

Electron Collisional Excitation of S XII

H. P. Saha and E. Treffitz

Max-Planck-Institut für Physik und Astrophysik, Garching bei München

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To Professor Arnulf Schlüter on his 60th Birthday

Atomic data have been obtained for the coronal ion S XII using the UCL program codes. Energy levels and radiative transition probabilities have been computed with different target descriptions allowing for configuration interaction and relativistic effects. Multi-configuration Hartree-Fock method is used to calculate the target wave functions. Collisional excitation cross sections between the $2s^2 2p^2 P^0$, $2s2p^2^4P$, 2D , 2S , 2P and the $2p^3 4S^0$, $2D^0$, $2P^0$ eigenstates of S XII have been calculated using eight-state close coupling and distorted wave approximations with a target description employing a $3\bar{d}$ pseudo orbital. Collision strengths between the lowest five eigenstates of S XII have also been computed in five-state close coupling and distorted wave approximations for comparison. The results are compared with available theoretical work. It is found that the use of elaborate target wave functions and the choice of a more accurate scattering approximation may change the cross sections by more than 25% in some of the transitions.

1. Introduction

In the universe sulphur is one of the most abundant heavier elements which are of astrophysical interest. In the solar corona the highly ionized atom S XII of the boron-isoelectronic sequence has been found to be present. Lines from S XII have been identified in the extreme ultraviolet solar emission spectra of quiet, active, and flaring solar regions. On a spectrum obtained with the Harvard College Observatory spectrometer (300–1350 Å), flown aboard Skylab, many XUV lines are observed some of which may belong to S XII, cf. Reeves et al [1]. Observation of the optically allowed transitions $2s^2 2p^2 P^0 - 2s 2p^2^2L$ have been made by Behring et al. [2] from the full disk of the sun photographed under quiet solar conditions by a rocket-borne spectrograph with a spectral resolution of less than 0.06 Å, flown in September 1973. Malinovsky and Heroux [3] also observed the same optically allowed transitions with a grazing incidence rocket spectrometer flown in April 1969. Observations of EUV emission spectra by the Goddard orbiting solar observatory (OSO-7), launched in September 1971, also show the presence of the lines $2s^2 2p^2 P^0 - 2s 2p^2^2P$, cf. Kastner and Mason [4]. These lines are potentially useful for density diagnostics in the solar corona. For the interpretation of these observational results it is

necessary to have accurate atomic data both for the radiative and for the electron excitation cross sections of these transitions.

Atomic data have been calculated by Flower and Nussbaumer [5] in similar approximations as we employ here. The present paper discusses and compares different approximations and their effect on the different kinds of transitions. The analysis follows closely the one given by Saha and Treffitz [6] for the case $e + Si^{+9}$, hence forth called paper I. Chapter 2 gives details on the target description, energy levels and oscillator strengths. Chapter 3 describes the methods used to calculate collision strengths. The results are discussed in Chapter 4.

2. Target Description

As for Si^{+9} we determined the wave functions in multiconfiguration Hartree-Fock approximation. For practical reasons the same set of orbitals is used to describe all target states of interest. Therefore the program of Fischer [7, 8] was generalized to allow the minimization of the energy expectation value of a linear combination of two states. As in I we minimized

$$\langle 2s^2 2p^2 P^0 | H | 2s^2 2p^2 P^0 \rangle + \langle 2s2p^2^4P | H | 2s2p^2^4P \rangle = \text{Min.} \quad (1)$$

A "simple" ansatz (characterized by index a) was compared with an "elaborate" ansatz b. Ansatz a described the target states by 3 configurations $2s^2 2p$, $2s 2p^2$, $2p^3$ with orbitals $1s$, $2s$, $2p$, while ansatz b added a pseudo orbital $3\bar{d}$ and used 7 con-

Reprint requests to Dr. Eleonore Treffitz, Max-Planck-Institut für Physik und Astrophysik, D-8046 Garching.

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Index	Term	<i>J</i>	<i>E</i> ^a (cm ⁻¹)	<i>E</i> ^b (cm ⁻¹)	observed ^c (cm ⁻¹)
1	2s ² 2p ² P ^o	1/2	0	0	0
2		3/2	12706	12765	13135
3	2s 2p ² ⁴ P	1/2	187541	191140	193970
4		3/2	192252	195876	198774
5		5/2	198861	202506	205487
6	² D	3/2	351756	348751	346748
7		5/2	352072	349098	347015
8	² S	1/2	443203	444815	439627
9	² P	1/2	476634	469548	464799
10		3/2	483709	475993	471461
11	2p ³ ⁴ S ^o	3/2	606589	613741	610178
12	² D ^o	3/2	698837	697584	689990
13		5/2	699253	697957	690495
14	² P ^o	1/2	785154	788585	774115
15		3/2	786768	790156	775834

Table 1. Observed and calculated energy levels of the configurations 2s² 2p, 2s 2p² and 2p³.^a 3 configurations.^b 7 configurations.^c Edlen, [16].

figurations: 2s² 2p, 2p³, 2s 2p $\overline{3d}$ for odd states, 2s 2p², 2p² $\overline{3d}$, 2s $\overline{3d^2}$, 2s² $\overline{3d}$ for even states, the last configuration entering only in ²D. The wave functions are the same as the ones used by Dankwort and Treffitz [9].

Care has to be taken that in all parts of the calculation consistent phase conventions are employed. Since the collision problem was solved with the University College London program set (Eissner and Nussbaumer [10], Seaton [11], Eissner et al. [12], Crees et al. [13], Saraph [14, 15]) we used the program SUPERSTRUCTURE [12] to determine intermediate coupling effects. SUPERSTRUCTURE differs from the program WAVANG employed by Dankwort and Treffitz [9] in the neglect of orbit-orbit interactions. Also in WAVANG states LS have been added which appear only in admixed configurations.

SUPERSTRUCTURE was also used by Flower and Nussbaumer [5] in their calculation of S XII data together with orbitals calculated in a scaled Thomas-Fermi potential. These authors used the "simple" 3-configuration ansatz. For calculating intermediate coupling effects they corrected the non-relativistic energies semiempirically. For highly ionized systems the difference in the orbitals of the two calculations is negligible compared to differences in other details of approximation.

Table 1 compares our calculated energy levels with those determined by Edlen [16] from observation. Their numbering, column 1, is used in the further tables. For the lower levels ansatz b is an appreciable improvement over ansatz a.

In Table 2 weighted oscillator strengths for electric dipole transitions are given. In general there

Table 2. Weighted oscillator strengths for the transitions. Numbers in brackets are powers of 10.

Transition <i>i j</i>	gf ^a	gf ^b	gf ^c
1 3	8.172 (−5)	7.847 (−5)	9.23 (−5)
1 4	3.494 (−6)	3.321 (−6)	3.93 (−6)
1 6	1.388 (−1)	1.267 (−1)	1.36 (−1)
1 8	1.216 (−1)	1.327 (−1)	1.41 (−1)
1 9	1.525 (−1)	1.270 (−1)	1.25 (−1)
1 10	9.540 (−2)	9.236 (−2)	9.10 (−2)
2 3	6.655 (−5)	5.864 (−5)	7.36 (−5)
2 4	3.115 (−5)	3.417 (−5)	3.82 (−5)
2 5	1.779 (−4)	1.850 (−4)	1.99 (−4)
2 6	1.750 (−2)	1.537 (−2)	1.65 (−2)
2 7	2.238 (−1)	2.032 (−1)	2.17 (−1)
2 8	8.178 (−2)	5.342 (−2)	6.55 (−2)
2 9	1.540 (−1)	1.635 (−1)	1.66 (−1)
2 10	5.312 (−1)	5.144 (−1)	5.11 (−1)
3 11	1.253 (−1)	1.191 (−1)	1.81 (−1)
3 12	6.985 (−6)	5.093 (−6)	
3 14	5.741 (−5)	5.639 (−5)	
3 15	9.079 (−7)	1.472 (−6)	
4 11	2.475 (−1)	2.350 (−1)	2.33 (−1)
4 12	3.010 (−4)	3.047 (−4)	
4 13	2.959 (−5)	2.661 (−5)	
4 14	1.100 (−5)	1.136 (−5)	
4 15	2.198 (−4)	2.292 (−4)	
5 11	3.656 (−1)	3.472 (−1)	3.43 (−1)
5 12	1.540 (−5)	1.293 (−5)	
5 13	1.059 (−3)	1.057 (−3)	
5 15	8.781 (−5)	8.859 (−5)	
6 11	6.115 (−6)	9.244 (−6)	
6 12	2.506 (−1)	2.308 (−1)	
6 13	4.254 (−2)	3.916 (−2)	
6 14	1.745 (−1)	1.578 (−1)	
6 15	4.552 (−2)	4.007 (−2)	
7 11	5.616 (−6)	1.983 (−6)	
7 12	5.263 (−2)	4.702 (−2)	
7 13	4.352 (−1)	3.990 (−1)	
7 15	2.707 (−1)	2.455 (−1)	
8 11	1.097 (−5)	1.840 (−5)	
8 12	1.659 (−2)	2.373 (−2)	
8 14	1.789 (−2)	9.817 (−3)	
8 15	1.274 (−1)	1.273 (−1)	
9 11	7.183 (−5)	6.676 (−5)	

Table 2 continued

Transition <i>i j</i>	gf ^a	gf ^b	gf ^c
9 12	1.713 (−1)	1.423 (−1)	
9 14	1.692 (−1)	1.583 (−1)	
9 15	1.989 (−2)	1.023 (−2)	
10 11	2.320 (−4)	2.245 (−4)	
10 12	1.975 (−2)	1.863 (−2)	
10 13	2.829 (−1)	2.511 (−1)	
10 14	6.069 (−2)	5.305 (−2)	
10 15	3.782 (−1)	3.331 (−1)	

^a 3 configurations.^b 7 configurations.^c Flower and Nussbaumer [5].

is close agreement between our 7-configuration approximation b and the energy improved 3-configuration approximation of Flower and Nussbaumer. Larger deviations up to 25% are found in the intercombination transitions, which are naturally more sensitive towards details of approximation.

3. Collision Cross Sections, Methods

Collision cross sections Q are related to collision strengths Ω by

$$Q(i \rightarrow j) = \frac{\Omega(i, j)}{g_i k_i^2} \pi a_0^2, \quad (2)$$

where g_i is the statistical weight of the initial state and k_i is the velocity of the colliding electron in the initial state in atomic units, a_0 is the Bohr radius. $\Omega(i, j) = \Omega(j, i)$ is symmetric in initial and final target state. The collision problem is first solved non-relativistically by a partial wave expansion as described by Eissner and Seaton [17]. For low total angular momentum L close coupling approximation (CCA) as well as distorted wave approximation (DWA) has been used as described in paper I. For higher L distorted wave approximation suffices since the interaction between channels is small compared to centrifugal forces on the free electron. Therefore what is called CCA results use CCA up to $L=4$ by employing the program IMPACT [13]. The collision algebra is done by the program COLLALG which belongs to the SUPER-STRUCTURE set as does the DWA program for higher L and for the DWA results.

So far relativistic effects are neglected. For highly ionized ions like S^{+11} the target states are strongly affected by spin orbit coupling while at the relevant temperatures the velocity of the

colliding electron is still small compared to light velocity. For this case the program JAJOM has been written by Saraph [14, 15]. In a first step the reactance matrix element

$$RLSp(\Gamma_i L_i S_i l, \Gamma'_i L'_i S'_i l', E)$$

which refers to the total multiplet $\Gamma_i L_i S_i - \Gamma'_i L'_i S'_i$ is algebraically transformed to refer to fine structure levels with the help of recoupling coefficients. $LSJp$ are the total angular momenta and parity. The indexed quantities refer to the target states, and l, l', s is the free electron's orbital angular momentum before and after the collision and its spin:

$$\begin{aligned} & R^{Jp}(\Gamma_i L_i S_i J_i l K, \Gamma'_i L'_i S'_i J'_i l' K') \\ &= \sum_{L, S} ((L_i S_i) J_i l (K) J | (L_i l) L (S_i s) S J) \\ & \quad \times R^{LSp}(\Gamma_i L_i S_i l, \Gamma'_i L'_i S'_i l') \quad (3) \\ & \quad \times ((L'_i l') L (S'_i s) S J | (L'_i S'_i) J'_i l' (K') J), \end{aligned}$$

where $\mathbf{K} = \mathbf{J}_i + \mathbf{l}$ and $\mathbf{J} = \mathbf{K} + \mathbf{s} = \mathbf{L} + \mathbf{S}$.

The resulting fine structure matrix elements are then again transformed with the "term coupling coefficients" $f_{J_i}(\Delta_i, \Gamma_i L_i S_i)$ which describe the intermediate coupling effects in the target:

$$\begin{aligned} \Psi^{\text{ion}}(\Delta_i J_i) &= \sum_{\Gamma_i L_i S_i} f_{J_i}(\Delta_i, \Gamma_i L_i S_i) \\ & \quad \times \Psi^{\text{ion}}(\Gamma_i L_i S_i J_i), \quad (4) \end{aligned}$$

$$\begin{aligned} & R^{Jp}(\Delta_i J_i l K, \Delta'_i J'_i l' K') \\ &= \sum_{\substack{\Gamma_i L_i S_i \\ \Gamma'_i L'_i S'_i}} f_{J_i}(\Delta_i, \Gamma_i L_i S_i) \\ & \quad \times R^{Jp}(\Gamma_i L_i S_i J_i l K, \Gamma'_i L'_i S'_i J'_i l' K') \\ & \quad \times f_{J'_i}(\Delta'_i, \Gamma'_i L'_i S'_i). \quad (5) \end{aligned}$$

The validity of this approach is discussed in paper I.

In optically allowed excitations dipole interactions have a very long range so that very high angular momenta l of the free electron still contribute. These may be summed up by the Coulomb-Bethe approximation, cf. Burgess and Sheorey [18]. This approximation was applied for $l > 11$ using the oscillator strengths of Table 2. Care has to be taken that in adding up DWA partial waves and "Bethe tails" no contribution is either counted twice or left out.

In all the approximations (CCA, DWA and Coulomb-Bethe approximation) observed target energies [16] are used instead of calculated ones. As discussed in paper I a difficulty in the present approach is the appearance of "bound channel

resonances". Each bound channel resonance corresponds to a true resonance but since the orbitals are chosen to describe the target states well they are not suited for the description of a true resonance state. The energy at which a bound channel resonance appears is often far from the energy of the corresponding true resonance. We cut these unrealistic resonances out by approximating the collision strength outside the resonance by a smooth analytic expression:

$$\Omega = A + B \exp(-\alpha E) + C \log(E/\Delta E), \quad (6)$$

where E is the energy of the incoming electron relative to the ground level $2s^2 2p^2 P_{1/2}^0$, and ΔE is the energy difference between the ground level and the upper level of the transition. This analytic expression was then used to calculate excitation rates.

4. Collision Cross Sections, Results

Collision strengths have been calculated at the following energy values (measured from the target

ground state $2s^2 2p^2 P^0$):

$$E = 9, 12, 15, 20, 25, 30, 34, 37, 40, 45, 50, \\ \text{and } 70 \text{ Ryd}$$

in close coupling and distorted wave approximation (CCA and DWA). The calculations with the "simple" ansatz a included 5 target terms with 10 fine structure levels, those with ansatz b included 8 target terms with 15 fine structure levels. Table 3 shows the results for excitations from the ground state at three energies.

The lowest energy, $E=9$ Ryd is just above the highest threshold, $2p^3 2P^0$ at 7 Ryd. At this energy the collision strength between the ground levels is very sensitive towards the approximations. There is about 29% difference between the close coupling (CCA^b) and the distorted wave (DWA^b) result with the elaborate ansatz. At energy 15.0 Ryd close coupling results (CCA^a) with the simple ansatz and close coupling results (CCA^b) with the elaborate ansatz differ by about 5% whereas the difference between distorted wave (DWA^b) and close coupling

Table 3. Comparison of fine structure collision strengths calculated in different approximations at three different energies (Rydbergs).

Transition $i \rightarrow j$		Energy 9			15			70		
		DWA ^c	DWA ^b	CCA ^b	CCA ^a	DWA ^b	CCA ^b	DWA ^a	DWA ^b	CCA ^b
1	2	0.092	0.0703	0.0993	0.0868	0.0702	0.0912	0.0526	0.0514	0.0537
1	3	0.011	0.0126	0.0118	0.0102	0.0101	0.0101	0.0039	0.0039	0.0040
1	4	0.015	0.0172	0.0160	0.0136	0.0135	0.0136	0.0043	0.0045	0.0045
1	5	0.009	0.0107	0.0100	0.0084	0.0084	0.0085	0.0026	0.0028	0.0028
1	6	0.54	0.5373	0.5426	0.6414	0.5954	0.5974	0.9032	0.8542	0.8537
1	7	0.017	0.0166	0.0165	0.0135	0.0135	0.0141	0.0045	0.0049	0.0048
1	8	0.37	0.3985	0.4033	0.4131	0.4446	0.4440	0.5868	0.6448	0.6433
1	9	0.41	0.3445	0.3520	0.4531	0.3841	0.3876	0.6505	0.5632	0.5640
1	10	0.25	0.2521	0.2563	0.2846	0.2797	0.2817	0.4049	0.4082	0.4085
1	11		0.0010	0.0005		0.0005	0.0004		0.0001	0.0001
1	12		0.0040	0.0042		0.0040	0.0041		0.0046	0.0043
1	13		0.0031	0.0028		0.0026	0.0027		0.0027	0.0026
1	14		0.0025	0.0029		0.0015	0.0028		0.0016	0.0021
1	15		0.0046	0.0022		0.0018	0.0019		0.0017	0.0016
2	3	0.007	0.0075	0.0070	0.0060	0.0060	0.0060	0.0024	0.0024	0.0025
2	4	0.019	0.0214	0.0199	0.0170	0.0168	0.0170	0.0056	0.0059	0.0059
2	5	0.042	0.0481	0.0448	0.0322	0.0382	0.0384	0.0138	0.0142	0.0142
2	6	0.095	0.0901	0.0906	0.1011	0.0923	0.0933	0.1230	0.1112	0.1110
2	7	0.91	0.9144	0.9231	1.0932	1.0018	1.0056	1.5201	1.3957	1.3949
2	8	0.26	0.1733	0.1740	0.2885	0.1901	0.1883	0.4035	0.2643	0.2627
2	9	0.44	0.4711	0.4783	0.4875	0.5193	0.5211	0.6896	0.7370	0.7366
2	10	1.46	1.4341	1.4610	1.6213	1.5908	1.6010	2.3141	2.2981	2.2992
2	11		0.0021	0.0010		0.0009	0.0008		0.0002	0.0002
2	12		0.0041	0.0036		0.0033	0.0034		0.0035	0.0033
2	13		0.0089	0.0088		0.0084	0.0086		0.0094	0.0089
2	14		0.0052	0.0028		0.0024	0.0026		0.0024	0.0022
2	15		0.0106	0.0092		0.0059	0.0087		0.0062	0.0071

^a 3 configurations.

^b 7 configurations.

^c Flower and Nussbaumer [5].

(CCA^b) results with the elaborate ansatz is about 23%. This indicates that at low energies for this particular transition the type of approximation is more important than the target description. At high energy, 70.0 Ryd, the difference between DWA^b and CCA^b is very small as expected. In optically allowed transitions the deviations between DWA and CCA results are small, of the order of 1%. For these transitions the effect of the improved target description is appreciably larger than the difference between the approximations DWA and CCA. As discussed in I exchange transitions are more sensitive towards the approximation, because only low angular momenta contribute. Here larger deviations show for $E=9$ Ryd. The quadrupole transitions, $2s^2 2p-2p^3$, are also sensitive because they refer to a two-electron jump. A transition is possible only through configuration interaction (admixture of $2p^3$ to the ground state $2s^2 2p$) or through higher order effects in the relation between Ω and the reactance matrix R , cf. paper I [6] or [17], Eqs. (2.25) and (2.28). Deviations between DWA and CCA of a few percent are even found for $E=70$ Ryd. This holds especially for transitions 1–14 and

2–15 where a monopole contribution from inside the ion is sensitive to the approximation.

At $E=9$ Ryd our results may be compared with those of Flower and Nussbaumer [5]. In general the agreement is very good. There are larger discrepancies for transitions 1–9 and 2–8. Level 8 and 9 are strongly mixed levels of $2s 2p^2 {}^2S_{1/2}$ and ${}^2P_{1/2}$. In the calculations of Dankwort and Trefftz [9] these levels showed an avoided crossing higher up in the isoelectronic series at $Z \approx 23$, V^{+18} . In a transition to one of these levels the R-matrix element is a linear combination of the 2S and 2P contribution. In any pair of transitions i–8, i–9 one transition is strengthened while the other is weakened by the mixture, i.e. in one of the transitions the signs of the 2S and 2P contributions are the same while in the other they are opposite to each other. In our case 1–9 and 2–8 are weakened while 2–9 and 1–8 are strengthened by the mixing effects. In the weakened cases the collision strength is essentially the square of a difference of two contributions and therefore sensitive to details of the target description.

At $E=9$ Ryd a few of the $2s^2 2p-2p^3$ transi-

Transition			Collision strength		Parameters			
<i>i</i>	<i>j</i>	type ⁺	calculated	fitted	<i>A</i>	<i>B</i>	<i>C</i>	α
1	2	q	0.0947	0.0949	0.2364	– 0.0379	– 0.0287	0.1166
1	3	ex	0.0109	0.0110	– 0.0072	0.0205	0.0026	0.0370
1	4	ex	0.0147	0.0148	– 0.0117	0.0300	0.0038	0.0370
1	5	ex	0.0092	0.0092	– 0.0070	0.0186	0.0023	0.0369
1	6	d	0.5714	0.5717	0.8580	– 0.4162	0.0370	0.0179
1	7	ex	0.0153	0.0153	– 0.0028	0.0237	0.0017	0.0338
1	8	d	0.4246	0.4249	0.6774	– 0.3417	0.0284	0.0155
1	9	d	0.3706	0.3708	0.6003	– 0.3066	0.0231	0.0158
1	10	d	0.2696	0.2698	0.4393	– 0.2240	0.0165	0.0153
1	11	ex	0.0005	0.0005	0.0	0.0007	0.0	0.0360
1	12	q	0.0042	0.0042	0.0063	– 0.0022	– 0.0005	0.0167
1	13	q	0.0027	0.0027	0.0024	0.0008	0.0001	0.0760
1	14	q	0.0028	0.0028	0.0012	0.0021	0.0003	0.0289
1	15	q	0.0020	0.0020	0.0036	– 0.0015	– 0.0006	0.0153
2	3	ex	0.0065	0.0065	– 0.0042	0.0120	0.0016	0.0371
2	4	ex	0.0184	0.0184	– 0.0139	0.0366	0.0047	0.0370
2	5	ex	0.0415	0.0417	– 0.0289	0.0802	0.0102	0.0368
2	6	d	0.0920	0.0920	0.2270	– 0.1413	0.0022	0.0020
2	7	d	0.9666	0.9669	1.4039	– 0.6327	0.0606	0.0167
2	8	d	0.1815	0.1816	0.2929	– 0.1423	0.0100	0.0126
2	9	d	0.5008	0.5010	0.7969	– 0.3874	0.0315	0.0137
2	10	d	1.5344	1.5352	2.4656	– 1.2301	0.0959	0.0149
2	11	ex	0.0009	0.0009	0.0	0.0013	0.0	0.0362
2	12	q	0.0035	0.0035	0.0051	– 0.0015	– 0.0004	0.0100
2	13	q	0.0087	0.0087	0.0127	– 0.0041	– 0.0009	0.0136
2	14	q	0.0027	0.0027	0.0046	– 0.0018	– 0.0007	0.0140
2	15	q	0.0089	0.0089	0.0072	0.0028	– 0.0001	0.0402

Table 4. Fitting parameters, Eq. (6), and comparison of calculated (CCA^b) and fitted collision strengths at electron energy $E=12.0$ Rydbergs.

⁺ type of collisional excitation:
q quadrupole,
ex exchange,
d dipole.

tions show large deviations between DWA and CCA. Closer inspection shows that the DWA results are affected by bound channel resonances of configuration $2p^3 3d$. The parent term of the highest of these is $2p^3 {}^2P$ which explains the large effect on 1–15 and 2–14. Using the smooth approximation (6), the “wiggling” structure of the original collision strengths near $E=9$ Ryd is seen in most transitions. In the CCA calculation the values are unaffected by the bound channel resonance. Probably the better approximation shifts the resonance towards its true position below the $2p^3 {}^2P$ threshold so that it is not seen at 9 Rydbergs.

Another group of bound channel resonances is described in paper I. It consists of configurations $2s^2 \overline{3d^2}$, $2s \ 2p \ \overline{3d^2}$, $2p^2 \ \overline{3d^2}$. For S^{+11} these bound channel resonances lie near 40 Ryd (between 36 and 47 Ryd). To determine the parameters of the smooth analytic fit (6) we therefore used CCA collision strengths calculated at $E \leq 30$ Ryd and at $E = 70$ Ryd in a least square fit. Table 4 gives the parameters. It also shows the quality of the fit at $E = 12$ Ryd. This energy corresponds to the temperature of maximum abundance of S^{+11} in the solar corona. Figure 1 shows a few examples of collision strengths as functions of energy, one of each type: dipole, quadrupole, and exchange collisional excitation. The calculated points are connected by straight lines since we did not determine the exact structure of the resonance. It is seen that the bound channel resonances have the largest effect on the transition 1–2 between the ground state levels. On the optically allowed transition 2–8 their effect is lowest. Correspondingly the effect of true resonances is important for transition 1–2 while for optically allowed transitions it may be neglected, cf. Saha and Trefftz [19].

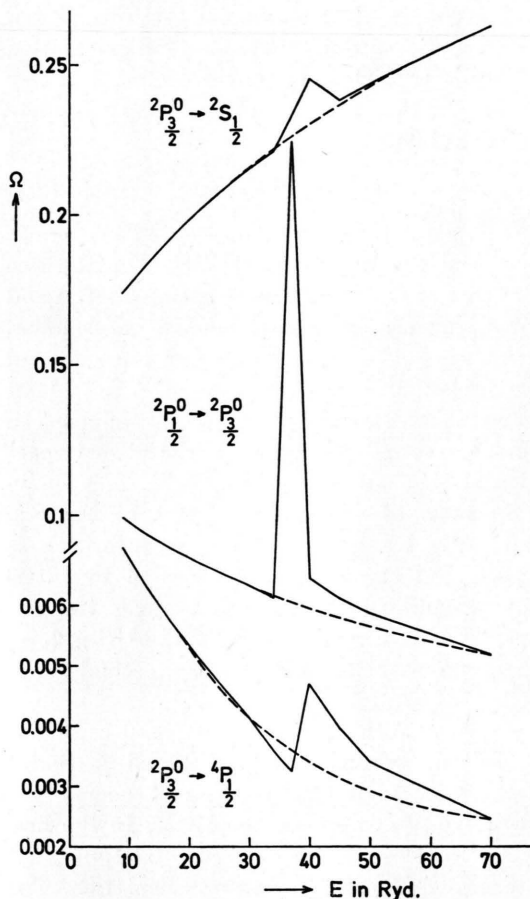


Fig. 1. Fine structure collision strengths for three transitions of different type: $2-8(2P_{3/2}^0-2S_{1/2})$ dipole excitation, $1-2(2P_{1/2}^0-2P_{3/2}^0)$ quadrupole excitation (upper scale), $2-3(2P_{3/2}^0-4P_{1/2})$ exchange excitation (lower scale).

For transitions between excited states collision strengths at $E=12$ Ryd are given in Table 5. Because of the low population of excited states in

Table 5. Collision strengths $\Omega(i, j)$ (CCA^b) for transitions between levels of excited states of S⁺¹¹ at $E = 12$ Ryd.

[illegible]

the solar corona electron impact transitions between these levels don't influence the population and may be neglected. If they are needed in any other context the authors will be happy to supply the full set of data.

5. Conclusions

Comparing the present results for S^{+11} with those for Si^{+9} we expect the difference between DWA and CCA collision strengths to have become smaller. This effect is not pronounced enough to be verified in the tables. The relative differences are about the same. More striking is the larger influence of intermediate coupling effects on the electron impact collision strengths in the case of S^{+11} . This shows most in ratio of collision strengths to the two ground state levels in which one transition is weakened and the other strengthened by intermediate coupling effects. Table 6 gives two examples. The first refers to the $2s\ 2p^2\ ^2S_{1/2}$ level which mixes with $2s\ 2p^2\ ^2P_{1/2}$, the second refers to $2s\ 2p^2\ ^2D_{3/2}$ mixing with $^2P_{3/2}$.

The ratios of the Ω 's are compared with the ratios of the corresponding weighted oscillator strengths. For high electron impact energy the ratios of the Ω 's approach the latter. In the first case, $2s^2\ 2p\ ^2P^0 - 2s\ 2p^2\ ^2S$, $\Omega(2, 8)/\Omega(1, 8)$ is almost energy independent in our calculation. The S^{+11} value of Flower and Nussbaumer [5] deviates somewhat. In the second case, $2s^2\ 2p\ ^2P^0 - 2s\ 2p^2\ ^2D_{3/2}$ Flower and Nussbaumer's and our

calculation agree very well. $\Omega(1, 6)/\Omega(2, 6)$ changes appreciably with energy. The low energy ratio is close to the non-relativistic value. It should be kept in mind that the same term coupling coefficients have been used in the intermediate coupling transformation of the reactance matrix R^{Jp} , Eq. (5), as in that of the radiative matrix elements for gf. Differences between the Ω — and gf — ratios are due to differences in the relative sizes of the coupled matrix elements and also to higher order effects in the calculation of Ω from R , cf. paper I.

For diagnostics of low density plasmas the most important cross section is that between the two state levels. The present calculations show that ground here a careful choice of target description and scattering approximation is necessary. On the other hand for optically allowed transitions intermediate coupling effects are most important. Reliable term coupling coefficients are needed. While Flower and Nussbaumer [5] improved these by a semiempirical correction to their simple target model we used a more elaborate target description. The difficulty introduced by the elaborate target description of unwanted bound channel resonances was circumvented by fitting a smooth analytic approximation to the collision strength values outside the resonance region. Since the ion S^{+11} is most abundant at temperatures $kT \approx 12$ Ryd, $T \approx 1.9 \cdot 10^6$ K, we extended the calculation of collision strength as compared to Flower and Nussbaumer's work to high energies to allow reliable determinations of electron collision rates.

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Table 6. Ratios of collision strengths from the two ground state levels to $2s2p^2\ ^2S_{1/2}$ and $^2D_{3/2}$ at 9 Ryd and ratios of weighted oscillator strengths for Si^{+9} and S^{+11} .

	Here:		Flower and Nussbaumer [5]	
	$\Omega(2, 8)$ $\Omega(1, 8)$	gf(2, 8) gf(1, 8)	$\Omega(2, 8)$ $\Omega(1, 8)$	gf(2, 8) gf(1, 8)
S^{+11}	0.43	0.40	0.70	0.46
Si^{+9}	0.81	0.78	0.87	0.83
non-relativistic	2		2	
	$\Omega(1, 6)$ $\Omega(2, 6)$	gf(1, 6) gf(2, 6)	$\Omega(1, 6)$ $\Omega(2, 6)$	gf(1, 6) gf(2, 6)
S^{+11}	5.99	8.24	5.68	8.24
Si^{+9}	5.19	6.80	5.14	6.75
non-relativistic	5		5	

- [1] E. M. Reeves, M. C. E. Huber, and J. G. Timothy, *Appl. Optics* **16**, 837 (1977), J. E. Vernazza and E. M. Reeves, *Astrophys. J. Suppl. S.* **37**, 485 (1978).
- [2] W. E. Behring, L. Cohen, U. Feldman, and G. A. Doschek, *Astrophys. J.* **203**, 521 (1976).
- [3] M. Malinovsky and L. Heroux, *Astrophys. J.* **181**, 1009 (1973).
- [4] S. O. Kastner and H. E. Mason, *Astron. Astrophys.* **67**, 119 (1978).
- [5] D. R. Flower and H. Nussbaumer, *Astron. Astrophys.* **45**, 349 (1975).
- [6] H. P. Saha and E. Trefftz, *J. Phys. B* **15**, 1089 (1982) (Paper I).
- [7] C. F. Fischer, Private Communication (1975).
- [8] C. F. Fischer, *Comp. Phys. Commun.* **14**, 145 (1978).
- [9] W. Dankwort and E. Trefftz, *Astron. Astrophys.* **65**, 93 (1978).
- [10] W. Eissner and H. Nussbaumer, *J. Phys. B* **2**, 1028 (1969).
- [11] M. J. Seaton, *J. Phys. B* **7**, 1817 (1974).
- [12] W. Eissner, M. Jones, and H. Nussbaumer, *Comp. Phys. Commun.* **8**, 270 (1974).
- [13] M. A. Cree, M. J. Seaton, and P. M. H. Wilson, *Comp. Phys. Commun.* **15**, 23 (1978).
- [14] H. E. Saraph, *Comp. Phys. Commun.* **3**, 256 (1972).
- [15] H. Saraph, *Comp. Phys. Commun.* **15**, 247 (1978).
- [16] B. Edlen, *Phys. Scripta* **23**, 1079 (1981).
- [17] W. Eissner and M. J. Seaton, *J. Phys. B* **5**, 2187 (1972).
- [18] A. Burgess and V. B. Sheorey, *J. Phys. B* **7**, 2403 (1974).
- [19] H. P. Saha and E. Trefftz, *Astron. Astrophys.*, submitted (1982).