COLLISION STRENGTHS FOR ELECTRON EXCITATION OF CORONAL IONS

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1. Method

Using general purpose computer programmes developed by Drs. Eissner and Nussbaumer at University College London for the solution of atomic structure and atomic collision problems, collision strengths have been obtained for transitions between terms of the ground and first few excited configurations of ions of interest in studies of the solar corona. The atomic structure programme is written in a configuration interaction representation and uses a scaled Thomas-Fermi potential as described by Eissner and Nussbaumer (1969). The bound state wave functions generated by the structure programme are used by the collision programme (Eissner, 1970) to calculate the *R*-matrix solution of the collision problem by means of the distorted wave approximation (Saraph *et al.*, 1969). This approximation should be valid for highly ionized ions such as exist in the corona and this prediction is fully confirmed where comparison can be made with calculations using the more rigorous but more time-consuming close coupling method (Burke *et al.*, 1966; Petrini, 1969).

2. Results

Tables of collision strengths are presented for transitions between terms of the following configurations of the following ions:

Nv, SixII: $1s^2 2s, 2p, 3s, 3p, 3d;$ FexIII: $3s^2 3p^2, 3s 3p^3, 3s^2 3p 3d;$ FexIV: $3s^2 3p, 3s 3p^2, 3s^2 3d;$ Fexv: $3s^2, 3s 3p, 3p^2, 3s 3d;$ FexvII: $2p^6, 2p^5 3s, 3p, 3d.$

The calculations are in L-S coupling but the resultant *R*-matrices may be transformed to intermediate coupling using coefficients obtained from a version of the atomic structure programme incorporating relativistic terms in the Hamiltonian (Jones, 1970). This transformation has, to date, been applied only to Fexv, configurations $3s^2$ and 3s 3p, with the results shown in Table VII.

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De Jager (ed.), Highlights of Astronomy, 512–517. All Rights Reserved Copyright C 1971 by the IAU

Nv			
	c	 d	-

Transition	$\Omega(i-j)$			
i–j	а	b	с	d
$k_1^2 = 2.25$				
2s ² S-2p ² P	8.05	8.64	8.01	
$k_1^2 = 6.0$				
$2s {}^{2}S - 2p {}^{2}P$	9.94	10.58	9.84	10.44
${}^{2}S - 3s {}^{2}S$	0.224	0.302		0.305
${}^{2}S - 3p {}^{2}P$	0.122	0.126	0.170	0.196
$^{2}S-3d$ ^{2}D	0.458	0.542		0.546
$2p ^{2}P - 3s ^{2}S$	0.144	0.108		
$^{2}P - 3p ^{2}P$	1.01	1.27		
$^{2}P-3d^{2}D$	3.42	4.54		

TABLE I Collision strenghts in Nv

a = DW (this paper)

b = CBI (Bely, 1966a, b; Bely and Petrini, 1970)

c = Strong coupling with exchange (Burke *et al.*, 1966)

d = Five-state close coupling without exchange (Burke et al., 1966)

TABLE II

Collision strengths in SixII

Transition	Ω(<i>i–j</i>)	
i–j	a	b
$k_1^2 = 5.0$		
$2s {}^{2}S - 2p {}^{2}P$	1.79	
$k_{1^2} = 22.4$		
$2s {}^{2}S - 2p {}^{2}P$	2.29	
${}^{2}S - 3s {}^{2}S$	0.0485	0.0620
${}^{2}S-3p {}^{2}P$	0.0336	0.0353
$^{2}S-3d$ ^{2}D	0.0984	0.124
2p ² P-3s ² S	0.0152	0.0089
² P-3p ² P	0.209	0.227
$^{2}P-3d$ ^{2}D	0.642	0.766
$k_{1^2} = 30.0$		
2s ² S-2p ² P	2.44	
² S-3s ² S	0.0534	0.0630
${}^{2}S-3p {}^{2}P$	0.0424	0.0482
$^{2}S-3d$ ^{2}D	0.106	0.131
2p ² P-3s ² S	0.0145	0.0110
² P -3p ² P	0.213	0.230
$^{2}P-3d$ ^{2}D	0.729	0.866

a = DW (this paper)

b = CBI (Bely, 1966a, b; Bely and Petrini, 1970)

3. Notes on the Tables

The notation used is as follows:

- DW distorted wave approximation
- CBI Coulomb-Born I approximation
- Ω collision strength:

 $\Omega(i, j) = k_i^2 \omega_i Q(i, j)$ where k_i^2 is numerically equal to the energy of the incident electron, in Rydbergs, relative to state i; $\omega_i = (2S_i + 1)(2L_i + 1)$ is the statistical weight of state *i*, and Q(i, j) is the cross-section for the $i \rightarrow j$ transition in units of πa_0^2 .

Table I: $k_1^2 = 2.25$ is above the calculated $1s^2 2s^2 S - 2p^2 P$ threshold (0.732 Ry) but below the $1s^2 2s^2 S - 3s^2 S$ threshold (4.144 Ry) and the calculations at this energy therefore included only the $1s^2 2s$ and $1s^2 2p$ configurations; $k_1^2 = 6.0$, on the other hand, is above the $1s^2 2s^2 S - 3d^2 D$ threshold (4.396 Ry) and all five configurations were included in these calculations. The tabulated results of Bely (1966a, b) and Bely and Petrini (1970) were obtained by interpolation of the values actually given by these authors to the same value of $x(x=k_i^2/\Delta E_{ij})$, the ratio of incident and transition energies for the i-j transition.)

Transition		$\Omega(i-j)$	Transition		$\Omega(i-j)$	
<i>i–j</i>		a	i-j		a	
		$k_{1^2} = 5.1$			$k_1^2 = 5.1$	
$3s^2 3p^2 {}^3P - 3s^2 3p^2$	1 D	0.134	1 <i>D</i> -	1 <i>P</i>	2.73	
³ P-	^{1}S	0.014	¹ D-	³ S	0.0006	
³ P-3s 3p ³	⁵ S	0.060	$^{1}D-3s^{2}$ 3p 3	∂d ³F	0.180	
³ P-	зD	2.82	¹ D	³ P	0.061	
³ P-	³ P	2.53	${}^{1}D$ –	^{1}D	6.85	
³ P	¹ D	0.095	¹ <i>D</i> -	³ D	0.0 76	
³ P-	1 P	0.034	¹ <i>D</i> -	${}^{1}F$	6.45	
³ Р_	³ S	6.36	1 D -	1 P	0.154	
⁸ P-3s ² 3p 3d	^{3}F	0.255				
³ P-	3Р	6.10	$^{1}S-3s \ 3p^{3}$	³ D	0.0009	
³ P-	1 D	0.032	1 <i>S</i> -	3Р	0.039	
³ P	3 D	15.82	1 <i>S</i> _	${}^{1}D$	0.003	
³ P-	${}^{1}F$	0.076	1 <i>S</i> _	1 P	0.712	
³ P-	1 P	0.020	$^{1}S-3s^{2}$ 3p 3	$d^{3}F$	0.029	
			1 <u>S</u> _	³ Р	0.016	
$^{1}D - 3s^{2} \ 3p^{2}$	1 <i>S</i>	0.358	1 <i>S</i> _	1 D	0.009	
$^{1}D - 3s \ 3p^{3}$	³ D	0.116	¹ S_	³ D	0.009	
¹ D	3Р	0.030	1 <u>S</u> _	${}^{1}F$	0.023	
¹ <i>D</i> -	¹ D	2.20	¹ <i>S</i> -	1 P	2.90	

TABLE III

 $\mathbf{a} = \mathbf{D}\mathbf{W}$ (this paper)

Table II: similarly, for SixII, the results at $k_1^2 = 5.0$ are from a two configuration $(1s^2 2s \text{ and } 1s^2 2p)$ calculation. The calculated $1s^2 2s^2 S - 2p^2 P$ threshold is at 1.735 Ry and the $1s^2 2s^2 S - 3d^2 D$ threshold at 22.343 Ry. The results of Bely (1966a, b) and Bely and Petrini (1970) were obtained by double interpolation – to the same values of x and to the same member of the isoelectronic sequence.

Table III: the calculated $3s^2 3p^2 {}^3P - 3s^2 3p 3d {}^1P$ threshold is 5.069 Ry.

Table IV: $k_1^2 = 4.309$ corresponds to the $3s^2 3p {}^2P - 3s^2 3d {}^2D$ threshold in Petrini's calculations; the calculated threshold in the present work is 4.150 Ry.

Table V: $k_1^2 = 3.1$ is just above the calculated $3s^2 {}^1S - 3s {}^3p {}^1P$ threshold (3.073 Ry) and the calculations at this energy include only the $3s^2$ and $3s {}^3p$ configurations.

The $3s^2 {}^1S$ - $3s {}^3d {}^1D$ threshold is 6.837 Ry and the calculations at $k_1^2 = 6.9$ therefore include all four configurations. Results of Bely and Blaha (1968) obtained by interpolation to the same values of x.

Table VI: the calculated $2p^{6} {}^{1}S - 2p^{5} {}^{3}d {}^{1}P$ threshold is 60.220 Ry. Note that $10^{2} \Omega$ is tabulated for this ion.

Table VII: a two configuration $(3s^2, 3s 3p)$ calculation. Results of Bely and Blaha (1968) are at threshold.

Collision strengths in Fexiv				
Transition	Ω(<i>i</i> -j)			
i-j	a	b	b	
	$k_1^2 = 4.309$	$k_{1^2} = 4.2$	$k_{1^2} = 6.0$	
3s ² 3p ² P-3s 3p ² ⁴ P		0.092	0.085	
$^{2}P_{-}$ ^{2}D	1.81	2.43	2.41	
${}^{2}P_{-}$ ${}^{2}S$	1.19	1.17	1.20	
² P- ² P	10.40	9.85	10.14	
${}^{2}P-3s^{2} 3d {}^{2}D$	9.06	8.19	8.43	
3s 3p ² 4P-3s 3p ² ² D		0.169	0.152	
$^{4}P_{-}$ ^{2}S		0.019	0.017	
4 <i>P</i> _ 2 <i>P</i>		0.028	0.025	
${}^{4}P-3s^{2} \; 3d \; {}^{2}D$		0.023	0.020	
${}^{2}D-3s \; 3p^{2} \; {}^{2}S$	0.860	0.670	0.661	
$^{2}D ^{2}P$		0.096	0.086	
$^{2}D-3s^{2}$ 3d ^{2}D		0.125	0.113	
² S-3s 3p ² ² P		0.017	0.015	
${}^{2}S - 3s^{2} 3d {}^{2}D$	0.180	0.084	0.083	
$^{2}P ^{2}D$		0.039	0.036	

TABLE IV

a = close coupling without exchange (Petrini, 1969)

b = DW (this paper)

TABLE V Collision strengths in Fexv				
<i>i–j</i>	a	b		
$k_1^2 = 3.1$				
3s ² 1S-3s 3p ³ P	0.0332	0.0314		
$^{1}S_{-}$ ^{1}P	3.33	3.37		
$3s \ 3p \ ^3P - \ ^1P$	0.0523			
$k_{1}^{2} = 6.9$				
3s ^{2 1} S-3s 3p ³ P	0.0332	0.0269		
${}^{1}S_{-} - {}^{1}P$	2.67	3.62		
${}^{1}S - 3p^{2} {}^{1}D$	0.106			
¹ <i>S</i> → ³ <i>P</i>	0.0003			
¹ S- ¹ S	0.0031			
¹ S–3s 3d ³ D	0.0465			
$^{1}S ^{1}D$	0.187	0.312		

a = DW (this paper)

b = CBI and Coulomb-exchange approximations (Bely and Blaha, 1968)

TABLE VI

Collision strengths in Fexvii

Transition		$10^2 imes \Omega(i-j)$	
i–j		a	
		$k_1^2 = 61.0$	
$2p^{6} {}^{1}S - 2p^{5} 3s$	³ P	0.346	
¹ S-	^{1}P	0.307	
${}^{1}S-2p^{5} 3p$, ³ S	0.471	
1 <i>S</i>	³ D	1.16	
1 <i>S</i> _	¹ D	0.512	
1 <i>S</i> _	3P	0.467	
1 <i>S</i> _	${}^{1}P$	0.160	
1 <i>S</i> _	1 <i>S</i>	5.19	
$^{1}S-2p^{5} 3c$	l³P	2.07	
1 <i>S</i> _	${}^{3}F$	1.98	
1 <i>S</i> _	${}^{1}F$	0.409	
1 <i>S</i> _	3 D	0.842	
¹ S	^{1}D	0.285	
1 <i>S</i> _	1 P	10.42	

a = DW (this paper)

TABLE VII

Collision strengths for fine structure transitions in Fexv

Transition <i>i–j</i>		$\Omega(i-j)$		
		a	b	
		$k_{1^2} = 3.1$		
$3s^{2} {}^{1}S_{0} - 3s {}^{3}p$	${}^{3}P_{0}$	0.0037	0.004	
${}^{1}S_{0-}$	³ P ₁	0.0265	0.045	
${}^{1}S_{0-}$	${}^{3}P_{2}$	0.0185	0.018	
${}^{1}S_{0}-$	¹ P ₁	3.32	3.37	
3s 3p ³ P ₀ -	³ P ₁	0.0328		
³ P ₀ -	${}^{3}P_{2}$	0.105		
³ P ₀ -	${}^{1}P_{1}$	0.0062		
${}^{3}P_{1}-$	${}^{3}P_{2}$	0.277		
³ P ₁	${}^{1}P_{1}$	0.0211		
${}^{3}P_{2}$ -	¹ P ₁	0.0296		

a = DW (this paper)

b = CBI and Coulomb-exchange approximations (Bely and Blaha, 1968)

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DISCUSSION

R. H. Garstang: I wish to draw attention to an important feature in Table I. The transition $2p^2P$ - $3p^2P$ is forbidden for electric dipole radiation, but it has a relatively large cross-section. The transition $2p^2P$ - $3s^2S$ is allowed for electric dipole radiation, but its cross-section is much smaller than that for the 2p-3p transition. A similar situation was found earlier in FexvII in work by Bely. One must, therefore, be exceptionally careful when making rough estimates of the cross-sections from their approximate proportionality to the *f*-values.

E. Trefftz: Concerning the same subject of quadrupole transitions, I noticed that in Table IV you do not include the transition $3s^2 3p-3s 3p 3d$.

D. R. Flower: The Eissner and Nussbaumer atomic structure programme was used to calculate energy levels for the $3s^2 3p$, $3s 3p^2$, $3s^2 3d$ and 3s 3p 3d configurations. The energy of the lowest term of the 3s 3p 3d configuration ($3s 3p 3d ^4F^0$) was found to be more than 1 Ry greater than the energy of the highest term of the other three configurations ($3s^2 3d ^2D$). Consequently, the mixing between the $3s 3p 3d ^2P^0$ and $3s^2 3p ^2P^0$ terms was small and it was realized that the results given in Table IV would not be significantly changed by inclusion of the 3s 3p 3d configuration. Therefore, in order to economize on storage when using the atomic collision programe, the 3s 3p 3d configuration was not included in the calculations.

R. H. Garstang: There are other cases where quadrupole transitions are important, for example, $3s^2-3s$ 3d in Fexv.