

Atomic data from the IRON Project

XXX. Collision data for the ${}^2P^{\circ}_{\frac{1}{2}} - {}^2P^{\circ}_{\frac{3}{2}}$ fine-structure lines of P III, S IV and Cl V

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Abstract. This is the third paper in a series giving collision rates for electron excitation of the ${}^2P^{\circ}_{\frac{1}{2}} - {}^2P^{\circ}_{\frac{3}{2}}$ ground state fine-structure transition in aluminium-like ions. In this paper we give data for the transitions in P III (17.9 μm), S IV (10.5 μm) and Cl V (6.71 μm). For the P and Cl ions the only existing results are nearly 30 years old and were obtained using a method which does not incorporate resonance effects. For S IV, previous close-coupling calculations do exist but we show that our more elaborate calculation changes the rate coefficients by about 50% at lower temperatures.

Key words: atomic data

1. Introduction

In the two previous papers on Al-like ions, IP XI: Saraph & Storey (1996) and IP XIV: Storey et al. (1996), effective collision strengths for excitation of the ground state fine-structure transition ${}^2P^{\circ}_{\frac{1}{2}} - {}^2P^{\circ}_{\frac{3}{2}}$ in Ar VI, K VII, Ca VIII and Fe XIV, respectively, were presented. Of the three ions discussed in the present paper S IV is astrophysically the most interesting since the $\lambda 10.5 \mu\text{m}$ line is an important diagnostic tool. The calculations by Johnson et al. (1986) showed that the effective collision strengths increased by a factor four compared to earlier determinations (Brocklehurst 1972) when the effects of resonances were included. We show in this paper that a still higher degree of sophistication is required to calculate the positions of these resonances accurately. Only then can reliable collision rates be obtained. Our results are 30% higher than those of Johnson et al. (1986) at 10000 K.

The three ions discussed in the present paper are only two to four times ionised and thus have a rather open target structure, with $n = 4$ valence electron states lying

Table 1. Target description for P III, S IV and Cl V: 32 configurations with closed shells $1s^2 2s^2 2p^6$

10	configs	$3s^2 nl$	with	$n \leq 5$	$l \leq 3$
5	configs	$3s 3p nl$	with	$n \leq 4$	$l \leq 2$
5	configs	$3p^2 nl$	with	$n \leq 4$	$l \leq 2$
4	configs	$3s 3d nl$	with	$n \leq 4$	$l \leq 2$
4	configs	$3p 3d nl$	with	$n \leq 4$	$l \leq 2$
4	configs	$3d^3$	$3s 4s^2$	$3s 4s 4p$	$3s 4p^2$

among the states of the $n = 3$ complex. The construction of the target model is therefore more complicated than for the heavier ions. The details are given in Sect. 2. The collision strengths were calculated on a very fine energy mesh. In the near threshold region the details of the resonances were accurately delineated. For higher energies a sampling technique was developed as described in Sect. 3. The results are presented in Sect. 4, where a detailed discussion is devoted to the differences between the current work and that of Johnson et al. (1986).

We refer readers to the paper by Hummer et al. (1993) for details of the theory, numerical methods and a description of the computer programs. All energies are given in Rydberg units.

2. Target representations

Table 1 lists the 32 electron configurations that are used to represent the target states for the scattering problem.

A schematic diagram of the term structure of Cl V is given in Fig. 1, where the dashed line indicates the cutoff in the close-coupling expansion for this ion. As the effective charge of the ions in the series decreases, the separation in energy between states of the $n = 3$ complex and the $3s^2 nl$ Rydberg states decreases so that for P III the

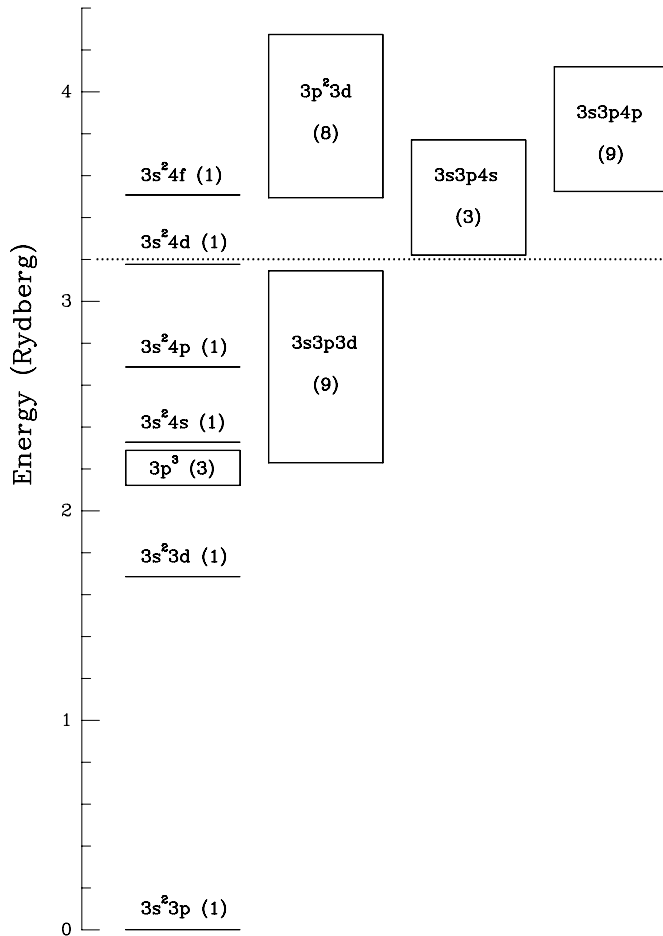


Fig. 1. The term structure of Cl v. The horizontal dashed line indicates the cutoff of the CC expansion. The number of terms in each electron configuration is given in brackets

close-coupling expansion needs to be extended to include terms $3s^2 5s \ ^2S$ and $3s^2 5p \ ^2P$, which lie among the terms of the configuration $3s3p3d$. The cutoff of the close-coupling expansion for the three ions, P III, S IV and Cl v, was such that respectively 22, 21 and 21 target states were included, as shown in Tables 2, 3 and 4.

The program SUPERSTRUCTURE by Eissner et al. (1974) as modified by Nussbaumer & Storey (1978) was used to construct the target wavefunctions. The scaling parameters were optimised in two stages, first, the sum of the energies of all configurations was minimised, and in the second stage, the potential parameters for orbitals with principal quantum numbers $n = 4$ and 5 were kept fixed whilst the others were optimised so as to minimise the energies of all the target terms that were to be retained in the CC expansion. This method ensured that the $n = 4$ and 5 valence electron states were not dragged into the core by the optimisation process. Whilst this optimisation was carried out in LS coupling the contributions of the mass and Darwin relativistic operators were included at all further stages of the calculation.

The term systems of P III and S IV are well known (Martin et al. 1985) so that the calculated energies could be checked against experiment. The analysis is less complete for Cl v. The term structure of these ions shows some interesting configuration interaction. Terms of configurations $3p^3$ and $3s3p3d$ are strongly mixed. This led to the configuration assignment $3s3p3d$ to the lowest term of symmetry $^2D^o$ and the third term $^2P^o$ in P III (Magnusson & Zetterberg 1977). In S IV the pattern is further complicated by terms of configurations $3s^2 4l$ appearing among those of the $n = 3$ complex (Reistadt & Engström 1989). In Tables 2 to 4 we give the centres of gravity of the experimental term energies (E_{exp}) and the energies that were actually used in the scattering calculation (E_{target}). The latter are as close as practicable to the experimental values without changing the calculated order of the target terms. E_{exp} and E_{target} differ only for a few of the higher terms. But it is evident from the tables that the term structure of P III is much more difficult to represent than that of the more highly ionised systems. For some terms of Cl v, which we have indicated with an “*”, term energies are not available experimentally and the corresponding E_{target} were obtained by interpolation.

Martin et al. (1985, 1990) ask for further calculations of mixing coefficients. They give leading percentages alongside their term table. Therefore we give in the last Cols. of Tables 2 to 4 the theoretical target term energies (E_{calc}) including contributions from the mass and Darwin terms, and calculated leading percentages where we adopt the presentation of Martin et al. Aashamar et al. (1984) give mixing coefficients for some terms of Al-like ions. Reistadt & Engström (1989) give leading percentages for all experimentally determined terms of S IV. Martin et al. also quote some unpublished eigenvector components from Froese-Fischer (1981).

For most terms we agree very well with other calculated leading percentages. However, where our calculated term energy disagrees significantly with experiment the associated mixing coefficients are unreliable. Tables 2 to 4 would suggest a few changes to the configuration assignments that might be of interest to experimentalists. Particularly the order of terms $3s^2 5p \ ^2P^o$ and $3s3p(^3P^o)4s \ ^2P^o$ in P III should be interchanged. In S IV terms $^2P^o$ and $^2D^o$ appear more strongly mixed in our calculation than in that of Reistadt & Engström (1989). For Cl v we give, in Table 4, identifications according to our calculated leading percentages that do differ from those given by Baudinet-Robinet et al. (1982) for some terms, we have indicated the affected terms by an *. For a more comprehensive theoretical treatment of the term structure of Al-like ions, Al I, Si II, S IV, Ar VI, Ca VIII, and Fe XIV, see Mendoza et al. (1995).

Table 2. Target energies (E_{target}) for all terms included in the CC expansion for P III. Columns 1 to 3 are from Martin et al. (1985) but (E_{exp}) are the centres of gravity of the experimental energies. Calculated energies (E_{calc}) include the mass and Darwin type relativistic contributions. The abbreviations $^1\text{P}^\circ$ and $^3\text{P}^\circ$ stand for $3s3p(^1\text{P}^\circ)$ and $3s3p(^3\text{P}^\circ)$ respectively

config.	term	E_{exp}	E_{target}	E_{calc}	leading percentages			
$3s^23p$	$^2\text{P}^\circ$	0.0	0.0	0.0	94	$3p^3$	3	
$3s3p^2$	^4P	.5184	.5184	.4961	99			
	^2D	.6795	.6795	.6778	76	$3s^23d$	21	
	^2S	.9097	.9097	.9338	95	$3s3d^2$	3	$3s^24s$ 2
	^2P	.9925	.9925	1.0210	93	$3p^23d$	6	
$3s^23d$	^2D	1.0617	1.0617	1.0944	74	$3s3p^2$	20	$3p^23d$ 4
$3s^24s$	^2S	1.0704	1.0617	1.0665	93	$3p^24s$	4	$3s3p^2$ 2
$3s^24p$	$^2\text{P}^\circ$	1.2858	1.2858	1.2790	94	$3p^24p$	4	
$^3\text{P}^\circ 3d$	$^2\text{D}^\circ$	1.3395	1.3395	1.3258	48	$3p^3$	50	
	$^4\text{F}^\circ$	1.4492	1.4492	1.4419	98			
$3p^3$	$^4\text{S}^\circ$	1.4520	1.4520	1.4476	98			
$3p^3$	$^2\text{P}^\circ$	1.5470	1.5470	1.5643	59	$^3\text{P}^\circ3d$	27	$^1\text{P}^\circ 3d$ 8
$3s^24d$	^2D	1.5679	1.5679	1.5733	94	$3p^24d$	4	
$^3\text{P}^\circ 3d$	$^4\text{P}^\circ$	1.5815	1.5815	1.5746	96	$^3\text{P}^\circ4s$	2	
	$^4\text{D}^\circ$	1.5947	1.5947	1.5923	98			
$3s^25s$	^2S	1.6008	1.6008	1.6743	99			
$3s^24f$	$^2\text{F}^\circ$	1.6246	1.6008	1.6866	87	$^1\text{P}^\circ3d$	11	
$^3\text{P}^\circ 4s$	$^4\text{P}^\circ$	1.6807	1.6008	1.6588	96	$^3\text{P}^\circ3d$	2	
$3s^25p$	$^2\text{P}^\circ$	1.6808	1.6832	1.7202	30	$^3\text{P}^\circ4s$	64	
$3p^3$	$^2\text{D}^\circ$	1.6832	1.6832	1.7029	11	$^3\text{P}^\circ3d$	50	$^1\text{P}^\circ3d$ 13 $3s3p4d$ 22
$^3\text{P}^\circ 3d$	$^2\text{F}^\circ$	1.7142	1.7142	1.7481	81	$^1\text{P}^\circ3d$	13	$3s^24f$ 4
$^3\text{P}^\circ 4s$	$^2\text{P}^\circ$	1.7419	1.7419	1.7820	26	$3s^25p$	69	

Table 3. Target energies (E_{target}) for all terms included in the CC expansion for S IV. Columns 1 to 3 are from Martin et al. (1990) but (E_{exp}) are the centres of gravity of the experimental energies. Calculated energies (E_{calc}) include the mass and Darwin type relativistic contributions. The abbreviations $^1\text{P}^\circ$ and $^3\text{P}^\circ$ stand for $3s3p(^1\text{P}^\circ)$ and $3s3p(^3\text{P}^\circ)$ respectively

config.	term	E_{exp}	E_{target}	E_{calc}	leading percentages			
$3s^23p$	$^2\text{P}^\circ$	0.0	0.0	0.0	95	$3p^3$	3	
$3s3p^2$	^4P	.6480	.6480	.6285	99			
	^2D	.8520	.8520	.8534	80	$3s^23d$	17	$3p^23d$ 2
	^2S	1.1197	1.1197	1.1475	97	$3s3d^2$	3	
	^2P	1.2157	1.2157	1.2469	94	$3p^23d$	6	
$3s^23d$	^2D	1.3806	1.3806	1.4289	78	$3s3p^2$	17	$3p^23d$ 3
$3s^24s$	^2S	1.6477	1.6477	1.6516	94	$3p^24s$	4	$3s3p4p$ 2
$3p^3$	$^2\text{D}^\circ$	1.6811	1.6811	1.6720	57	$^3\text{P}^\circ3d$	41	
	$^4\text{S}^\circ$	1.7845	1.7845	1.7844	98	$3p3d^2$	1	
$^3\text{P}^\circ 3d$	$^4\text{F}^\circ$	1.8524	1.8524	1.8526	98			
$3p^3$	$^2\text{P}^\circ$	1.9204	1.9204	1.9300	46	$3s^24p$	27	$^3\text{P}^\circ3d$ 16 $^1\text{P}^\circ3d$ 5
$3s^24p$	$^2\text{P}^\circ$	1.9412	1.9412	1.9554	66	$3p^3$	22	$^3\text{P}^\circ3d$ 9 $^1\text{P}^\circ3d$ 2
$^3\text{P}^\circ 3d$	$^4\text{P}^\circ$	2.0207	2.0207	2.0257	98			
	$^4\text{D}^\circ$	2.0403	2.0403	2.0509	98			
	$^2\text{D}^\circ$	2.1232	2.1232	2.1503	40	$^1\text{P}^\circ3d$	33	$3p^3$ 23 $3p3d^2$ 2
	$^2\text{F}^\circ$	2.2003	2.2003	2.2499	67	$^1\text{P}^\circ3d$	30	
$3s^24d$	^2D	2.3216	2.3216	2.3397	94	$3p^24d$	4	
$3s^24f$	$^2\text{F}^\circ$	2.3423	2.3423	2.4128	36	$^1\text{P}^\circ3d$	36	$^3\text{P}^\circ3d$ 23 $3p3d^2$ 4
$^3\text{P}^\circ 4s$	$^4\text{P}^\circ$	2.3972	2.3423	2.3834	98			
$^3\text{P}^\circ 3d$	$^2\text{P}^\circ$	2.4085	2.4085	2.4623	49	$^3\text{P}^\circ4s$	35	$3p^3$ 10
$^3\text{P}^\circ 4s$	$^2\text{P}^\circ$	2.4659	2.4659	2.4930	55	$^1\text{P}^\circ3d$	28	$3p^3$ 8

Table 4. Target energies (E_{target}) for all terms included in the CC expansion for Cl v. (E_{exp}) are the centres of gravity of the experimental energies taken from Moore (1971) and from Baudinet-Robinet et al. (1982). The identifications (Col. 1) that are marked with an * do not agree with those by Baudinet-Robinet et al., see Sect. 2. Calculated energies (E_{calc}) include the mass and Darwin type relativistic contributions. The abbreviations $^1\text{P}^\circ$ and $^3\text{P}^\circ$ stand for $3s3p(^1\text{P}^\circ)$ and $3s3p(^3\text{P}^\circ)$ respectively

config.	term	E_{exp}	E_{target}	E_{calc}	leading percentages						
$3s^23p$	$^2\text{P}^\circ$	0.0	0.0	0.0	95	$3p^3$	2	$^1\text{P}^\circ3d$	1		
$3s3p^2$	^4P	.7826	.7826	.7592	99						
	^2D	1.0232	1.0232	1.0257	82	$3s^23d$	15	$3p^23d$	2		
	^2S	1.3273	1.3273	1.3564	97	$3s3d^2$	3				
	^2P	1.4360	1.4360	1.4700	94	$3p^23d$	5				
$3s^23d$	^2D	1.6848	1.6848	1.7416	80	$3s3p^2$	15	$3p^23d$	3		
$3p^{3*}$	$^2\text{D}^\circ$	2.0196	2.0196	2.0112	61	$^3\text{P}^\circ3d$	37				
	$^4\text{S}^\circ$	2.1211	2.1211	2.1189	98	$3p3d^2$	1				
$^3\text{P}^\circ 3d$	$^4\text{F}^\circ$	–	2.2436	2.2532	99						
$3p^{3*}$	$^2\text{P}^\circ$	2.2961	2.2961	2.3183	72	$^3\text{P}^\circ3d$	17	$^1\text{P}^\circ3d$	7	$3s^23p$	2
$3s^24s$	^2S	2.3266	2.3266	2.3315	95	$3p^24s$	3	$3s3p4p$	2		
$^3\text{P}^\circ 3d$	$^4\text{P}^\circ$	2.4537	2.4537	2.4595	99						
	$^4\text{D}^\circ$	2.4777	2.4777	2.4909	99						
	$^2\text{D}^\circ$	–	2.5775	2.5872	44	$^1\text{P}^\circ3d$	32	$3p^3$	21	$3p3d^2$	2
$3s^24p$	$^2\text{P}^\circ$	–	2.6824	2.6920	92	$3p^24p$	3	$3s3p4s$	2		
$^3\text{P}^\circ 3d$	$^2\text{F}^\circ$	–	2.7206	2.7302	64	$^1\text{P}^\circ3d$	34				
$^1\text{P}^\circ 3d$	$^2\text{F}^\circ$	–	2.9754	2.9850	56	$^3\text{P}^\circ3d$	33	$3s^24f$	8	$3p3d^2$	3
$^3\text{P}^\circ 3d$	$^2\text{P}^\circ$	3.0437	3.0437	3.0039	80	$3p^3$	17	$3p3d^2$	1		
$^1\text{P}^\circ 3d$	$^2\text{P}^\circ$	–	3.1391	3.1487	86	$3p3d^2$	5	$3p^3$	4	$3s^23p$	2
$^1\text{P}^\circ 3d$	$^2\text{D}^\circ$	–	3.1625	3.1723	62	$^3\text{P}^\circ3d$	17	$3p^3$	16	$3p3d^2$	4
$3s^24d$	^2D	3.1759	3.1759	3.1951	94	$3p^24d$	3				

3. The scattering calculation

The close-coupling method in the R-matrix formulation was employed, using the programs developed for the IRON Project (Hummer et al. 1993). The mass and Darwin terms of the Breit-Pauli operator were included explicitly. Calculated target energies were replaced by the energies E_{target} listed in Col. 4 of Tables 2 to 4, to ensure that the series limits of resonances were as accurately positioned as possible. Orbitals of high valence states extend far out and can cause numerical problems in the scattering calculations. Therefore, the radius of the “inner region” of the R-matrix method was relatively large, 19.2 au for Cl v, 24.3 au for S IV and 32.0 au for P III. Up to 20 basis functions had to be used in the R-matrix method to span these extended inner regions. We considered scattering electron energies up to 1.5 Ryd; this range being sufficient for the determination of collision rates in plasmas with temperatures up to 30000 K. The expansion over total angular momenta converged for these energies by $J = 8$.

The collision strengths are completely dominated by resonances. Since the aim of this calculation is to provide collision rates the delineation of the resonances has to be detailed enough so as to avoid errors when the collision strengths are sampled by the Maxwell velocity distribution function. This is particularly critical near the excitation threshold where we used small steps $\delta\nu = 0.0002$

with ν the effective quantum number relative to the nearest higher threshold. When $\nu > 25$ resonances due to the corresponding threshold were averaged using the Gailitis method (Seaton 1983) and ν was taken relative to the next higher threshold. At energies between about 1 Ryd and 1.5 Ryd the closely-packed target states made this approach impractical and instead we used a small constant step in energy. In order to ensure that no essential information was lost the calculation was repeated at points shifted by half that steplength. This process was repeated with the steplength halved until it was found that the results obtained from two sets of non-overlapping data points differed by less than 1%. The final results were obtained by integrating over all datapoints.

These scattering calculations were performed in LS coupling and in order to obtain collision strengths for the fine-structure transition the T-matrix elements were transformed algebraically to pair coupling. The spin-orbit interaction between the target terms was included as a perturbation by a second transformation that incorporated the so-called term coupling coefficients (Saraph 1978). In practice, at the low energies considered here the collision strengths are hardly affected by term coupling.

The fine-structure splitting of the target terms was neglected. This leads to some inaccuracy in the collision rate at the lowest temperature, but is not as serious for

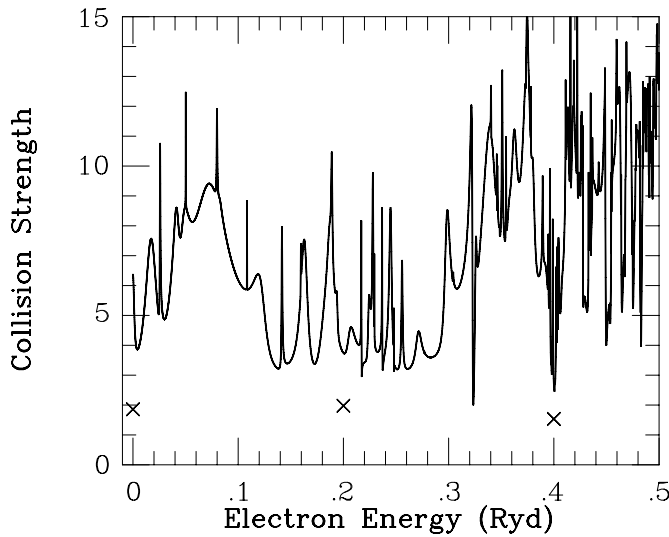


Fig. 2. Low energy collision strength for excitation of $3s^23p(^2P^{\circ}_{1/2} - ^2P^{\circ}_{3/2})$ in P III, obtained using a 22 term CC expansion. $\times \times \times$ DW calculations by Krüger & Czyzak (1970)

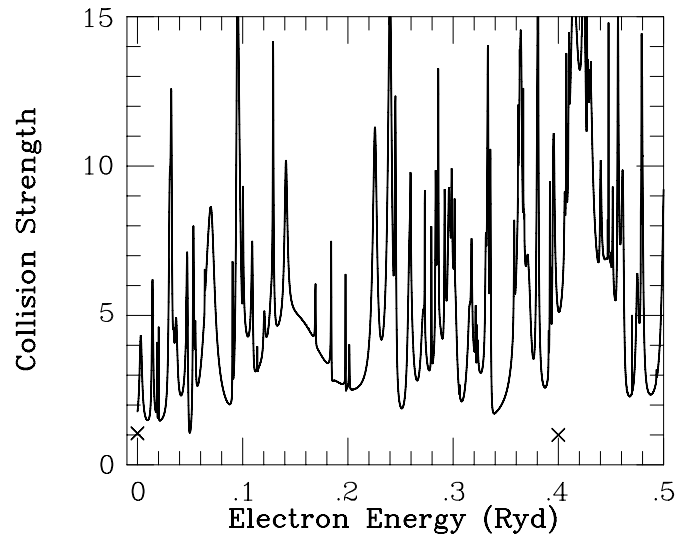


Fig. 4. Low energy collision strength for excitation of $3s^23p(^2P^{\circ}_{1/2} - ^2P^{\circ}_{3/2})$ in Cl V, obtained using a 21 term CC expansion. $\times \times \times$ DW calculations by Krüger & Czyzak (1970), the point at 0.4 Ryd was obtained by interpolation

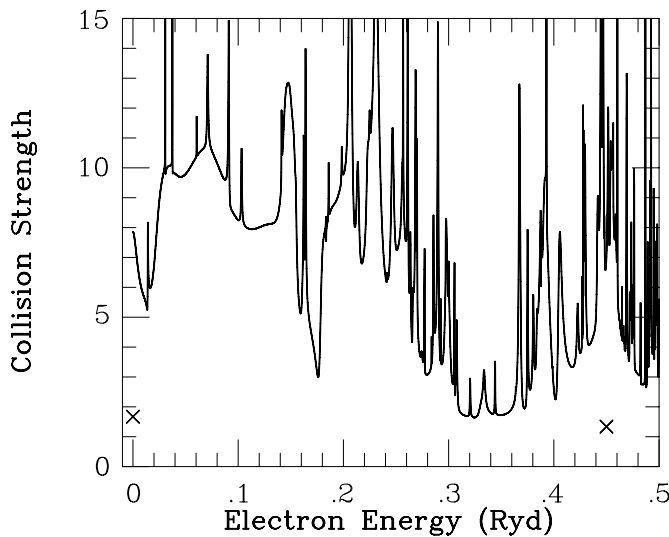


Fig. 3. Low energy collision strength for excitation of $3s^23p(^2P^{\circ}_{1/2} - ^2P^{\circ}_{3/2})$ in S IV, obtained using a 21 term CC expansion. $\times \times \times$ DW calculations by Krüger & Czyzak (1970)

these light ions as for the ions discussed in IP XI due to the relatively smaller fine-structure splittings. The low energy collision strengths are shown in Figs. 2 to 4 where the results of the distorted wave calculations of Krüger & Czyzak (1970) are included for comparison.

4. Collision rates

The effective collision strength $\mathcal{Y}(T)$ was obtained from the calculated collision strengths as described in Hummer et al. (1993) and discussed in IP XI.

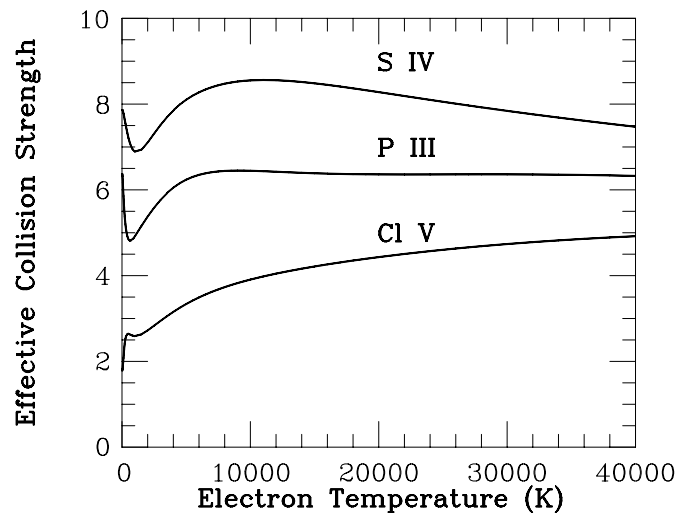


Fig. 5. Thermally averaged collision strengths \mathcal{Y} for excitation of the ground state fine-structure line in P III, S IV and Cl V

The collisional de-excitation rate coefficient $q(T)$ is related to $\mathcal{Y}(T)$ by

$$q = \frac{8.63 \cdot 10^{-6} \mathcal{Y}}{\omega T^{\frac{1}{2}}} \text{ cm}^3 \text{ s}^{-1}, \quad (1)$$

where ω is the statistical weight of the upper state and T is the electron temperature in K. Our values for $\mathcal{Y}(T)$ for the three ions are given in Table 5 and in Fig. 5.

4.1. Comparison with earlier calculations.

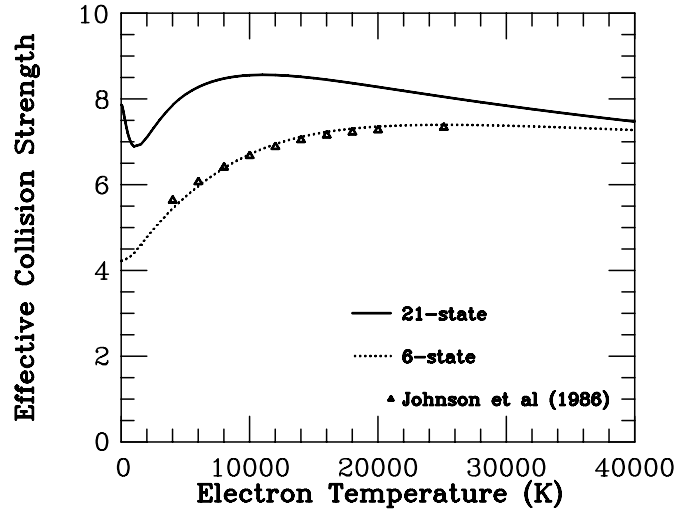
The present results for S IV differ significantly from those of Johnson et al. (1986), that were also obtained from

Table 5. Effective collision strengths for excitation of the $2P^{\circ}_{1/2} - 2P^{\circ}_{3/2}$ fine-structure lines in P III, S IV and Cl V

T (K)	$\Upsilon(\text{P III})$	$\Upsilon(\text{S IV})$	$\Upsilon(\text{Cl V})$
1000.	4.92	6.89	2.59
1500.	5.16	6.93	2.63
2000.	5.38	7.11	2.72
2500.	5.59	7.32	2.83
3000.	5.77	7.52	2.94
3500.	5.92	7.70	3.05
4000.	6.05	7.85	3.15
5000.	6.23	8.10	3.33
6000.	6.35	8.27	3.49
7000.	6.41	8.39	3.62
8000.	6.44	8.47	3.73
9000.	6.45	8.52	3.82
10000.	6.44	8.55	3.90
11000.	6.43	8.56	3.98
12000.	6.42	8.55	4.04
13000.	6.41	8.54	4.10
14000.	6.39	8.51	4.16
15000.	6.38	8.48	4.21
16000.	6.37	8.44	4.26
18000.	6.36	8.36	4.35
20000.	6.36	8.28	4.43
24000.	6.36	8.09	4.57
28000.	6.36	7.92	4.68
32000.	6.35	7.76	4.78
36000.	6.34	7.61	4.85
40000.	6.32	7.47	4.92

a close-coupling calculation. In order to understand the cause of the discrepancy we simulated their calculation by cutting off our CC expansion at six target terms. We found that as a result the resonances were all shifted to higher energies, particularly the broad and tall feature between .03 and .1 Ryd. Analysis of this feature shows that it is chiefly made up of resonances with configurations $3s3p^2nl$. Johnson et al. had included all parent terms to these resonances and correlation configurations in their calculation, but they omitted the channel coupling effects to higher terms. As a result the resonance positions were shifted and the overlap between the Maxwell velocity distribution function at low temperatures and the collision strength is very much smaller.

Figure 6 shows a comparison of our present results including 21 target terms with the results obtained when the CC expansion is cut short at six terms and with the results of Johnson et al. (1986) who included the same six terms. Our six term results agree with those of Johnson et al., although they used different CI and target orbitals. It is clear that the migration of the resonances to higher energies effected by the omission of channel coupling effects causes the discrepancy.

**Fig. 6.** Thermally averaged collision strengths for excitation of the ground state fine-structure line in S IV. Full line: 21 term CC calculation, dotted line: 6 term CC calculation, triangles: results of Johnson et al. (1986)

5. Discussion

The results of the present calculation differ significantly from the earlier data.

We note first the enormous increase of the averaged collision strength effected by resonant coupling to dipole-allowed transition channels. This increase extends from the excitation threshold to energies of roughly 1.2 Ryd. The early distorted wave calculations (Krüger & Czyzak 1970) neglected channel coupling completely and the present results for the averaged collision strength differ from theirs by factors three to five. As can be seen from Figs. 2 to 4 the distorted wave results do not even come close to the background values of the collision strengths. Earlier CC calculations have attempted to address this problem, see Johnson et al. (1986), and have obtained an increase by a factor of four for the averaged collision strength compared to the distorted wave calculations. It must be mentioned that the earlier calculations were limited by the computer power that was available at the time.

Secondly, we find that inclusion of resonances alone does not necessarily give the full answer. The proper delineation of the resonance structure is crucial for accurate determinations of the thermally averaged collision strength, particularly at low temperatures, as discussed by Storey et al. (1996) and noted by Johnson et al. (1986).

A third non-negligible effect is caused by any shift of these resonances, especially if they are large features that compare in width with the Maxwell velocity distribution function. The extent of the overlap will determine the magnitude of the thermally averaged collision strength at a given temperature. Significant resonance shifts can result from the use of calculated rather than experimental term energies, from the inclusion or neglect of relativistic

effects, or from an early cutoff of the CC expansion, (see the detailed discussion for Ca VIII and Ar VI in Saraph & Storey 1996). We have shown that the discrepancy between the current results and those of Johnson et al. for S IV is due to the difference in the cutoff of the CC expansion, (Fig. 6). By cutting off the present 21 state CC expansion after only six terms we obtain results that are remarkably close to those of Johnson et al. (1986).

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References

- Aashamar K., Luke T.M., Talman J.D., 1984, Phys. Scr. 30, 121
- Baudinet-Robinet Y., Dumont P.D., Garnir H.P., 1982, Nucl. Instr. Met. 202, 33
- Brocklehurst M., 1972, MNRAS 160, 19p
- Eissner W., Jones M., Nussbaumer H., 1974, Comput. Phys. Commun. 8, 270
- Froese-Fischer C., 1981, Phys. Scr. 23, 38
- Hummer D.G., Berrington K.A., Eissner W., et al., 1993, A&A 279, 298
- Johnson C.T., Kingston A.E., Dufton P.L., 1986, MNRAS 220, 155
- Krüger T.K., Czyzak S.J., 1970, Proc. R. Soc. London Ser. A318, 531
- Magnusson C.E., Zetterberg P.O., 1977, Phys. Scr. 15, 237
- Martin W.C. Zalubas R., Musgrove A., 1985, J. Phys. Chem. Ref. Data 14, No. 3
- Martin W.C. Zalubas R., Musgrove A., 1990, J. Phys. Chem. Ref. Data 19, No. 4
- Mendoza C., Eissner W., Le Dourneuf M., Zeippen C.J., 1995, J. Phys. B: At. Mol. Opt. Phys. 28, 1
- Moore C.E., 1971, Atomic Energy Levels 1, NBS Circular No. 467, U.S. Government Printing Office, Washington DC
- Nussbaumer H., Storey P.J., 1978, A&A 64, 139
- Reistad N., Engström L., 1989, Phys. Rev. A 39, 4518
- Saraph H.E., 1978, Comput. Phys. Commun. 15, 247
- Saraph H.E., Storey P.J., 1996, A&AS 115, 151
- Seaton M.J., 1983, Rep. Prog. Phys. 46, 167
- Storey P.J., Mason H.E., Saraph H.E., 1996, A&A 309, 667