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Forbidden transitions in Li-like ions: Compact effective collision strengths for 2s − *n*s, *n*d where *n* = 3, 4, 5⋆

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Abstract. Using an extension of the method for compacting atomic data set out by Burgess & Tully (1992), we make concise fits to a selection of the set of collision strengths Ω given by Zhang et al. (1990) for Li-like ions from O^{+5} to U^{+89}. We carry out thermal averaging and fit the resulting effective collision strengths Υ. A compact 5×5 or 4×4 table of cardinal values for each transition allows one to reproduce the T and Z dependent Υ to better than 1 per cent. The present study is for the forbidden transitions $2s \rightarrow 3s, 4s, 5s$ and $2s \rightarrow 3d, 4d, 5d$.

Key words: Li-like ions — electron excitation — compact atomic data

1. Introduction

Zhang et al. (1990) (hereafter referred to as ZSF) give extensive tables of collision strengths Ω for transitions in Li-like ions with atomic numbers Z_0 ranging from 8 to 92. They obtained their data for $Z_0 = 8, 14, 22, 30, 42, 56, 74, 92$ by making detailed calculations with a relativistic distorted wave approximation. They then used an eight parameter analytic fit in Z_0 to complete their tabulation for the remaining ions in the sequence between O^{+5} and U^{+89}.

In order to simplify the storage of these data we examine the possibility of fitting them, both as functions of energy and of ion charge number Z. We then carry out thermal averaging and fit the resulting effective collision strengths Υ as functions of temperature T and Z. The basis for carrying out each of these processes was set out in detail by Burgess & Tully (1992) (hereafter referred to as B&T) and we use their notation. B&T also described the interactive program OMEUPS and used it to obtain such isoelectronic fits for the 2s−2p transition in all the Li-like ions of charge 1 to 23, and for the 2^1S-2^1P transition in all the Be-like ions of charge 2 to 10.

Our present purpose is to extend the treatment in three ways:

First, we fit the ZSF data for the non-optically allowed transitions 2s−3s, 2s−4s, 2s−5s, 2s−3d, 2s−4d and 2s−5d. To help achieve this, we calculate the Born high energy limit points following the procedure described by Burgess et al. (1997).

Secondly, we incorporate some of the relativistic corrections required for larger values of Z than those treated in B&T.

Finally, we illustrate the use of types of fit other than the 5-point cubic spline adopted as standard in the previous work and in current plasma modelling computer programs.

We use a recent version of the interactive program, renamed OmeUpZ, designed to handle these extensions. Details will be given elsewhere (Burgess 2001).

2. Compacting atomic collision data

We use notation as established in B&T. All the transitions treated in the present paper are of type 2. In this section we specify the changes required for these transitions as a consequence of including relativistic effects. We use the same equation numbers as in B&T, with * added to the number of the modified equation. Derivations, and details for other types of transition, will be given elsewhere.

In order to distinguish the adjustable parameter C occurring in the different fits we denote it by C_E, C_T, C_Z

⋆ Appendix available on the on-line version of A&AS.

Table 1. High energy Born collision strengths $\Omega(nlj)$ for transitions $2s_{1/2} \rightarrow nlj$

Z_0	$\Omega(3s_{1/2})$	$\Omega(4s_{1/2})$	$\Omega(5s_{1/2})$
8	2.355−1	4.583−2	1.804−2
10	1.396−1	2.707−2	1.077−2
12	9.222−2	1.790−2	7.078−3
14	6.549−2	1.269−2	4.992−3
16	4.894−2	9.472−3	3.719−3
18	3.791−2	7.343−3	2.868−3
20	3.025−2	5.858−3	2.285−3
26	1.737−2	3.360−3	1.303−3

Z_0	$\Omega(3d_{3/2})$	$\Omega(4d_{3/2})$	$\Omega(5d_{3/2})$
8	2.625−1	4.363−2	1.560−2
10	1.604−1	2.511−2	8.814−3
12	1.081−1	1.628−2	5.646−3
14	7.772−2	1.139−2	3.914−3
16	5.857−2	8.403−3	2.870−3
18	4.570−2	6.457−3	2.194−3
20	3.665−2	5.114−3	1.729−3
26	2.125−2	2.888−3	9.687−4

Z_0	$\Omega(3d_{5/2})$	$\Omega(4d_{5/2})$	$\Omega(5d_{5/2})$
8	3.938−1	6.544−2	2.340−2
10	2.407−1	3.767−2	1.322−2
12	1.162−1	2.442−2	8.469−3
14	1.166−1	1.708−2	5.871−3
16	8.785−2	1.260−2	4.304−3
18	6.854−2	9.685−3	3.292−3
20	5.498−2	7.671−3	2.594−3
26	3.188−2	4.331−3	1.453−3

according to whether the fit is over the range of energy E, temperature T or ion charge Z.

2.1. Fitting the collision strengths Ω

Equation (9) of B&T is unchanged except that C is denoted by C_E, but (10) becomes

$$y(x) = \Omega/(1 + \epsilon\, E_i)(1 + \epsilon\, E_j)\,, \qquad (10^*)$$

where $\epsilon = I_\infty/mc^2 = \alpha^2/2 = 2.6626\ 10^{-5}$, α being the fine structure constant.

2.2. Limiting values of $\Omega(E_j)$ *when* $E_j \rightarrow \infty$

We use the interactive FORTRAN program BORN written by Burgess (1998) to compute the non relativistic high energy limit points presented in Table 1. We take radial orbitals $P_{1s}\,, P_{2s}$ from Clementi & Roetti (1974) and calculate $P_{3s}\,, P_{3d}\,, P_{4s}\,, P_{4d}\,, P_{5s}\,, P_{5d}$ using Hibbert's (1975) program CIV3. The parameterised form of $P_{nl}(r)$ is

$$P_{nl}(r) = \sum_{p=1}^{k} c_{nlp} \Big[\frac{(2\zeta_{nlp})^{2q_{nlp}+1}}{(2q_{nlp})!}\Big]^{1/2} r^{q_{nlp}} \exp(-\zeta_{nlp} r). \qquad (1)$$

Our choice for the integers $(k,\, q_{nlp})$ in Eq. (1) is $(n,\, p)$ for $l = 0$ and $(n-2,\, p+2)$ for $l = 2$. Results for four ions in the sequence, namely $Z_0 = 8, 16, 26, 36$, are given in Table 2. We obtained the values for ζ_{nlp} and c_{nlp} by using CIV3 to minimise the $1s^2nl$ term energy. Since in general many local minima exist it can be quite an arduous task locating the one that seems to be the lowest. A similar investigation has in the past been carried out for some of the orbitals included here (see Tully et al. 1990 and Berrington & Tully 1997). A comparison of the present and past data shows that they are not always the same. Although we have not compared the orbitals it is our belief that they do not differ significantly. The numerical differences alluded to here reflect the fact that in the present work we have given greater attention to locating the term minima than in the past. In all cases we use the minimization code MODDAV by setting the CIV3 parameter IDAVID = 0. We assume each orbital P_{nl} to have the minimum number of exponents dictated by nl and therefore the coefficients c_{nlp} are determined by the conditions of orthonormality, but for convenience we include their numerical values in Table 2.

2.3. Values of Ω *when* Z *is large*

It is extremely useful, when fitting collision data along an entire isoelectronic sequence, to have an indication of the behaviour of the collision strengths when Z becomes large. The true limiting values do not exist since the relativistic wave functions for the ion collapse when Z is too large (e.g. for s-states, when $Z \rightarrow 137$). Nevertheless, the non-relativistic values, scaled by a factor $(Z+1)^2$, do exist in the limit and are useful in this context.

D. H. Sampson and his co-workers have, over the past two decades, produced an enormous amount of reliable collision data in just this limit, and we make use of their Coulomb Born Oppenheimer results for the hydrogenic transitions $2s \rightarrow 3s, 4s, 5s$ and $2s \rightarrow 3d, 4d, 5d$. These are available in Golden et al. (1981) and Clark et al. (1982). However it should be noted that the values they tabulate for the collision strength need to be multiplied by a factor 2 in order to be consistent with the definitions of Ω and statistical weight given in equations (2) and (3) in Golden et al. (1981)

We have made only approximate allowance for the relativistic corrections to these limiting values. However, the uncertainties arising from this affect only values beyond the range of the ZSF tabulation (i.e. for $Z > 89$ or

Table 2. Radial orbital parameters $\zeta_{nlp}(Z_0)$ and $c_{nlp}(Z_0)$

nlp	$\zeta_{nlp}(8)$	$c_{nlp}(8)$	$\zeta_{nlp}(16)$	$c_{nlp}(16)$	$\zeta_{nlp}(26)$	$c_{nlp}(26)$	$\zeta_{nlp}(36)$	$c_{nlp}(36)$
301	5.4321	0.256172	9.9500	0.341894	15.2480	0.394217	20.3310	0.427254
302	1.6773	−3.238590	3.8972	−3.437766	6.7498	−3.513345	9.6590	−3.540427
303	1.9696	3.843596	4.5091	3.959569	7.7225	3.978447	10.9620	3.967328
321	2.0026	1.0	4.6709	1.0	8.0050	1.0	11.3387	1.0
401	5.1737	0.175261	6.7500	0.394362	5.7200	1.110070	5.2300	2.118666
402	1.3916	−3.594468	2.8294	−7.799553	4.9287	−9.663204	6.8298	−10.899624
403	1.3812	11.231169	6.0044	2.308520	9.5746	3.017685	12.9950	3.305530
404	1.5007	−8.564409	4.7669	5.612881	7.9133	6.074342	10.9956	5.853544
421	1.6232	1.619651	3.7563	1.664016	6.3752	1.720715	8.9680	1.762298
422	1.4881	−2.110174	3.4771	−2.157408	5.9706	−2.217847	8.4672	−2.262205
501	5.5738	0.113692	9.9500	0.158703	13.3459	0.222186	17.3693	0.249660
502	1.9058	−1.051693	4.1499	−1.378359	5.4367	−3.261515	5.1748	−9.206321
503	1.0217	11.740236	2.3899	13.663345	4.9773	12.275513	7.1928	15.609117
504	1.3242	−6.908209	3.5020	−5.265064	4.4549	−26.207598	6.8440	−15.466590
505	1.5917	−4.277071	3.4121	−7.837612	4.7145	18.034602	6.7466	10.256049
521	1.2966	2.700849	2.9715	2.896201	5.1075	2.864325	7.4530	2.580420
522	1.2577	−6.342879	2.9346	−6.565149	4.9810	−6.810249	6.9767	−6.778766
523	1.1915	4.309127	2.7800	4.323400	4.7782	4.617560	6.7798	4.904312

$E_j > 10^4$ Ryd, $T > 10^9$). Further work on this will be given elsewhere.

2.4. Calculation of the effective collision strength $\Upsilon(T)$

The definition of Υ in terms of Ω, Eq. (21) of B&T, is unchanged, (as is the detailed balance Eq. (22)), so that the OmeUpZ program can be used to calculate Υ from the fitted Ω as described in Sects. 6.3 and 7.2 of B&T. However, Eq. (20) for the rate coefficient is altered by replacing the factor Υ, on the right hand side, by Υ/Φ, where

$$\Phi = (2mc^2/\pi kT)^{1/2} \exp(mc^2/kT)\, K_2(mc^2/kT)\,, \quad (20^*)$$

K_2 being a modified Bessel function (Abramowitz & Stegun 1965). This result is for a low density, high temperature plasma corresponding to the nondegenerate Maxwell-Juttner case discussed by Chandrasekhar (1957, pp. 394-8).

Except for very large values of T, we have $\Phi \approx 1 + (15/8)(kT/mc^2) = 1 + 3.1619\ 10^{-10}\, T$.

2.5. Fitting Υ *as a function of* T

Equation (27) of B&T is unchanged except that C is denoted by C_T, but (28) becomes

$$y(x) = \Upsilon/(1 + \epsilon E_{ij} + \mu T(2 + \epsilon E_{ij} + 2\mu T))\,, \quad (28^*)$$

where $\mu = k/mc^2 = 1.6864\ 10^{-10}$.

2.6. Fitting the nodal values of $\Omega_{\rm r}$ *and* $\Upsilon_{\rm r}$ *as functions of* $Z_{\rm r}$

As described in Sects. 7.5 and 8.2 of B&T, for a given transition, the standard 5-point cubic spline fitting procedure produces 5 nodal values of $\Omega_{\rm r}$ or $\Upsilon_{\rm r}$ for each Z, which may themselves then be fitted as a function of a reduced Z variable, so as to produce the doubly reduced quantities $\Omega_{\rm rr}$ or $\Upsilon_{\rm rr}$. As in B&T, use of a common value of C_E or C_T for all the values of Z is obviously most convenient and leads to no significant loss of accuracy.

Equations (58) and (59) of B&T are unchanged except that C is denoted by C_Z.

This gives a 5×5 matrix S_{mn} of nodal values of $\Omega_{\rm rr}(E_{\rm r}, Z_{\rm r})$ or $\Upsilon_{\rm rr}(T_{\rm r}, Z_{\rm r})$ from which Ω or Υ may be obtained for all energies or temperatures and all charges.

Values of the S_{mn} matrix elements, together with the values of C_E or C_T and C_Z are given in Tables 3 and 4.

The fitted values of Ω given by Table 3 were compared with all the original tabulated values given by ZSF for these transitions (i.e. for all 6 energies × all 85 charges × 9 transitions); the rms error was 0.3% and the maximum error was 0.9%. The rms error involved in fitting Υ, to obtain Table 4, was also found to be about 0.3%.

As noted in Sect. 2.3, there is some uncertainty in the values of Ω beyond the range of the ZSF tabulation. We estimate that the resulting uncertainty in values obtained from Table 3 and 4 exceeds 1% only if $Z_0 > 92$ or $E_j > 10^4$ Ryd, $T > 10^9$).

Table 3. Program data to obtain Ω for all charges $8 \le Z_0 \le 92$

Omega 2s−3s (Type,CE,CZ,Smn)
12 3.8 30

5.148	5.847	6.229	6.434	6.764
7.535	8.387	8.914	9.201	9.312
8.307	9.182	9.725	10.004	9.945
8.959	9.616	9.890	9.712	8.757
10.287	9.453	7.810	5.319	1.376

Omega 2s−4s (Type,CE,CZ,Smn)
12 1.8 25

1.0300	1.1009	1.1714	1.2316	1.2828
1.4780	1.5651	1.6642	1.7474	1.7701
1.6410	1.7307	1.8330	1.9183	1.9318
1.7886	1.8543	1.9294	1.9687	1.9240
2.2511	2.1340	1.9707	1.6627	1.4938

Omega 2s−5s (Type,CE,CZ,Smn)
12 1.5 20

0.3814	0.3973	0.4177	0.4408	0.4417
0.5514	0.5744	0.6082	0.6434	0.6809
0.6229	0.6467	0.6825	0.7182	0.7404
0.6739	0.6926	0.7228	0.7478	0.7412
0.8401	0.8046	0.7705	0.6927	0.5632

Omega 2s−3d 3/2 (Type,CE,CZ,Smn)
12 2.2 32

2.251	2.733	3.603	4.639	6.403
5.483	6.353	7.749	9.454	11.077
6.139	7.053	8.513	10.318	11.960
3.917	4.388	5.249	6.345	7.972
−8.680	−10.512	−12.811	−15.348	−13.725

Omega 2s−4d 3/2 (Type,CE,CZ,Smn)
12 1.8 31

0.7174	0.7802	0.9510	1.1806	1.4309
1.0990	1.0992	1.2316	1.4487	1.6322
1.1637	1.1416	1.2567	1.4616	1.6321
0.9449	0.9147	1.0070	1.1757	1.3859
−0.4518	−0.4914	−0.5076	−0.5302	0.1589

Omega 2s−5d 3/2 (Type,CE,CZ,Smn)
12 1.6 31

0.3098	0.3208	0.3750	0.4587	0.5522
0.4322	0.4025	0.4291	0.4968	0.5631
0.4524	0.4105	0.4282	0.4896	0.5486
0.3867	0.3491	0.3660	0.4211	0.4905
−0.0428	−0.0376	−0.0142	0.0108	0.2313

Table 3. continued

Omega 2s−3d 5/2 (Type,CE,CZ,Smn)
12 2.2 32

3.378	4.102	5.408	6.959	9.604
8.219	9.524	11.621	14.180	16.616
9.162	10.545	12.750	15.471	17.941
5.592	6.366	7.737	9.443	11.958
−14.063	−16.595	−19.814	−23.464	−20.595

Omega 2s−4d 5/2 (Type,CE,CZ,Smn)
12 1.8 32

1.0866	1.1807	1.4366	1.7803	2.1596
1.6553	1.6550	1.8537	2.1797	2.4526
1.7508	1.7239	1.9040	2.2182	2.4667
1.4100	1.4096	1.5981	1.8945	2.2393
−0.8245	−0.6956	−0.5277	−0.3766	1.0619

Omega 2s−5d 5/2 (Type,CE,CZ,Smn)
12 1.6 32

0.4682	0.4842	0.5651	0.6903	0.8312
0.6506	0.6056	0.6453	0.7468	0.8450
0.6817	0.6214	0.6511	0.7457	0.8287
0.5885	0.5531	0.6018	0.7019	0.7888
−0.0675	0.0404	0.1785	0.2852	0.6170

3. Generating $\Omega(E, Z)$ or $\Upsilon(T, Z)$ from the S_{mn} matrices

Since we have type 2 transitions (instead of type 1) and include relativistic corrections, Eqs. (62) to (65) of B&T become

$$\Upsilon = (Z+1)^{-2}\,(1 + \epsilon E_{ij} + \mu T(2 + \epsilon E_{ij} + 2\mu T)) \text{ spline}$$
$$(P_1, P_2, P_3, P_4, P_5, T_\mathrm{r})\,, \qquad (62^*)$$

where

$$P_n = \text{spline}(S_{1n}, S_{2n}, S_{3n}, S_{4n}, S_{5n}, Z_\mathrm{r}) \;\; (1 \le n \le 5)\,, \qquad (63^*)$$

$$T_\mathrm{r} = \frac{kT/E_{ij}}{kT/E_{ij} + C_T}\,, \qquad (64^*)$$

$$Z_\mathrm{r} = \frac{Z}{Z + C_Z}\,. \qquad (65^*)$$

Correspondingly, for Ω, we have

$$\Omega = (Z+1)^{-2}\,(1 + \epsilon\, E_i)(1 + \epsilon\, E_j) \text{ spline}$$
$$(P_1, P_2, P_3, P_4, P_5, E_\mathrm{r})\,, \qquad (62^{*\prime})$$

where

$$E_\mathrm{r} = \frac{E_j/E_{ij}}{E_j/E_{ij} + C_E}. \qquad (64^{*\prime})$$

4. Other types of fit

As well as the standard 5-point cubic spline fit, the new program OmeUpZ allows the options of varying the number of nodal points, and of using quadratic splines (in which case the knots are at mid-nodal points) or Tchebyshev polynomials.

In general, global fits with Tchebyshev polynomials are not suitable for this type of data, especially if resonance contributions are appreciable. For such data, piecewise fits with low-degree splines are more appropriate, and in extreme cases it may be best to resort to linear splines (see B&T Sect. 6.2).

Table 4. Program data to obtain Υ for all charges $8 \leq Z_0 \leq 92$

Upsilon 2s−3s (Type,CT,CZ,Smn)

12	3.0	28			
5.085		5.556	5.866	6.091	6.635
7.473		8.069	8.478	8.839	9.242
8.279		8.901	9.319	9.702	9.948
8.913		9.417	9.678	9.691	8.942
10.319		9.814	8.940	6.295	2.028

Upsilon 2s−4s (Type,CT,CZ,Smn)

12	3.0	25			
1.0315		1.1132	1.1659	1.2118	1.2830
1.4785		1.5850	1.6595	1.7203	1.7708
1.6413		1.7518	1.8285	1.8910	1.9332
1.7882		1.8711	1.9222	1.9448	1.9242
2.2519		2.0937	1.9158	1.6471	1.4834

Upsilon 2s−5s (Type,CT,CZ,Smn)

12	3.6	25			
0.3975		0.4269	0.4464	0.4642	0.4938
0.5697		0.6097	0.6391	0.6642	0.6984
0.6313		0.6733	0.7022	0.7252	0.7462
0.6894		0.7171	0.7334	0.7367	0.7286
0.8802		0.7880	0.6988	0.5733	0.4860

Upsilon 2s−3d 3/2 (Type,CT,CZ,Smn)

12	7.6	32			
2.249		3.431	4.292	5.108	6.384
5.487		7.485	8.774	9.835	11.072
6.138		8.266	9.652	10.839	11.980
3.904		5.257	6.421	7.414	7.974
−8.704		−11.710	−12.109	−13.151	−13.887

Upsilon 2s−4d 3/2 (Type,CT,CZ,Smn)

12	2.6	32			
0.7235		0.8222	0.9727	1.1325	1.4300
1.0980		1.1375	1.2607	1.3964	1.6298
1.1570		1.1766	1.2879	1.4216	1.6306
0.9194		0.9315	1.0380	1.1985	1.3742
−0.5466		−0.5620	−0.4709	−0.2169	0.0781

Upsilon 2s−5d 3/2 (Type,CT,CZ,Smn)

12	2.4	31			
0.3086		0.3343	0.3859	0.4419	0.5495
0.4293		0.4154	0.4463	0.4845	0.5615
0.4488		0.4232	0.4474	0.4827	0.5486
0.3828		0.3616	0.3886	0.4368	0.4921
−0.0444		−0.0291	0.0256	0.1327	0.2283

Table 4. continued

Upsilon 2s−3d 5/2 (Type,CT,CZ,Smn)

12	7.6	32			
3.374		5.149	6.441	7.663	9.576
8.224		11.224	13.159	14.751	16.608
9.161		12.376	14.465	16.255	17.970
5.574		7.741	9.560	11.101	11.960
−14.090		−18.131	−18.424	−19.821	−20.844

Upsilon 2s−4d 5/2 (Type,CT,CZ,Smn)

12	2.6	32			
1.0827		1.2314	1.4577	1.6987	2.1494
1.6478		1.7080	1.8934	2.0974	2.4468
1.7412		1.7784	1.9514	2.1566	2.4676
1.3990		1.4707	1.6772	1.9598	2.2471
−0.8267		−0.6233	−0.2672	0.3471	1.0465

Upsilon 2s−5d 5/2 (Type,CT,CZ,Smn)

12	2.4	31			
0.4621		0.5011	0.5788	0.6631	0.8259
0.6444		0.6239	0.6704	0.7279	0.8429
0.6762		0.6409	0.6794	0.7336	0.8294
0.5907		0.5820	0.6408	0.7214	0.7933
−0.0229		0.1104	0.2822	0.4817	0.6198

However, Tchebyshev fits are very useful for other types of data which might be expected to have a convergent power series expansion over the whole range. The ZSF data is very smooth so, as an example of using the program in this mode, we also give results obtained from 4-point Tchebyshev fits to $\Upsilon_{\rm rr}$. For these, the interpolation function poly4(P_1, P_2, P_3, P_4, X) is used in place of spline$(P_1, P_2, P_3, P_4, P_5, X)$, both these functions being defined in terms of FORTRAN listings in the Appendix. This gives an even more compact representation of the data, and still to about 1% accuracy provided the range of nuclear charge is limited to $8 \leq Z_0 \leq 30$, which covers most cases of astrophysical interest. The results are given in Table 5.

As an example to compare with we have run the interactive program described in the Appendix for the case of the 2s $\rightarrow$ 3s transition in Fe^{+23}. In Table 6 we give the corresponding Υ as a function of log$T$. The column headed ZSF(5) has results obtained by using as input to the interactive program the spline data in Table 4. The numbers in Col. ZSF(4) are obtained in a similar way but using the Tchebyshev data given in Table 5. In the final column of Table 6 we give results from the IRON Project (see Berrington & Tully 1997). There is good agreement for most of the temperatures in the table although at the lowest ones the IRON results clearly exceed those of ZSF(5) and ZSF(4). This is explained by the effect of resonances which Berrington & Tully take account of whereas ZSF do not. Most of the collision strengths considered by Berrington & Tully are greatly modified by resonances at relatively low energies. As a result of this the resonances only have a strong effect on the thermally averaged collision strengths at temperatures which are well below those of astrophysical importance, i.e. where Fe^{+23} is expected to be abundant under conditions of coronal ionization equilibrium. Another small difference can be seen to occur at the highest temperature where the ZSF results exceed those of the IRON Project by a few percent. This is explained by the fact that ZSF's calculation is fully relativistic and therefore takes account of both the magnetic

Table 5. Program data to obtain Υ for charges $8 \leq Z_0 \leq 30$

Upsilon 2s−3s (Type,CT,CZ,Smn)
212 3.0 20

4.439	5.070	5.655	6.177
7.553	8.299	8.791	9.321
8.507	9.252	9.744	10.036
10.393	11.032	10.730	10.513

Upsilon 2s−4s (Type,CT,CZ,Smn)
212 3.0 20

0.9165	1.0415	1.1380	1.2208
1.5175	1.6506	1.7391	1.8096
1.6969	1.8305	1.9182	1.9667
2.1242	2.1995	2.1979	2.1447

Upsilon 2s−5s (Type,CT,CZ,Smn)
212 3.0 20

0.3520	0.3965	0.4315	0.4429
0.5832	0.6302	0.6655	0.7118
0.6519	0.6979	0.7311	0.7575
0.8183	0.8362	0.8429	0.9259

Upsilon 2s−3d 3/2 (Type,CT,CZ,Smn)
212 3.0 20

1.476	2.255	3.178	5.179
5.362	6.824	8.359	10.857
6.134	7.658	9.362	11.963
6.083	7.278	8.860	11.631

Upsilon 2s−4d 3/2 (Type,CT,CZ,Smn)
212 3.0 20

0.5927	0.7890	1.0187	1.3509
1.0789	1.1817	1.3620	1.6207
1.1540	1.2207	1.3915	1.6191
1.2816	1.2871	1.4297	1.5939

Upsilon 2s−5d 3/2 (Type,CT,CZ,Smn)
212 3.0 20

0.2665	0.3369	0.4215	0.5354
0.4218	0.4273	0.4790	0.5592
0.4450	0.4310	0.4766	0.5426
0.4945	0.4494	0.4834	0.5347

Table 5. continued

Upsilon 2s−3d 5/2 (Type,CT,CZ,Smn)
212 3.0 20

2.242	3.390	4.766	7.761
8.037	10.233	12.537	16.286
9.135	11.447	14.024	17.946
8.743	10.729	13.232	17.478

Upsilon 2s−4d 5/2 (Type,CT,CZ,Smn)
212 3.0 20

0.8882	1.1761	1.5194	2.0136
1.6188	1.7741	2.0453	2.4333
1.7394	1.8542	2.1198	2.4598
1.9608	2.0555	2.3126	2.5678

Upsilon 2s−5d 5/2 (Type,CT,CZ,Smn)
212 3.0 20

0.3982	0.5020	0.6276	0.7993
0.6331	0.6418	0.7196	0.8396
0.6725	0.6575	0.7290	0.8238
0.7686	0.7320	0.8007	0.8572

Table 6. $\Upsilon(2s_{1/2} - 3s_{1/2})$: Comparison of results for Fe^{+23}. ZSF(5), present 5-point spline fit; ZSF(4), present 4-point Tchebyshev fit; IRON, from the IRON Project (Berrington & Tully 1997)

$\log T$	ZSF(5)	ZSF(4)	IRON
6.0	1.4364−2	1.4369−2	1.644−2
6.2	1.4434−2	1.4435−2	1.603−2
6.4	1.4540−2	1.4533−2	1.562−2
6.6	1.4693−2	1.4677−2	1.522−2
6.8	1.4905−2	1.4880−2	1.493−2
7.0	1.5179−2	1.5149−2	1.484−2
7.2	1.5503−2	1.5485−2	1.499−2
7.4	1.5858−2	1.5872−2	1.534−2
7.6	1.6246−2	1.6289−2	1.581−2
7.8	1.6685−2	1.6723−2	1.631−2
8.0	1.7169−2	1.7188−2	1.677−2

effects and the Lorentz transformation of electron velocities mentioned in Sect. 1.1 of B&T. On the other hand the IRON Project calculation allows only for the magnetic effects but treats the kinematics of the collision classically. A proper relativistic treatment of the colliding electron's velocity can profoundly modify the collision strength at high energies and hence affect Υ at high temperatures.

5. How high in energy does one need to go?

The effective collision strength Υ was originally introduced by Seaton (1953) and is now almost universally used in place of the rate coefficient for presenting computational results. We call attention to the fact that the two are connected by a very simple relationship in which the factor Υ should be replaced by Υ/Φ when relativistic effects are taken into account (see Sect. 2.4). The integral defining Υ extends from $E_j = 0$ to $E_j = \infty$. While we always integrate over the full range, the general practice is to replace the upper limit by the maximum value of E_j, which in the present case is $0.75(Z_0 - 1.66)^2$ (see ZSF). We have investigated whether this is high enough when calculating Υ at temperatures where the ion in question is expected to have maximum abundance under conditions of coronal ionization equilibrium. We denote this temperature by $T_{\max}(Z_0)$.

Arnaud & Rothenflug's (1985) tabulation allows us to obtain $T_{\max}(Z_0)$ for 13 ions in the range $6 \leq Z_0 \leq 28$. A result for $Z_0 = 42$ is also available from the molybdenum ion fractions calculated and plotted by Fournier et al.

Table 7. $\log T_{\max}$: logarithm of the temperature at which a Li-like ion has maximum abundance under conditions of coronal ionization equilibrium as a function of atomic number Z_0. Results obtained from 5-point cubic spline fits (a) to Arnaud & Rothenflug's (1985) data points, and (b) also including the data point from Fournier et al. (1997)

Z_0	(a)	(b)
6	5.023	5.025
16	6.446	6.440
26	7.162	7.169
36	7.703	7.777
46	8.142	8.294
56	8.510	8.736
66	8.826	9.118
76	9.102	9.452
86	9.347	9.749
92	9.482	9.912
96	9.568	10.015

(1997). Their Fig. 1a shows that Mo^{+39} has maximum abundance at a temperature corresponding to $kT_{\max} = 1.1\ 10^4$ eV. Dr. Fournier (private communication) has informed us that the precise value is 10720 eV. We use the program OmeUpZ to plot and extrapolate the reduced quantity $\log T_{\max}(Z_0)\,/\,\log(Z_0)$ as a function of $Z_{\rm r} = Z/(Z + C_Z)$. We have made two fits, one including the data point for Mo^{+39} and the other excluding it. A graphical comparison of the spline fits and original data points is shown in Fig. 2. The fit which makes use only of the data from Arnaud & Rothenflug (1985) is a smooth monotonically decreasing curve which tends to 4.8090 at $Z_{\rm r} = 1$. From this fit we estimate that $T_{\max}(42) = 9.47\ 10^7$, which is 40% lower than the temperature calculated by Fournier et al. (1997). A set of results obtained along the sequence from both fits is presented in Table 7. The most highly charged ion in the sequence considered by ZSF is U^{+89}. According to Table 7 this ion has maximum abundance at a temperature of either $3.0\ 10^9$ or $8.2\ 10^9$. We obtain the higher temperature when we include the data point from Fournier et al. (1997) in the fitting process.

For the 2s → 3s transition the value of $\Upsilon(Z_0 = 92)$ at $T = 3.0\ 10^9$ is underestimated by more than 90% if the contribution from energies above the highest one considered by ZSF is neglected. With decreasing Z_0 the value of $T_{\max}(Z_0)$ falls and so does the high energy contribution. Our spline fit predicts $T_{\max}(36) = 6.1\ 10^7$ and at this temperature the high energy contribution to Υ is only of the order of 10%.

Our conclusion is that although $E_j = 0.75(Z_0 - 1.66)^2$ is high enough for ions at the lower end of the sequence this is not so at the top end. Consequently one really needs to extrapolate some of ZSF's data, or interpolate them if the high energy limit points are known.

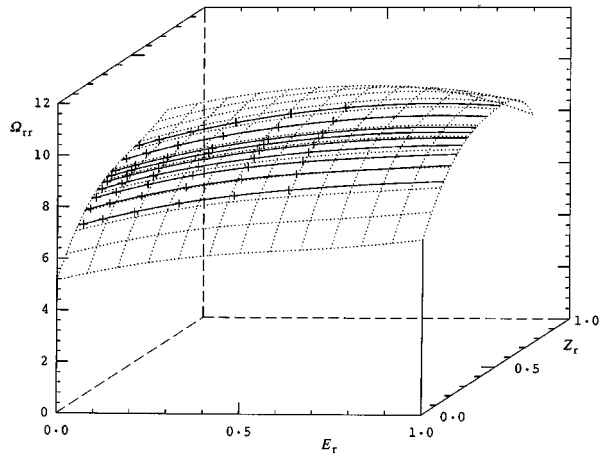

Fig. 1. Reduced collision strength $\Omega_{\rm rr}(2{\rm s} - 3{\rm s})$ for $C_E = 3.8$ (rms error = 0.004%) and $C_Z = 30$ (rms error = 0.15%). + points and full curves show data and spline fits for $Z_0 = 8, 10, 12, 14, 16, 18, 20, 22, 26$. The dotted mesh shows the double fit for $3 \le Z_0 \le 92$

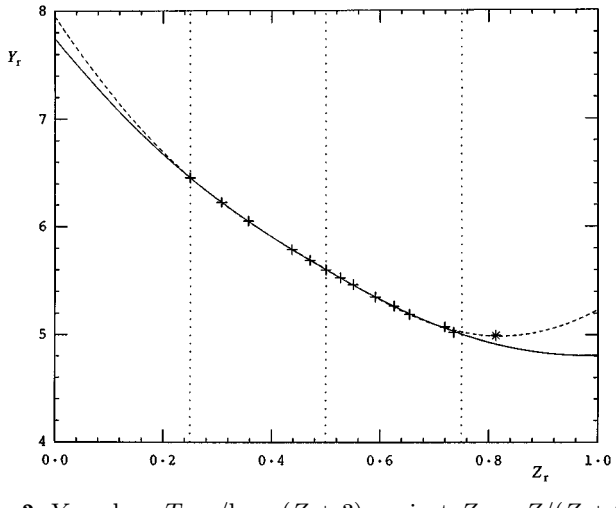

Fig. 2. $Y_{\rm r} = \log_{10} T_{\max}/\log_{10}(Z + 3)$ against $Z_{\rm r} = Z/(Z + 9)$. + Arnaud & Rothenflug (1985) data points; * Fournier et al. (1997) data point. Full curve, fit to + data points only; dashed curve, fit to both sets of data

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