range $6.3 \leq \log T \leq 8.1$ which is centred on the temperature where Fe^{+22} is abundant under conditions of coronal ionization equilibrium (see Arnaud & Rothenflug 1985). For temperatures below five million degrees the abundance of Fe^{+22} will be negligeable. Astrophysical situations may exist where Fe^{+22} is abundant at temperatures lower than this; in these cases one would need to extend the temperature range below $10^{6.3}$ K. Anyone interested in obtaining copies of our energy dependent collision strengths for the transitions dealt with here should send a request to tully@obs-nice.fr. We plan to install them eventually in the TIPbase databank that is being set up at the CDS (Centre de données astronomiques de Strasbourg). Files containing the thermally averaged collision strengths are available now from the A&A databank at CDS.

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CHRX CT920013 and by the NSERC (Natural Sciences and Engineering Research Council of Canada). The figures were drawn using the graphics package TVB developed by Georges Gonczi at the Observatoire de la Côte d'Azur. An English version of this is now available at http://www.obs-nice.fr/tvb/tvb.html. We wish to thank Alan Burgess of Cambridge University for providing us with the latest version of his interactive program OmeUps. We are grateful to Guo-xin Chen, D.G. Hummer and Hannelore E. Saraph for reading and commenting on an earlier version of the paper. Some convenient merging of tables and the inclusion of a discussion on the quality of results are the important modifications which we incorporated after studying the helpful report supplied by the referee, Professor Harry Nussbaumer of Zurich.

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