

A distorted-wave methodology for electron-ion impact excitation: calculation for two-electron ions

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Abstract. A distorted-wave program is being developed for calculating the excitation of few-electron ions by electron impact. It utilises the exchange approximation to represent the exact initial-state wavefunction in the T -matrix expression for the excitation amplitude. The program has been implemented for excitation of the $2^{1,3}(S,P)$ states of two-electron ions. Comparison is made with other results where available. The first part of the paper discusses some of the astrophysical applications of these cross sections as well as the motivation and requirements of the calculational methodology.

1. Introduction[†]

Among many applications, the interpretation of x-ray and EUV emissions in the solar corona requires the knowledge of electron-ion impact excitation cross sections. Figure 1 is an example of an x-ray spectrum, taken by the Goddard group (Neupert 1971) from OSO-5, in which the lines of two-electron iron (Fe xxv) figure prominently. Such ions can be produced in flare-excited plasmas ($T_e \simeq (10-40) \times 10^6$ K) and the object of the astrophysical studies is to determine the temperature and densities (as a function of time and space) of the various species from the spectral observations. The analysis is usually done in terms of an energy-averaged rate coefficient (in $\text{cm}^3 \text{s}^{-1}$)

$$C_{ni}(T) = \int f_T(v) v \sigma_{ni}(v) dv \quad (1.1)$$

where for the disturbed coronal problem $f_T(v)$ can be taken as a Maxwellian electron velocity distribution function of temperature T , and $\sigma_{ni}(v)$ is the excitation cross section (from state i to state n) whose decay emission is what is observed.

The calculation of σ_{ni} is the problem of concern here. It is not trivial, for, in spite of the high energy of the exciting electrons, the mean energy of the distribution $f_T(v)$ at the prevailing temperature T may well be comparable to, or even below, the excitation threshold of the ions, particularly if those ions are ionised sufficiently highly. This has the following effect: since only electrons in the high-energy tail of the distribution can be responsible for the excitation, and since the number of

[†] The material of the introduction follows Temkin (1974). Some of these points have also been made by Seaton (1975a) and Gabriel and Jordan (1972).

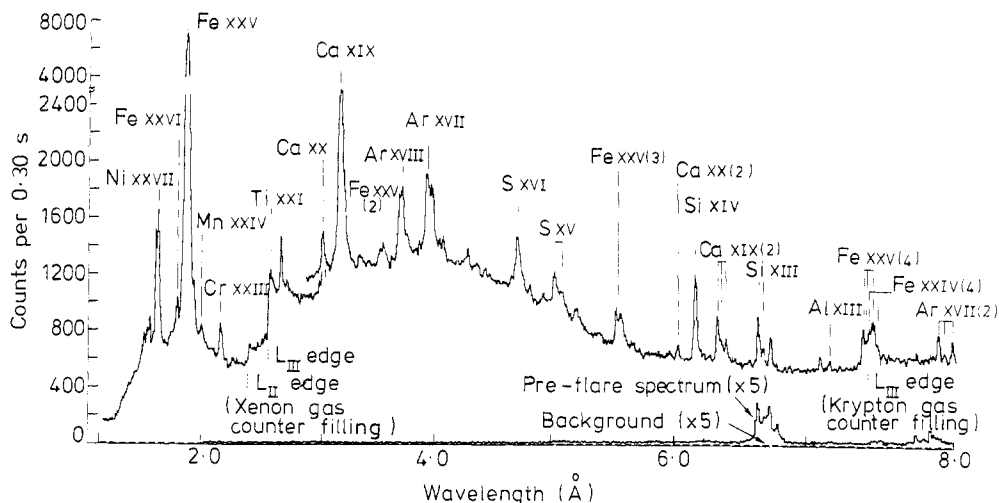


Figure 1. Solar flare spectrum obtained by crystal spectrometers on OSO-5 (Neupert 1971).

such electrons decreases exponentially with energy, there will only be a sufficient number of electrons in a narrow energy band (starting at the threshold and extending to slightly above the requisite energy threshold) that will effectively cause excitation. This is equivalent to saying that only those impacting electrons whose velocities are close to the velocity of the orbital electrons will be responsible for the excitation. This in turn is tantamount to the requirement, quantum-mechanically speaking, that low-energy methods of calculation are required! This conclusion, then, is quite contrary to what one might at first think, given the energies of the exciting electrons under conventional circumstances. It means, in particular, that Born, Born-Oppenheimer and other Born-like methods of calculation will not suffice the needs of reliability for the required cross sections.

What, then, are the essential items of low-energy methods which will be relevant here? The first is a *partial-wave expansion of the scattered amplitude*. Those methods which attempt to calculate the whole scattered amplitude at once are generally not reliable below impacting energies of several times the threshold energy. Although great advances over the Born approximation have been made in methods which calculate the whole scattered amplitude, the two major ones being the Glauber approximation (cf Gerjuoy and Thomas 1974) and eikonal-Born series approximation (Byron and Joachain 1973), none of these methods reliably surmounts the low-energy problem. It is true that these methods do lower the energy to which the approximations give good results and, furthermore for charged targets (i.e. ions), Coulomb-Born methods in electron-ion scattering are assuredly better to lower energies than plane-wave Born methods for neutral targets. Nevertheless within, say, three times the threshold energy we believe one cannot have uniform confidence in such results.

The second item that we know is important in calculating 'low-energy' scattering is the consistent incorporation of exchange—the identity of incoming and orbital electrons (Morse and Allis 1933). Here one derives a major advantage from a partial-wave expansion, for if one starts with a definite ansatz for the total function describing any specific partial wave, then one can include exchange consistently by antisymmetrising that ansatz to derive that appropriate dynamical equation. Furthermore, the

resulting integro-differential equations pose no particular problem for present-day machine calculation.

There is one simplification deriving from highly charged targets that does not hold for scattering from a neutral atom and that is the fact that induced polarisation (Temkin 1957) can confidently be expected to be small. Similarly, for the accuracy with which we are concerned here, the excess of nuclear charge over the number of orbital electrons should allow the use of a simplified form (i.e. Hartree-Fock in most cases) of the target-state wavefunctions without serious error.

Counterbalancing these advantages, there is the one giant problem, not yet generally solved, of the effect of resonances of the compound (electron-plus-ion) system. The effect of such resonances can completely dominate the 'low-energy' scattering. We shall have more to say about that later, but with this hiatus aside we are here initiating a program which is intended modestly to meet the essential requirements stated above. Specifically, we use the exchange approximation to describe, in partial-wave form, the scattering from the initial state. This automatically includes the requirement of exchange but no polarisation. For two-electron ions, which is the subject of the present calculations, we use a *modification* of the bound-state wavefunction of Morse *et al* (1935) (to be referred to as MYH), which we believe are then suitably accurate for the distorted-wave part of the calculation. (Distorted wave means we substitute the exchange-approximate wavefunction into the excitation matrix element whose final state is the appropriate unperturbed (Coulomb-Born) wavefunction describing the final state.)

The word 'modestly' used above is invoked with deliberate purpose. A very elaborate distorted-wave program has been developed at University College, London (UCL) over many years, involving many people (see e.g. Saraph *et al* 1969, Eissner and Seaton 1972, Eissner 1972). A useful review of this as part of the general problem of electron impact excitation of positive ions has recently been given by Seaton (1975a). The UCL distorted-wave program is itself part of a larger package which includes close-coupling plus correlation and quantum-defect parts (Seaton 1975a). A copy of the distorted-wave UCL program has been acquired here at Goddard and is being used by one of us (AKB) for cases of interest to Goddard.

The essence of the UCL program is that, following Mott and Massey (1965), it calculates distorted waves for both the initial and final states. This has the nice formal advantage that it renders the error in the amplitude of the order

$$\delta f_{ni}^{(UC)} = \langle \delta \Psi^- | H - E | \delta \Psi^+ \rangle. \quad (1.2)$$

This is formally bilinear (i.e. quadratic) and, other things being equal, would appear to be smaller than our own error (see §2)

$$\delta f_{ni}^{(BT)} = \langle \psi | \tilde{V} | \delta \Psi^+ \rangle \quad (1.3)$$

which is formally of first order. However, this comparison can be misleading. For example, if one is contemplating using the exchange approximation (as we are) for the distorted waves, then the absence of induced polarisation for scattering from the initial state (assumed to be the ground state) is truly justified. However, not including polarisation for scattering from the final state, whose polarisability can be orders of magnitude larger than the ground state and thus not negligible even for more highly charged ions, constitutes a much more uncertain degree of approximation. Furthermore, and most important, treating the scattering from an excited state as a one-channel problem is quantitatively a much less justifiable approximation

than doing the same for ground-state scattering. This latter, then, is the chief uncertainty of the UCL program[†] (since their one-channel code goes beyond the simple exchange approximation). Another limitation of their code derives from its use of Thomas–Fermi orbitals. This implies the charge Z of the ionic nucleus is such that $Z > \mu N$ with $\mu \gtrsim 1.5$, where N is the number of orbital electrons. (A stronger condition $\mu \gtrsim 3$ has been proposed (Parks and Sampson 1976) which seems overly restrictive.) Since, however, we would like to include cases in which both Z and N are small (but always $Z > N$) while at the same time testing the appropriateness of the exchange approximation for distorted waves, we shall in this paper be reporting on our own completely separate distorted-wave program.

Our results here are strictly confined to two-electron ion excitations from the ground to $2^{1,3}(S,P)$ states. Part of the motivation is to develop a program with very few options, so that it will be subject to as little likelihood of error in being run as possible. In so doing, we realise that we shall achieve less than optimum accuracy, but we believe that as long as the astrophysical and other needs require not optimum accuracy but rather uniform error limits plus simplicity, and speed of operation, then a program such as that initiated here will be worthwhile.

2. Application to two-electron ions

2.1. Formal aspects

The differential and total cross section from a state i to a state n can be written

$$\frac{d\sigma}{d\Omega} = \frac{k_n}{k_i} |f_{ni}|^2 \quad \sigma = \frac{k_n}{k_i} \int |f_{ni}|^2 d\Omega \quad (2.1)$$

where f_{ni} is a matrix element given by

$$f_{ni} = -(1/4\pi) \langle \psi_n | \hat{V}(1; 2, 3) | \Psi_i^+ \rangle. \quad (2.2)$$

The expression is exact if Ψ_i^+ is a solution of the three-particle Schrödinger equation

$$\left(T_i + \sum_{\text{cyclic } i,j,k} V(1; 2, 3) \right) \Psi_i^+ = E \Psi_i^+ \quad (2.3)$$

corresponding to outgoing radial wave solutions with the ion in initial state i with

$$V(1; 2, 3) = -\frac{2Z}{r_1} + \frac{2}{r_{12}} + \frac{2}{r_{13}}. \quad (2.4a)$$

Here ψ_n is an (unsymmetrised) final-state wavefunction which we choose to be the product of a Coulomb wave seeing the shielded charge of the ion multiplied by the

[†] This argument assumes a level structure, as occurs for two-electron targets, such that the excited-state energies are close to the ionisation energy, $\Delta E/I \lesssim 1$. If the level structure is such that $\Delta E/I \ll 1$, then the argument does not apply. A prime example of the latter is the excitation to states of the ground configuration of atoms (and ions) which have such structure. The Goddard group (Pindzola *et al* 1977) has used the Mott and Massey (1965) form of the distorted wave to calculate $^3P \rightarrow ^1D$ excitation in C and Si; for comparable ions the UCL program is similarly well suited.

final-state wavefunction of the ion. This means that the residual potential $\tilde{V}(1; 2, 3)$ in equation (2.2) is given by

$$\tilde{V} = V - \left(-\frac{2(Z-2)}{r_1} \right) = -\frac{4}{r_1} + \frac{2}{r_{12}} + \frac{2}{r_{13}}. \quad (2.4b)$$

(We use rydberg units throughout.)

In practice Ψ_i^+ is always approximate and the essence of the distorted-wave method, as we shall use it, is similar to that of McDowell *et al* (1973) in that *only the initial wavefunction is distorted*. (The latter, however, have concentrated on excitation of neutral and once-ionised systems where they have had to include induced polarisation in the context of the polarised-orbital method (Temkin 1957).) Not needing polarisation means that Ψ_i^+ can be approximated by the (one-channel) exchange approximation:

$$\Psi_i^+ = \sum_{\mathcal{L}} \sum_{l_i} [U_{l_i}(r_1) \phi_{L_i S_i}(r_2, r_3) y(l_i L_i, \mathcal{L}) x(\frac{1}{2} s_i, \mathcal{S}) + (2; 31) + (3; 12)]. \quad (2.5)$$

Here $\phi_{L_i S_i}$ is the eigenfunction of the target system in its initial state; y and x are appropriate angular and spin vector coupled combinations to form total \mathcal{L} and \mathcal{S} . In practice we shall confine ourselves to the initial state being the ground state ($^1S \Rightarrow L_i = S_i = 0$), so that $\mathcal{S} = \frac{1}{2}$ and $\mathcal{L} = l_i$ is the partial-wave index. The cyclic permutations $(2; 31) + (3; 12)$ in equation (2.5) give a totally antisymmetric function Ψ_i^+ assuming the target state is antisymmetric in its spin-space indices. Specifically this means for 1S states that $\phi_{0,0}(r_2, r_3)$ is symmetric with respect to $r_2 \leftrightarrow r_3$.

The radial functions U_l in (2.5) are further written as

$$U_l(r) = [4\pi(2l+1)]^{1/2} i^l \exp[i(\delta_l + \eta_l(k_i))] u_l(r)/k_i r \quad (2.6)$$

where the $u_l(r)$ are solutions of the appropriate radial equations (cf equation (2.17)) with asymptotic form

$$\lim_{r \rightarrow \infty} U_l(r) = \sin[k_i r - \frac{1}{2} l \pi + (z_e/k_i) \ln(2k_i r) + \eta_l(k_i) + \delta_l] \quad (2.7)$$

in which $\eta_l(k)$ is the Coulomb phase

$$\eta_l(k) = \arg \Gamma(l+1 - iz_e/k) \quad (2.8)$$

and δ_l is the residual phaseshift. In (2.7) and (2.8) z_e is the shielded charge, i.e. the nuclear charge minus the number of orbital electrons,

$$z_e = Z - 2. \quad (2.9)$$

The final state ψ_n is an unsymmetrised Coulomb wave multiplied by the excited target state

$$\psi_n = \mathcal{F}_{k_n}(r_1) \phi_{L_n S_n}(r_2, r_3) x(\frac{1}{2} s_n, \mathcal{S}) \quad (2.10)$$

where $\mathcal{F}_k(r)$ is a pure continuum Coulomb function† of energy k_n^2 which is given by

† It is perhaps worthwhile to reiterate that the phase factor $-i\eta_l(k)$ in equation (2.11a) is the appropriate phase factor when ψ_n is a (radially) ingoing Coulomb wave which it must be if Ψ_i^+ is taken to be a solution with radially outgoing scattered waves. Explicitly this means

$$i\eta_l = i \tan^{-1} \{ \text{Im}[\Gamma(l+1 - iz_e/k)] / \{ \text{Re}[\Gamma(l+1 - iz_e/k)] \} \}$$

where $-\pi/2 \leq \tan^{-1} x \leq \pi/2$. Note that in the matrix element the complex conjugate of ψ_n is what occurs (Pratt *et al* 1973; cf, in particular, p 290).

the expression

$$\mathcal{F}_{k_n}(r) = \frac{1}{k_n r} \sum_l [4\pi(2l+1)]^{1/2} i^l e^{-i\eta_l(k_n)} F_l(k_n r) Y_{10}(\Omega) \quad (2.11a)$$

and

$$F_l(kr) = C_l(z_e/k) (kr)^{l+1} e^{-ikr} F(l+1+i z_e/k, 2l+2, 2ikr) \quad (2.11b)$$

with asymptotic form (Abramowitz and Stegun 1964)

$$\lim_{r \rightarrow \infty} F_l(kr) = \sin[kr - \frac{1}{2}l\pi + (z_e/k)\ln(2kr) + \eta_l(k)]. \quad (2.12)$$

The transition matrix, equation (2.2) depends on θ where

$$\cos \theta = \hat{k}_i \cdot \hat{k}_n. \quad (2.13)$$

For final states ψ_n , we are contemplating excitation of all non-relativistically allowable states (i.e. $S_n = 1$ as well as 0, and $L_n \geq 0$).

Conservation of energy also requires the usual relation between the initial and final momenta

$$k_i^2 + \epsilon_i = k_n^2 + \epsilon_n = E \quad (2.14)$$

in which ϵ_i (here $\epsilon_i = \epsilon_0 =$ ground-state energy) and ϵ_n are the energies of the initial and final states.

The bound wavefunctions that we use in this two-electron target application are of the Morse *et al* (1935) form. The spatial part of the ground state is given by

$$\phi_i(r_2, r_3) = \phi_{00} = N e^{-\xi(r_2+r_3)} \quad (2.14a)$$

(i.e. the ground state is of closed-shell form, ξ is given in equation (2.18)) and the excited S states ($L_n = 0$) are given by

$$\phi_n(r_2, r_3) = A[e^{-a_n r_2}(e^{-b_n r_3} r_3 - B e^{-c_n r_3}) \pm (2 \leftrightarrow 3)] \quad (2.14b)$$

with the upper and lower signs for singlet and triplet ($S_n = 0, 1$) respectively. For P states we have

$$\phi_n(r_2, r_3) = A[e^{-a_n r_2} r_3 e^{-b_n r_3} Y_{1m}(\Omega_3) \pm (2 \leftrightarrow 3)]. \quad (2.14c)$$

However, it is to be noted that in MYH the method of determining the parameters is such that the 1S excited-state wavefunctions are *not* orthogonal to the ground state (2.14a). This, it turns out, can have large effects on the distorted-wave cross sections. Therefore, instead of determining the coefficients in (2.14b) using the procedure of MYH, we use the condition that the (2s) part of ϕ_n be orthogonal to the (1s) part of ϕ_i :

$$\int_0^\infty e^{-\xi r} (e^{-b_n r} r - B e^{-c_n r}) r^2 dr = 0. \quad (2.14d)$$

This guarantees the orthogonality of the wavefunction as a whole. In table 1 we give parameters and resultant energies that we have determined from (2.14d) (although all non- 1S wavefunctions are orthogonal in MYH, the use of (2.14d) will give slightly different parameters and therefore slightly different energies from MYH). It should be mentioned that this simple idea of modifying the MYH functions to be orthogonal to the ground state was used long ago by Marriott and Seaton (1957).

Table 1. Parameters of target state (equations (2.14b,c))†.

Z	State	a	b	c	B	E(Ryd)
3	³ S	3.0	1.14	2.07	1.5052	-10.216
	¹ S	3.0	0.90	2.07	1.9502	-10.072
4	³ S	4.0	1.65	2.66	0.9453	-18.587
	¹ S	4.0	1.40	2.67	1.1507	-18.359
5	³ S	5.0	2.15	3.26	0.6890	-29.460
	¹ S	5.0	1.88	3.34	0.8342	-29.144
6	³ S	6.0	2.65	3.85	0.5386	-42.834
	¹ S	6.0	2.38	3.94	0.6320	-42.430
7	³ S	7.0	3.15	4.43	0.4402	-58.707
	¹ S	7.0	2.88	4.52	0.5040	-58.216
8	³ S	8.0	3.65	5.00	0.3708	-77.081
	¹ S	8.0	3.38	5.10	0.4181	-76.502
9	³ S	9.0	4.05	6.05	0.3648	-97.958
	¹ S	9.0	4.05	4.62	0.2686	-97.286
10	³ S	10.0	4.55	6.63	0.3172	-121.332
	¹ S	10.0	4.55	5.16	0.2390	-120.572
14	³ S	14.057	6.253	10.192	0.2584	-239.816
	¹ S	14.184	6.09	9.783	0.2535	-238.644
	³ P	13.96	6.63			-238.814
	¹ P	14.01	6.56			-238.006
20	³ S	20.112	8.99	14.688	0.1802	-492.523
	¹ S	20.237	8.89	14.09	0.1733	-490.806
	³ P	19.96	9.63			-491.104
	¹ P	20.01	8.79			-489.451
26	³ S	26.109	12.533	10.564	0.0670	-835.290
	¹ S	26.186	12.49	11.195	0.0709	-833.086
	³ P	25.96	12.6			-833.394
	¹ P	26.0	12.4			-831.78

† For $Z \leq 10$ the P-wave parameters are those of Morse *et al* (1935).

The scattered partial waves u_l of the initial-state wavefunction are derived from the variational principle

$$\delta \left(\int \Psi_l^* (H - E) \Psi_l d\tau - k \tan(\eta_l + \delta_l) \right) = 0 \quad (2.15)$$

where Ψ_l is the l th component of Ψ^+ , from equation (2.5) (recall $\mathcal{L} = l$ for these applications). If the ground state were exact, (2.15) would reduce down to

$$\int \phi_i(r_2, r_3) Y_{10}(\Omega_i) x_{1/2}^*(1) x_0^*(2, 3) (H - E) \Psi_l dr_1^{-1} = 0. \quad (2.16)$$

Since this is not exactly true, (2.15) and (2.16) are not rigorously equivalent; our radial equations are actually determined from (2.16) (dr_1^{-1} means integration over all coordinates except r_1). The spin inner products are trivial in the process of carrying

out (2.16), and after straightforward spatial integrations one is left with the integro-differential equation for u_l

$$\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + 2 \frac{z_e}{r} + 4 \left(\xi + \frac{1}{r} \right) e^{-2\xi r} + k_i^2 \right] u_l + rT_4 = 0. \quad (2.17)$$

Equation (2.17) may be found in Bhatia *et al* (1975), equation (2.10a), where the polarisation (α , T_5 , T_6) terms there are here set equal to zero. T_4 is given in equation (A.1) and the constant ξ in equation (2.9b), both of Bhatia *et al* (1975). Repeating the latter, we have

$$\xi = Z - \frac{5}{16}. \quad (2.18)$$

With the details of the wavefunctions Ψ_i^+ and ψ_n now having been specified, we return to the evaluation of the excitation amplitude f_{ni} of equation (2.2). Again carrying out spin inner products, one can express the amplitude as a sum of two basic spatial integrals

$$f_{ni} = f_{ni}^{(d)} + f_{ni}^{(ex)} \quad (2.19)$$

where

$$f_{ni}^{(d)} = -\frac{1}{4\pi} \int \psi_n^*(1; 2, 3) \tilde{V}(1; 2, 3) \Psi_i(1; 2, 3) d\tau \quad (2.20)$$

and

$$f_{ni}^{(ex)} = +\frac{1}{4\pi} \int \psi_n^*(1; 2, 3) \tilde{V}(1; 2, 3) \Psi_i^{(ex)}(1; 2, 3) d\tau. \quad (2.21)$$

In equation (2.20) $\Psi_i(1; 2, 3)$ is the first term of Ψ_i^+ of equation (2.5); i.e.

$$\Psi_i(1; 2, 3) = \sum_{l_i} U_{l_i}(r_1) \phi_{L_i S_i}(r_2, r_3) Y_{10}(\Omega_1) x_{1/2}(1) x_0(2, 3) \quad (2.22)$$

where we have specialised to scattering from the ground state ($L_i = S_i = 0$). The exchange term, which derives from the second two terms of (2.5), is obtained from (2.22) by a cyclic permutation

$$\Psi_i^{(ex)}(1; 2, 3) = \Psi_i(2; 3, 1). \quad (2.23)$$

2.2. Results

In tables 2, 3 and 4 we give total (i.e. integrated) cross sections for various two-electron ions. Some of these cases are directly of astrophysical interest (cf figure 1). Both Coulomb-Born and distorted-wave results are presented. Here comparison is made with the Coulomb-Born results of Tully (1974) which differ from ours only in the target eigenfunctions; he uses the fixed-core Hartree-Fock functions of Cohen and McEachran (1967) and McEachran and Cohen (1969). One can see that the differences get smaller as Z gets larger but on the other hand, for a given Z , the percentage change remains roughly constant as k^2 increases. This is what one expects when differences between bound-state functions are responsible. Nevertheless we believe that, for larger Z , the differences are small enough to be tolerable for astrophysical applications.

Next we examine changes in going from the Coulomb-Born to the distorted-wave calculation†. Here referring again to tables 2-4, we see that the differences can be significant, even for larger Z at lower energies. (Energies are to be judged in threshold units; the first entry (in parentheses) for each ion in tables 2, 3 and 4 is the threshold of the excited state relative to the ground $1S$ state.) For larger Z we believe it is legitimate, as discussed above, to use and judge the University College program also. In particular one sees that excited-state energies from our wavefunctions compare very favourably with the results of the University College SUPERSTRUCTURE program (Eissner *et al* 1974, Jones 1974).

On the whole we consider the comparison with UCL results excellent! The agreement is generally considerably better than 10%. There is some tendency for greater discrepancy in the triplet cross sections but this is to be expected since those cross sections arise only from the exchange terms. In exchange terms one expects greater sensitivity to the target-state wavefunctions and the UCL program utilises a far more elaborate approximation than the modified MYH functions of this calculation. A more incisive test of the effect of the target-state ansatz is provided by the comparison with the results of McDowell *et al* (1977) who used a distorted-wave polarised-orbital methodology. Those results (cf figures 2 and 3 of our paper also) are for singlet transitions and thus include both direct and exchange parts; they also involve more elaborate excited-state wavefunctions. They are in even closer accord with our results than those of UCL, except at the lowest Z . This agreement, we feel, shows that both induced polarisation and target-state correlations are not important except possibly at the lowest Z .

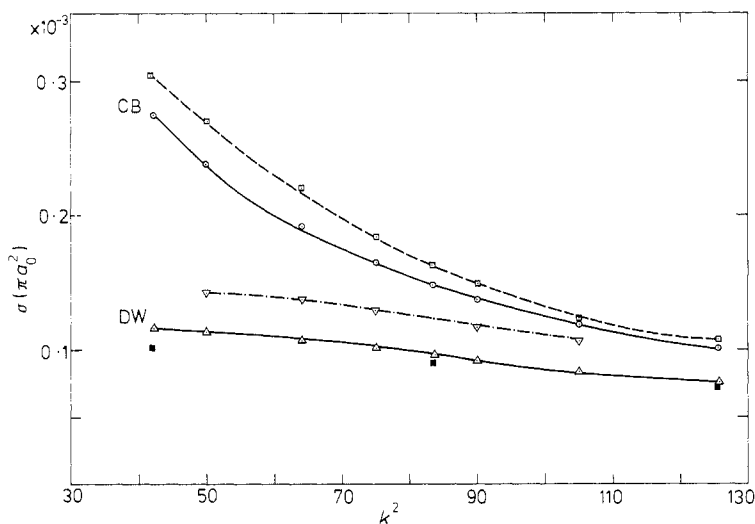


Figure 2. 2^1S excitation cross section in O^{6+} : \circ present Coulomb-Born results; \square Coulomb-Born results of Tully (1974); \triangle present distorted-wave results; ∇ distorted-wave results using the UCL program; \blacksquare calculation of McDowell *et al* (1977).

† We acknowledge the valuable suggestion of Dr D W Norcross about appropriately reducing the mesh size for high Z quadratures. This correction has changed the results from a previous preprint of this material.

Table 2. $n = 2$ 1S excitation cross sections† (units $10^{-3} \pi a_0^2$).

Ion	$k^2(\text{Ryd})$	Present‡	Tully‡	Present§	Ion	$k^2(\text{Ryd})$	Present§	Tully‡	Present§	UCL§
Li^+		(4.373 Ryd)			O^{6+}					(41.782 Ryd)
	5.0	11.405	15.57	2.691		50.0	0.239	0.269	0.115	0.141
	9.0	6.551	9.14	3.092		64.0	0.191	0.217	0.108	0.137
	13.41	4.476	6.43	2.704		75.0	0.165	0.184	0.101	0.129
	20.0	3.037		2.208		90.0	0.139	0.148	0.093	0.117
Be^{2+}					F^{7+}	105.0	0.120	0.124	0.085	0.106
						125.2	0.101	0.110	0.075	
		(8.836 Ryd)					(53.659 Ryd)			
	10.0	3.925	4.69	1.210		60.0	0.159		0.074	
	12.0	3.357	4.11	1.247		81.0	0.122		0.069	
	15.0	2.744	3.37	1.248	Ne^{8+}	160.0	0.064		0.048	
	20.0	2.097	2.47	1.170			(67.123 Ryd)			
	25.0	1.692	1.99	1.068		75.0	0.105		0.050	
						100.0	0.081		0.047	
						200.0	0.042		0.032	
B^{3+}		(14.801 Ryd)			Si^{12+}					(136.128 Ryd)
	18	1.500		0.602			(136.051 Ryd)			
	27	1.044		0.569		138.0	0.032		0.014	0.016
	50	0.578		0.423		196.0	0.023		0.013	0.015
						400.0	0.011		0.0083	

C^{4+}		(22.265 Ryd)					
25	0.784	0.323					
27	0.734	0.317					
36	0.569	0.306					
50	0.418	0.270					
60	0.351	0.245					
80	0.265	0.203					
100	0.212	0.172					
			Ca^{18+}		(284.389 Ryd)		(284.411 Ryd)
				288.0	0.0070	0.0039	0.0040
				400.0	0.0052	0.0033	0.0037
				600.0	0.0035	0.0026	
N^{5+}		(31.229 Ryd)					
36	0.418	0.187					
49	0.318	0.176					
75	0.213	0.145					
			Fe^{24+}		(486.609 Ryd)		(486.693 Ryd)
				493.3	0.0026	0.00130	0.0014
				510.0	0.0025	0.00129	
				676.0	0.0021	0.00116	0.0013
				750.0	0.0020	0.00110	
				800.0	0.0019	0.00106	
				976.0	0.0013	0.00094	

† A new distorted-wave polarised-orbital calculation by McDowell *et al* (1977) for two-electron ions gives results similar to those presented here. The reader should consult that paper for details.

‡ Coulomb-Born results.

§ Distorted-wave results.

|| Numbers in parentheses are threshold energies in the respective calculations.

The UCL results are given by Jones (1974) with the exception of O^{6+} which was calculated by us using the UCL program. Coulomb-Born results of Tully (1974) have been interpolated.

Table 3. $n = 2$ 1P excitation cross sections† (units $10^{-3} \pi a_0^2$).

Ion	k^2 (Ryd)	Present‡	Tully‡	Present§	$\sigma_{\text{corr}} $	Ion	k^2 (Ryd)	Present‡	Tully‡	Present§	UCL§
Li^+		(4.465 Ryd)				O^{6+}					
	5.0	38.90	40.10	12.43	0.0		50.0		1.011	0.496	(42.170 Ryd)
	9.0	37.58	42.37	25.87	0.035		64.0		0.948	0.586	0.494
	13.41	32.53	38.60	27.18	0.632		75.0		0.903	0.618	0.600
	20.0	24.80		22.60	2.685		90.0		0.847	0.635	0.635
Be^{2+}		(8.983 Ryd)				F^{7+}	105.0		0.798	0.624	0.656
	10.0	14.10					126.3		0.739	0.593	0.650
	12.0	13.94	14.51	5.19	0.0						
	15.0	13.40	14.39	6.90	0.0						
	20.0	12.34	14.13	8.41	0.001		60.0	(54.081 Ryd)			
	25.0	11.20	13.48	9.35	0.033		81.0	0.635		0.297	
			12.56	9.30	0.151		160.0	0.583		0.369	
B^{3+}		(15.003 Ryd)				Ne^{8+}					
	18	6.09		2.79	0.0		75.0	(67.600 Ryd)			
	27	5.56		3.82	0.002		100.0	0.420		0.200	
	50	4.22		3.68	0.152		200.0	0.386		0.243	
								0.286		0.245	

C ⁴⁺	25	(22.523 Ryd)						(136.831 Ryd)
		3.07	1.32	0.0			0.0516	0.051
	27	3.03	1.45	0.0			0.0661	0.067
	36	2.82	1.81	0.0			0.0657	
	50	2.52	1.96	0.007				
	60	2.32	1.92	0.025				
N ⁵⁺	80	1.95	1.73	0.095				(285.450 Ryd)
	100	1.64	1.50	0.185			0.0103	0.013
							0.0130	0.016
							0.0140	
	36	(31.543 Ryd)	0.782					
	49	1.68	0.991					
Fe ²⁴⁺	75	1.33	1.064					(488.069 Ryd)
							0.00444	0.0046
							0.00458	
							0.00541	0.0056
							0.00558	
							0.00566	
Si ¹²⁺								
Ca ¹⁸⁺								
Fe ²⁴⁺								

† For explanation of symbols and other clarifications, see footnote to table 2.

|| Both our Coulomb-Born and distorted-wave (as well as those of UCL) cross sections have been calculated for partial waves $l = 0, \dots, 11$. The remaining contributions from $l = 12$ to ∞ have been calculated by using the Coulomb-Bethe approximation (Burgess and Sheorey 1974) and the oscillator strengths derived from our (MYH) target wavefunction; σ_{corr} should be added to those results. For $Z \geq 6$ this correction was less than 1%.

Table 4. $n = 2$ 3S , 3P excitation cross sections in the distorted-wave approximation (units $10^{-3} \pi a_0^2$).

Ion	$k^2(\text{Ryd})$	3S		3P	
		Present	UCL	Present	UCL
Li^+		(4.229 Ryd)		(4.398 Ryd)	
	5	0.487		25.00	
	9	0.811		9.12	
	13.41	0.990		2.92	
	20	0.379		0.81	
Be^{2+}		(8.608 Ryd)		(8.856 Ryd)	
	10	0.711		9.235	
	12	1.555		6.510	
	15	0.991		3.860	
	20	0.544		1.770	
	25	0.312		0.914	
B^{3+}		(14.485 Ryd)		(14.812 Ryd)	
	18	0.390		3.095	
	27	0.312		1.140	
	50	0.065		0.186	
C^{4+}		(21.861 Ryd)		(22.267 Ryd)	
	25	0.220		1.661	
	27	0.336		1.395	
	36	0.174		0.682	
	50	0.078		0.274	
	60	0.049		0.160	
	80	0.023		0.062	
	100	0.013		0.033	
N^{5+}		(30.738 Ryd)		(31.22 Ryd)	
	36	0.119		0.797	
	49	0.093		0.368	
	75	0.032		0.112	
O^{6+}		(41.115 Ryd)	(41.224 Ryd)	(41.672 Ryd)	(41.767 Ryd)
	50	0.066	0.062	0.405	0.366
	64	0.051	0.038	0.216	0.189
	75	0.036	0.028	0.141	0.122
	90	0.023	0.018	0.084	0.073
	105	0.016	0.013	0.054	0.046
F^{7+}		(52.987 Ryd)		(53.623 Ryd)	
	60	0.042		0.288	
	81	0.037		0.135	
	160	0.006		0.019	
Ne^{8+}		(66.363 Ryd)		(67.068 Ryd)	
	75	0.028		0.183	
	100	0.020		0.088	
	200	0.004		0.012	
Si^{12+}		(134.879 Ryd)	(134.981 Ryd)	(134.881 Ryd)	(135.989 Ryd)
	138	0.0071	0.0085	0.055	0.051
	196	0.0047	0.0042	0.023	0.021
	400	0.0001		0.003	

Table 4. (continued)

Ion	$k^2(\text{Ryd})$	^3S		^3P	
		Present	UCL	Present	UCL
Ca^{18+}		(282.672 Ryd)	(282.736 Ryd)	(284.091 Ryd)	(284.198 Ryd)
	288	0.0016	0.0020	0.0125	0.0118
	400	0.0011	0.0010	0.0054	0.0051
	600	0.0004		0.0018	
Fe^{24+}		(484.405 Ryd)	(484.492 Ryd)	(486.301 Ryd)	(486.407 Ryd)
	493.3	0.00076	0.00069	0.0042	0.0040
	510.0	0.00074		0.0039	
	676.0	0.00040	0.00036	0.0019	0.0018
	750.0	0.00032		0.0014	
	800.0	0.00028		0.0012	
	976.0	0.00017		0.00069	

See also footnote to table 2.

In order to assess further the astrophysically important O VII cross sections both for present and future comparisons, we plot the 2^1S and 2^1P cross sections for O VII (O^{6+}) in the various approximations in figures 2 and 3. Note, in particular, the rise in the distorted-wave cross sections for 2^1P as k^2 increases. However, for lower energies we emphasise that neither set of results includes the effect of Feshbach resonances (which we shall discuss below). We also present in tables 5 and 6 our own and UCL partial-wave contributions to the various cross sections at three energies. We see that there is less good agreement in the partial-wave results than in the total cross sections. It is still too early to assess the meaning of these results, particularly in the absence of including the effect of resonances in either calculation.

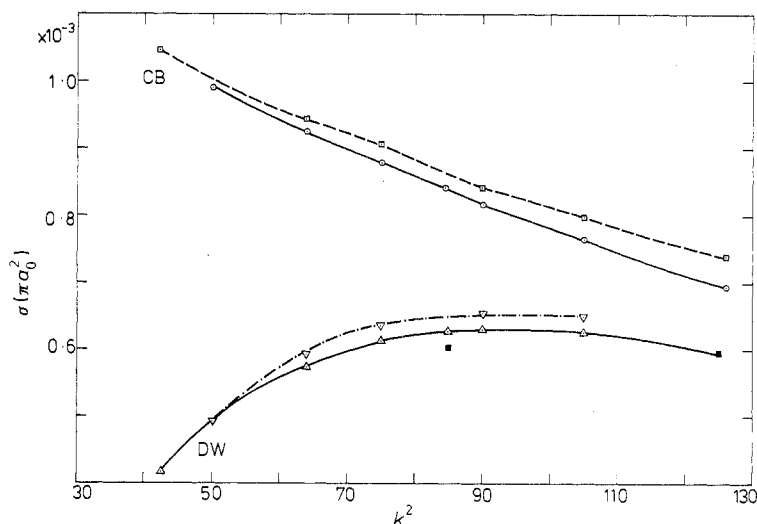


Figure 3. 2^1P excitation cross section in O^{6+} : \odot , \square , \triangle , ∇ and \blacksquare have the same representation as in figure 2.

Table 5. Partial-wave comparison of 1S and 1P excitation cross sections in O^{6+} in our own (BT) and UCL (UCL) distorted-wave approximations (units $10^{-3} \pi a_0^2$).

l	1S						1P					
	$k^2 = 50$		$k^2 = 75$		$k^2 = 90$		$k^2 = 50$		$k^2 = 75$		$k^2 = 90$	
	BT	UCL	BT	UCL	BT	UCL	BT	UCL	BT	UCL	BT	UCL
0	0.0110	0.0209	0.0107	0.0183	0.0100	0.0158	0.0217	0.0192	0.0186	0.0182	0.0161	0.0160
1	0.0733	0.0867	0.0499	0.0621	0.0412	0.0513	0.0159	0.0104	0.0161	0.0103	0.0144	0.0094
2	0.0279	0.0295	0.0316	0.0373	0.0297	0.0354	0.1588	0.1528	0.1007	0.1008	0.0781	0.0779
3	0.0025	0.0036	0.0076	0.0090	0.0093	0.0109	0.1989	0.2072	0.1758	0.1865	0.1458	0.1544
4	0.0001	0.0005	0.0012	0.0016	0.0020	0.0025	0.0772	0.0797	0.1440	0.1515	0.1411	0.1489
5	0.0	0.0001	0.0001	0.0004	0.0003	0.0006	0.0188	0.0194	0.0847	0.0891	0.1006	0.1060
6		0.0	0.0	0.0001	0.0001	0.0002	0.0037	0.0038	0.0427	0.0450	0.0618	0.0653
7				0.0	0.0	0.0001	0.0007	0.0007	0.0200	0.0211	0.0352	0.0372
8						0.0	0.0001	0.0001	0.0091	0.0096	0.0193	0.0205
9									0.0040	0.0043	0.0104	0.0111
10									0.0018	0.0019†	0.0056	0.0060†
11									0.0008	0.0008†	0.0030	0.0032†

† Coulomb-Bethe approximation.

One astrophysical application of these cross sections is presented at the end of the paper, and to our mind it emphasises the need for an accurate inclusion of the resonant contribution.

We next present a sample of angular distributions. In figure 4, 2^1S angular distributions are drawn for O^{6+} for three energies. The minimum around 60° is seen to vanish as k^2 increases. The minimum itself is well established in the excitation of $He(2^1S)$ (Hall *et al* 1973, Trajmar 1973) and its presence has emerged from distorted-wave calculations (Madison and Shelton 1973‡) and many-body Martin-Schwinger RPA calculations (Thomas *et al* 1974).

Table 6. Partial-wave comparison of 3S and 3P excitation cross sections in O^{6+} in our own (BT) and UCL (UCL) distorted-wave approximations (units $10^{-3} \pi a_0^2$).

l	3S						3P					
	$k^2 = 50$		$k^2 = 75$		$k^2 = 90$		$k^2 = 50$		$k^2 = 75$		$k^2 = 90$	
	BT	UCL	BT	UCL	BT	UCL	BT	UCL	BT	UCL	BT	UCL
0	0.0348	0.0315	0.0194	0.0123	0.0116	0.0076	0.0363	0.0230	0.0089	0.0071	0.0048	0.0040
1	0.0289	0.0265	0.0150	0.0141	0.0105	0.0099	0.0812	0.0652	0.0283	0.0167	0.0160	0.0089
2	0.0015	0.0029	0.0002	0.0001	0.0000	0.0	0.2545	0.2421	0.0774	0.0712	0.0431	0.0393
3	0.0006	0.0010	0.0007	0.0007	0.0005	0.0005	0.0312	0.0335	0.0221	0.0225	0.0161	0.0161
4	0.0001	0.0001	0.0002	0.0002	0.0002	0.0002	0.0017	0.0019	0.0035	0.0038	0.0035	0.0036
5	0.0	0.0	0.0	0.0	0.0001	0.0001	0.0001	0.0001	0.0004	0.0005	0.0006	0.0006
6					0.0	0.0	0.0	0.0	0.0001	0.0001	0.0001	0.0001
7									0.0	0.0	0.0	0.0

‡ 2^1S cross section quoted in Thomas *et al* (1974).

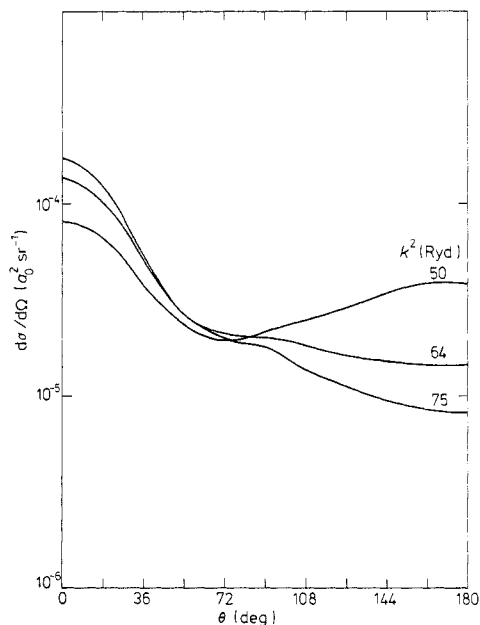


Figure 4. 2^1S differential excitation cross sections in O^{6+} for $k^2 = 50, 64$ and 75 Ryd. Results are from the present distorted-wave calculation.

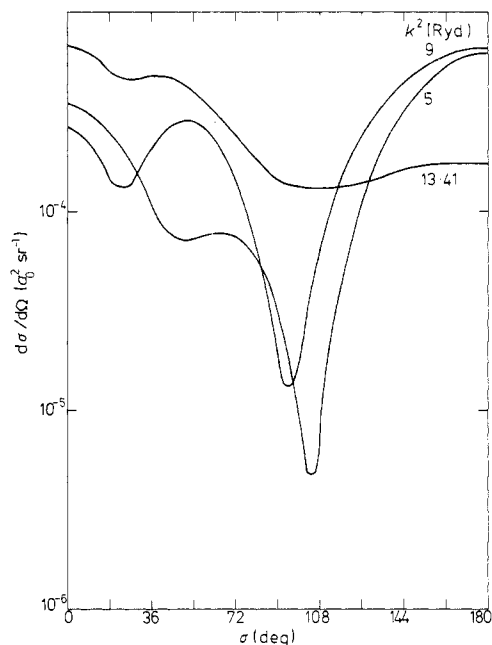


Figure 5. 2^3S differential excitation cross sections in Li^+ for $k^2 = 5, 9$ and 13.41 Ryd. Results are from the present distorted-wave calculation.

Qualitatively similar behaviour is seen to occur in excitation of the 2^3S state (figure 5). In fact, our calculation shows two minima for Li^+ at $k^2 = 5$ Ryd. Again the experimental results for excitation of $He(2^3S)$ show a pronounced minimum and an indication of a second minimum which diminishes at higher energies (Trajmar 1973, Crooks *et al* 1972).

The 2^1P excitation curves (figure 6) are characterised by the absence of any pronounced minima and again this behaviour is similar to the corresponding neutral ($He(2^1P)$) excitation both experimentally (Opal and Beaty 1972, Truhlar *et al* 1973) and theoretically (Madison and Shelton 1973, Thomas *et al* 1974).

Finally we present 2^3P excitation in figure 7. Here the neutral-atom ($He(2^3P)$) excitation shows experimentally (Trajmar 1973, Hall *et al* 1973) different behaviour from the calculations (Thomas *et al* 1974, W M Shelton, K Beluja and D H Madison quoted in Thomas *et al* 1974) with the theory being similar in shape to our own ionic results.

In the case of the neutral ($He(2^3P)$) Thomas *et al* (1974) attributed the difference to the absence of 2^3S – 2^3P coupling in the calculation, which is expected to have a large effect due to the closeness in energy of the target states. The effect of this coupling can be gauged by the ratio of the local wavelength of the scattered electron to the distance between S and P states (we assume the configurations $1s2s$ and $1s2p$ for $n = 2$ states). The latter is simply computed to be $\Delta r_n = |\bar{r}_{np} - \bar{r}_{ns}| = Z^{-1}$ (for $n = 2$) whereas the former depends on the energy of the scattered electron. At threshold $\lambda(r_n) \propto (Zr_n)^{1/2} \propto [Z(n^2/Z)]^{1/2} = \text{independent of } Z$. Thus $[\lambda(r_n)/\Delta r_n]_{n=2} \propto Z$ and the coupling is expected to be very important for large Z . However, because of the non-inclusion of resonances, the present cross sections are unreliable in any event.

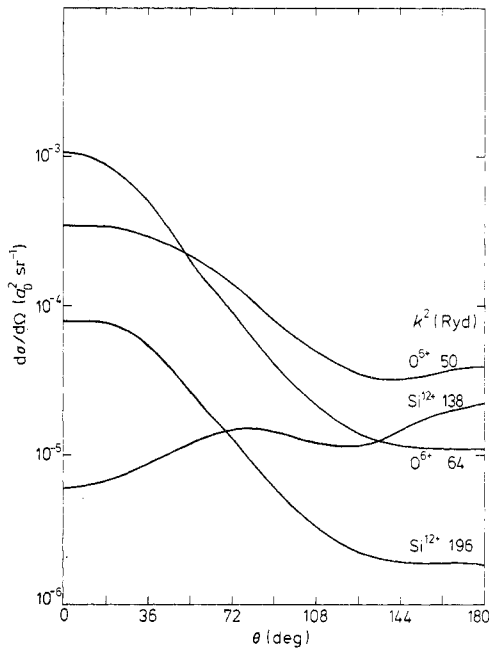


Figure 6. 2^1P differential excitation cross sections in O^{6+} for $k^2 = 50$ and 64 Ryd, and in Si^{12+} for $k^2 = 138$ and 196 Ryd. Results are from the present distorted-wave calculation.

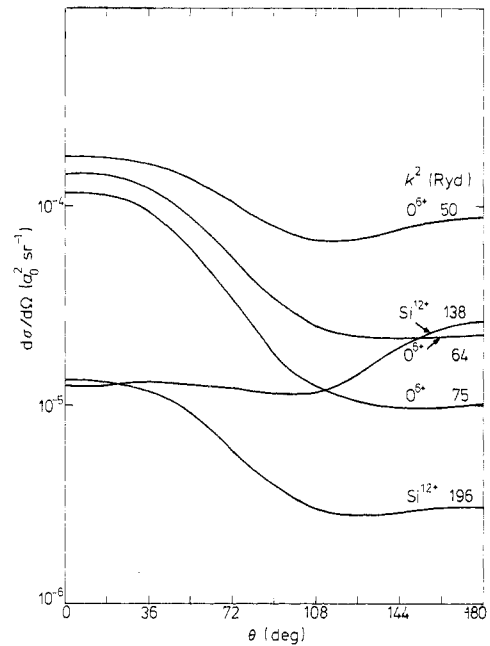


Figure 7. 2^3P differential excitation cross sections in O^{6+} for $k^2 = 50, 64$ and 75 Ryd, and in Si^{12+} for $k^2 = 138$ and 196 Ryd. Results are from the present distorted-wave calculation.

At about one threshold unit above threshold, the wavelength $\lambda \propto Z^{-1}$ and the ratio $\Delta r_n/\lambda$ becomes independent of Z . Thus the situation with regard to coupling is expected to be similar to that for e-He excitation.

It would clearly be desirable to have experimental verification in the ionic cases. However, we realise the great experimental difficulties attendant on direct observation of ionic rather than neutral systems. From solar-coronal line strengths of O VII, Gabriel and Jordan (1972) have inferred the ratio G of intercombination to allowed rates given by

$$G = [C(1^1\text{S} \rightarrow 2^3\text{P}) + C(1^1\text{S} \rightarrow 2^3\text{S})]/C(1^1\text{S} \rightarrow 2^1\text{P}). \quad (2.24)$$

In (2.24) the rate coefficient C is proportional to the cross section averaged over a Maxwell distribution of electrons of temperature T_e , cf equation (1.1). Explicitly this becomes

$$C(1^1\text{S} \rightarrow 2^\mu\text{L}) = \frac{1.36}{T_e^{3/2}} \int_{E_{\text{th}}}^{\infty} \sigma_{\mu\text{L}}(E) E e^{-E/k_B T_e} dE \quad (2.25)$$

(μ is the appropriate spin multiplicity for the respective transition in (2.23)). In table 7 we give G for three temperatures using our own and UCL cross sections. The solar value (Gabriel and Jordan 1972) favours our value slightly, but as discussed below this cannot be considered a convincing comparison. Rather, one might say on the basis of the T dependence of our results that, given accurate cross sections, this type of comparison is an accurate way of determining the temperature (T).

Table 7. The ratio G in our own (BT) and UCL (UCL) calculations.

T_e	G_{BT}	G_{UCL}	G_{exp}^\dagger
0.975×10^6	1.11	0.83	1.1
1.95×10^6	0.80	0.66	
9.75×10^6	0.36	0.30	

† Experimental values based on solar measurements (Gabriel and Jordan 1972), cf text for discussion.

We are not in a position to assess the accuracy of the solar measurement, but assuming it is correct we believe considerable caution should attend the respective calculational methodologies. Because the temperature in question, 1.95×10^6 K, corresponds to a $k_B T_e$ in (2.25) much less than the threshold energies E_{th} for any of these transitions, it follows that the exponential in (2.25) is a sharply decreasing function of E . Thus only $\sigma(E)$ near threshold $E \simeq E_{th}$ makes a significant contribution to C . This, then, is a specific example of the requirement of an accurate cross section near threshold, mentioned in the introduction. Although the average effects of resonances, using the incisive analysis of Gailitis (1963), have been included in specific cases (Hershkowitz and Seaton 1973, Presnyakov and Urnov 1975), resonances have not been included here. It is our belief that this effect may be very important, and furthermore one may *not* be able to average over resonances, for example in the case of O^{2+} (Seaton 1975b, Pindzola 1977). This problem deserves further study and until it is completed, we would urge caution in using the results of table 7 to compare methodologies for calculating what is in fact the non-resonant part of inelastic cross sections.

One can expect that beyond about two threshold units the resonant contribution will no longer be significant. Here we believe that our version of the distorted-wave method does give a reasonable description of the truth.

Acknowledgments

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