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WHAT WE DO AND DO NOT KNOW ABOUT

ELECTRON IMPACT EXCITATION OF ATOMIC HYDROGEN

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Abstract

The present state of knowledge derived from both theoretical and experimental information on electron impact excitation of atomic hydrogen is briefly reviewed. Suggestions are made for further calculations and for additional experiments.

Introduction

This note originated in a request from Collaborative Computational Project No. 7 (CCP7) (Atomic Processes in Astrophysics) of the U.K. Science and Engineering Research Council to CCP6 (Electron Scattering) for recommendations of best available values of electron impact excitation cross sections of H and He for $n \leq 5$. The theoretical groups at Queen's university of Belfast and Royal Holloway College (University of London) were tasked with this work. The present comment is at most a first step.

We found, to our dismay, that there was at this stage little hope of improving on the semi-empirical formula of Johnson¹ published almost twelve years ago for transitions involving states with n or $n' > 3$, although it is known² that this is in error for the $n = 2$ to $n = 3$ total excitation cross section at low energies by about a factor of two. We assume that for n and n' sufficiently large (say $n, n' \geq 5$) the classical treatment of Percival and Richards³ will be accurate to within $\pm 20\%$ for total excitation cross sections $\sigma_{nn'}$, but one aim of the programme of work being carried out by Queen's,

R.H.C., L.S.U. and Université Libre de Bruxelles, is to test both this assumption and the reliability of the Johnson semi-empirical formula.

The need for accurate values of the total (n, n') excitation cross sections arises not only from the astrophysicists' requirements but from low temperature plasma experiments. Burgess and his colleagues⁴ have shown that experiments on laser excited fluorescence of hydrogen plasmas at temperatures of a few eV imply either large errors in the currently accepted cross section values or highly non-maxwellian electron velocity distributions or both.

One purpose of this note is to remind our colleagues, both theorists and experimentalists, that while it is of great interest to measure or calculate such esoteric parameters as spin-flip ratios, differential cross sections and orientation and alignment parameters, we are still unable to give a satisfactory answer to the simple question "What is the absolute value of the cross section for the $|n\ell\rangle \rightarrow |n'\ell'\rangle$ transition at a specified energy?"

We find that the uncertainties are of the order of 20% at some energies for the simplest cases, of at least a factor of two in other apparently simple cases, while in many cases there is no reliable information at all, though First Born Approximation (FBA) results are known for $\sigma_{nn'}$ ($n, n' \leq 5$) in most cases.⁵

We will discuss the contributions to σ_{12} first, then σ_{13} and σ_{23} . We then consider the information available for other $\sigma_{nn'}$ ($n, n' \leq 5$).

Contributions to σ_{12}

The quality of the results depends on the incident energy.

(a) From the $n = 2$ threshold to the $n = 3$ threshold there

are very accurate variational calculations by Callaway⁶ using an eighteen state basis (seven exact and eleven pseudostates). These calculations give larger eigenphase sums than any other and are in excellent agreement with experiments of Williams⁷, except for fine detail of the Feshbach resonances below the $n = 3$ threshold. The important features are the finite threshold values and the shape resonance ($E_{rs} = 0.7512$ Ry) just above the $n = 2$ threshold. The width of this resonance is small ($\Gamma_r \sim 0.0015$ Ry) so for most purposes the low energy cross sections can be represented as a delta function at E_R superimposed on a linear background.

The Feshbach resonances are narrow and confined to a narrow region ($\Delta E \sim 0.03$ Ry) below the $n = 3$ threshold. The most prominent is a 3F resonance at $E_R = 0.877$ Ry of width $\sim 2 \times 10^{-4}$ Ry (though it is not seen in Williams' experiment). For astrophysical or plasma purposes, when $kT > 1$ eV it should cause no significant error to replace the actual cross section by a linear fit even in the resonance region. We recommend for the range $0.75 \leq E \leq 0.85$

$$\sigma_{1s \rightarrow 2s} = 1.3 \cdot 10^{-4} \delta(E - E_{rs}) + 0.13 + 0.89 (E - 0.75) \quad (1)$$

$$\sigma_{1s \rightarrow 2p} = 1.6 \cdot 10^{-3} \delta(E - E_{rs}) + 0.16 + 2.0 (E - 0.75) \quad (2)$$

in units of πa_0^2 . For 0.85 to 0.89 we take

$$\sigma_{1s \rightarrow 2s} = 0.204, \quad \sigma_{1s \rightarrow 2p} = 0.367. \quad (3)$$

The values given in (3) above are averages of the (numerical) cross sections calculated⁶ in the Feshbach resonance region.

(b) From the $n = 3$ threshold to the ionisation threshold there is little possibility of doing detailed calculations above, say, the $n = 5$ threshold. Otherwise we must represent the very large number of open channels by a few pseudostates.

The only accurate calculations for the contributions to σ_{12} are those of Callaway⁸ using a basis of the exact $1s, 2s, 2p,$

3d states and seven pseudostates. Results were given at $k_1^2 = 0.90, 0.95, 1.00$. The earlier six-state calculations are less reliable (see Hata et al²). The results are well represented by a linearly increasing function of energy in this range. There is some indication of a drop in the $1s \rightarrow 2s$ cross section at the $n = 3$ threshold. Calculations at 0.89 to 0.91 would be of interest.

We have for the range $0.89 \leq E \leq 1.0$

$$\sigma_{1s \rightarrow 2s} = 0.17 + 0.1 (E - 0.89) \quad (4)$$

$$\sigma_{1s \rightarrow 2p} = 0.36 + 0.8 (E - 0.89) \quad (5)$$

(c) For our third region we find it convenient to choose $13.6 < E \leq 54.4$ eV, since it is in this range that the most serious discrepancies occur, though we have an absolute measurement of $\sigma_{1s \rightarrow 2p}$ at 54.4 eV from Williams.⁹

The available calculations include the eleven state close-coupling (11CC) of Callaway,⁸ and a five state ($1s - 2s - 3p +$ two pseudostates) by Burke and Webb¹⁰ (5CC). These calculations are in reasonable agreement for $\sigma_{1s,2p}$ (Fig. 1) but not for $1s \rightarrow 2s$ (Fig. 2); the results are given in the figures as collision strengths

$$\Omega_{ij} = 2k_i^2 \sigma_{ij}. \quad (6)$$

At 20 eV the 5CC result for $\sigma_{1s,2s}$ is 12% higher than the 11CC, but are both at least a factor of two below the 3CC value.¹¹ At 30 eV the 5CC value is 55% higher than the 11CC but at 54.4 eV they agree closely. We note that the simple 3CC calculation is at its worst near 20 eV where even for $\sigma_{1s,2p}$ it is almost a factor of two higher than the 11CC result.

What does experiment say? The measurements of $\sigma_{1s,2p}$ by Long, Cox and Smith¹² can be renormalised to Williams⁷ at 11.02 eV or Williams⁹ at 54.4 eV: these normalisations are entirely consistent. The absolute measurement at 54.4 eV of $0.89 \pm 0.08 \pi a_0^2$

is consistent with both 5CC and 11CC calculated values. With this normalisation experiment and theory are in good agreement throughout the energy range under consideration and indeed up to 100 eV. However, the measurements in the range $100 < E_i \leq 199$ eV now lie above the Born, which is unlikely, though the discrepancy at 200 eV is less than 10%. More refined measurements would be desirable. From the collision strengths shown in Fig. 1 we find that from two to six times threshold

$$\Omega_{1s,2p} = 10 \log_{10} X - 0.60 \quad (7)$$

to within $\pm 10\%$. Over the whole range from the ionisation threshold to the FBA region we recommend

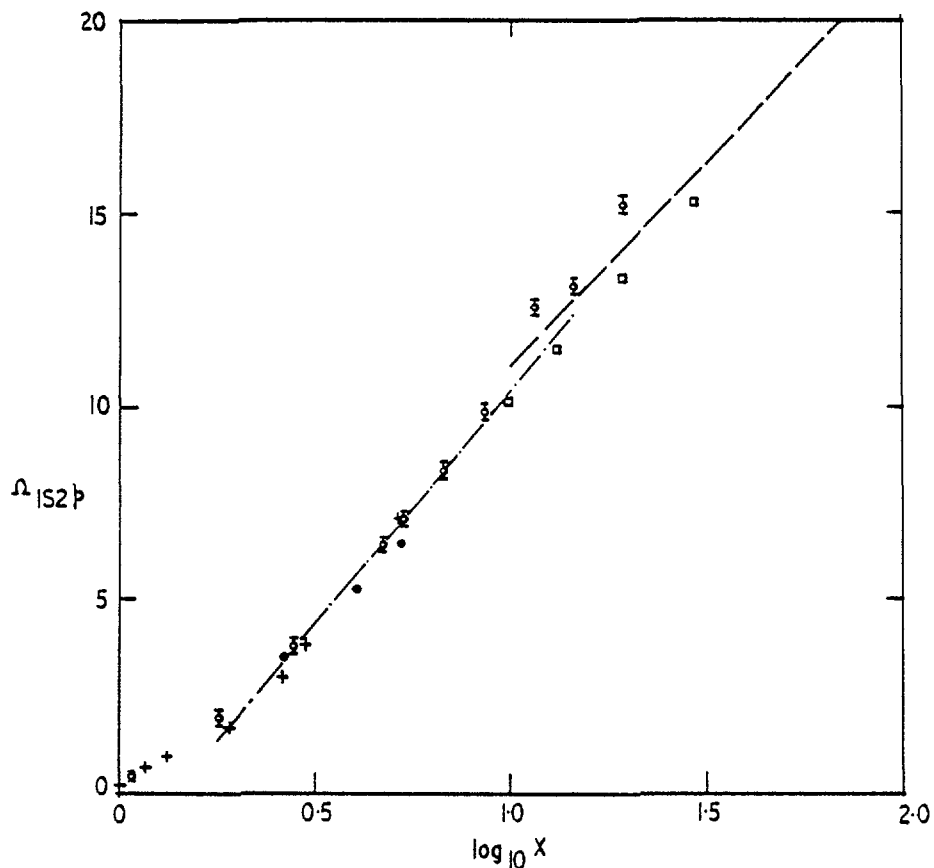


Fig. 1 Theoretical and experimental values of $\Omega_{1s,2p} = 2k_i^2 \sigma_{1s,2p}$. The experimental points (see text) are shown as \square . Theory + Ref. (6,8); \bullet Ref. 10; Ref. 11. The --- line is the Bethe approximation. The - o - o - line is eqn (8).

$$\Omega_{1s,2p} = 4.44 \ln X + 0.89 - 9.68 X^{-1} + 10.94 X^{-2} . \quad (8)$$

The situation is not so clear for the $1s \rightarrow 2s$ transition. The only absolute experimental point is that of Williams⁷ who finds $\sigma_{1s,2s} = 0.188^{+0.031}_{-0.022}$ at 11.0 eV. The measurements of Kauppila et al¹³ include cascade and are presented graphically. They quote a maximum value of 0.163 ± 0.02 at 11.6 ± 0.2 eV, though from the graph their measured value at 11.0 eV is very much smaller - perhaps 0.13? The threshold value indicated is 0.025 ± 0.005 , compared with Callaway's⁶ calculated value of 0.103. The calculated value at 11.0 eV of 0.187 ± 0.003 is in very close agreement with Williams' experiment. Bransden and McDowell¹⁴ have renormalised the Kauppila et al data

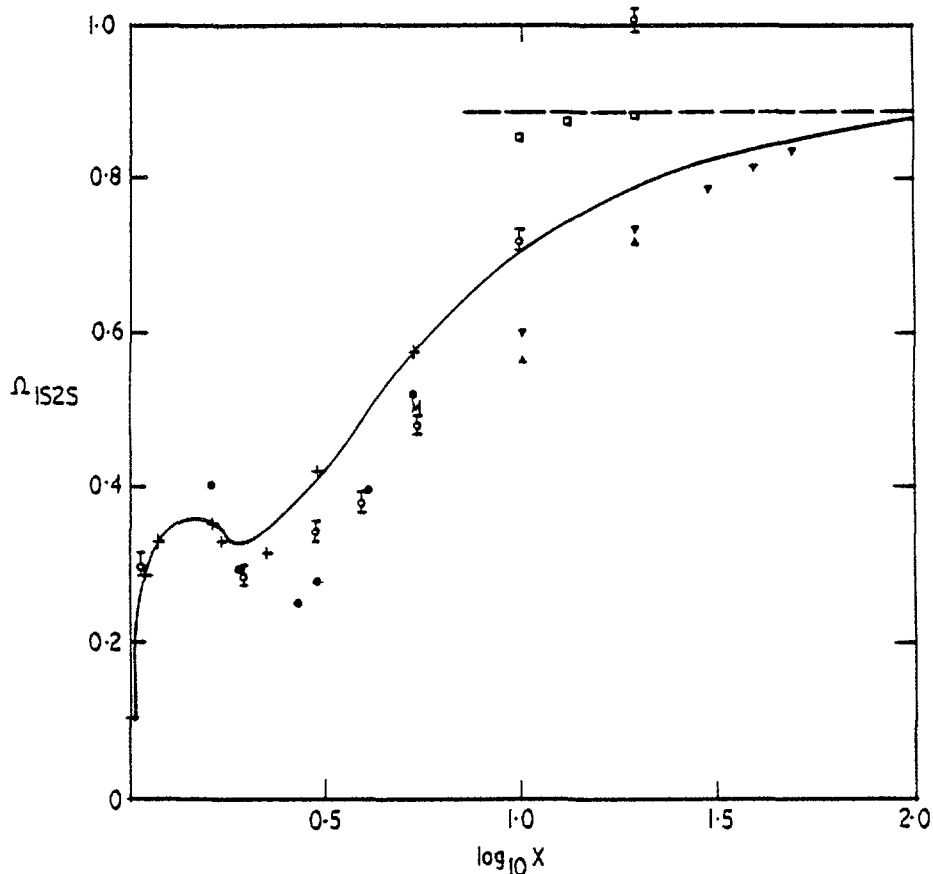


Fig. 2 As for Fig. 1 but $\Omega_{1s,2s}$. The — line is eqn (9) for $X \geq 2$ and Callaway's calculations (Ref. 6,8) for $X < 2$, while --- is the First Born Approximation. Theoretical values are shown as + Ref. (6,8); • Ref. 10; U Ref. 11; Δ Ref. 15; V Ref. 16; M Ref. 17.

upwards by 10% and attempted to correct for cascade in the usual way

$$\sigma_{1s,2s} = 1.1\sigma_{1s,2s}(\text{obs}) - 0.23\sigma_{1s,3p}$$

using theoretical values of $\sigma_{1s,3p}$. The cascade correction is large, and the results are very uncertain. We have followed Bransden and McDowell but used our best estimates of $\sigma_{1s,3p}$ (Fig. 3) to obtain the "experimental" points shown in Fig. 2. These lie about 10% above the values given by Bransden and McDowell, and are given in Table 1. This results in the value at 200 eV being 17% above the Born limiting value of $\Omega_{1s,2s}$, suggesting that the renormalisation may be incorrect and/or cascade may be underestimated above 100 eV.

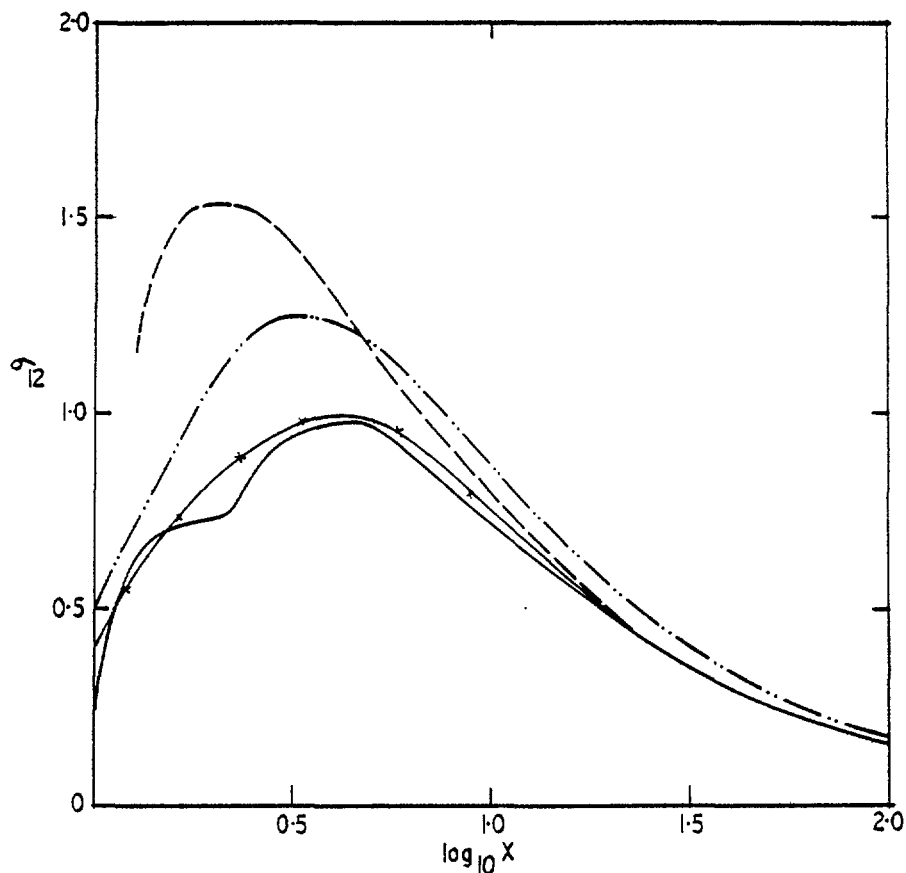


Fig. 3 Values of σ_{12} . The --- line is the FBA⁵, the solid curve — eqns (8) and (9) for $X \geq 2$ and Ref. (6,8) for $X < 2$. The -·-·- curve is the classical model³ and -x-x- the semi-empirical result of Johnson¹.

Table 1

E(eV)	k_i^2 (Ry)	X	log X	$Q_{1s,2s}$				
				Q_{obs}	0.23 Q_{3p}	$Q_{1s,2s}$	$\Omega_{1s,2s}$	
11.0	.808	1.08	.033	$0.188^{+0.03}_{-0.022}$	-	0.188	0.303	
20.0	1.47	1.96	.29	$0.112 \rightarrow .123$.025	0.098	0.288	
30.0	2.21	2.95	.47	$0.102 \rightarrow .112$	0.034	0.078	0.344	
40	2.94	3.92	.59	$0.088 \rightarrow .097$	0.033	0.064	0.38	
54.4	4.00	5.33	.73	$0.084 \rightarrow .092$	0.032	0.060	0.48	
100	7.35	9.8	.99	$0.068 \rightarrow .074$	0.025	0.049	0.72	
200	14.7	19.6	1.29	$0.046 \rightarrow .051$	0.016	0.035	1.03	

The cross section value at 11 eV is due to Williams⁽⁷⁾, the others in column 5 those of Kauppila et al, the second value following the arrow being the renormalised value, and column 7 the recommended value, all in πa_0^2 .

The agreement between 5CC¹⁰ and 11CC⁸ calculations is poor throughout this energy range, though both show a minimum in the collision strength between 20 and 30 eV, and there is some indication of this in the experimental data. At 30 eV the 11CC results are more than 50% higher than the 5CC though at 54.4 eV this discrepancy is only 11%. A thirteen state non-exchange calculation (13NECC) by Morgan¹⁷ gives $\Omega_{1s,2s} = 0.500$ at this energy, a surprisingly low result since exchange generally tends to lower the cross section for s - s transitions. Her calculation includes the exact n = 1, 2, 3 states and either six (35 eV) or seven (54.4 eV) pseudostates. A similar calculation using a ten state basis of exact n = 1, 2, 3, 4 states by Edmunds and McDowell¹⁸ gives $\Omega_{1s,2s} = 0.831$, which we think is more reasonable.

Much more accurate calculations are required in the range from the ionisation threshold to 54.4 eV, and are in hand. A preliminary (1s, 2s, 2p, $\overline{3s}$, $\overline{3p}$, 3d) result by Kingston and Lin (private communication) at 54.4 eV gives $\Omega_{1s,2s} = 0.544$ in good agreement with Callaway's value.

(d) Energies above 54.4 eV. For $\sigma_{1s,2p}$ theory and experiment represented by the 3CC calculation¹¹ and the re-normalised Long et al experiment are in close agreement from 50 to 100 eV and at higher energies the 3CC values tend smoothly to the FBA. The data are well represented by (8) above. There are two recent calculations of $\sigma_{1s,2s}$ which should be more accurate than earlier ones. First a Unitarised Eikonal Born Series (UEBS) calculation by Byron et al¹⁵, and a Distorted Wave Second Born Approximation (DWSBA) by Kingston and Walters¹⁶. They differ by 6% at 100 eV and by 2% at 200 eV. What is very surprising is the large disagreement with 3CC and the very slow approach to the FBA limit of $\Omega_{1s,2s} = 0.888$, the DWSBA results being 6% lower even at 500 eV.

There can be no really satisfactory representation of the 1s - 2s data until the major discrepancies are resolved. For the present we recommend

$$\Omega_{1s,2s}(X) = 0.888 - \frac{1.956}{X} + \frac{1.680}{X^2}, \quad X > 1.33. \quad (9)$$

The total $n = 1 \rightarrow n = 2$ cross section can now be obtained using these recommended values, and is shown in Fig. 3, where it is compared with the FBA⁵, the classical formula³, and the formula of Johnson¹. The classical result was not intended to apply for such low n and n' but below 50 eV it is a significant improvement on the FBA. Johnson's formula is in reasonable agreement with our recommendation, except very close to threshold the differences do not exceed about 14%. A brief table is given below (Table 2).

Near $X = 2$ the FBA overestimates by more than a factor of two. The Classical result is an improvement on the FBA only for

Table 2

X	1	2	4	6	8	10	20	30	40
$\sigma_{12}(X)$	0.29	0.73	0.97	0.91	0.80	0.72	0.48	0.37	0.30

X < 5. The large (n, n') form of Gee et al was used.

Contributions to σ_{13}

We have now very little information. Hata et al² have carried out sixteen to eighteen state close coupling calculations between the n = 3 and n = 4 thresholds. The earlier 6CC results are unreliable. Syms et al¹⁹ report distorted wave values (DWPO) while there are Glauber calculations²⁰ for 1s - 3d. Flannery and McCann²¹ used a multi-channel eikonal model in a (1s, 2s, 2p, 3s, 3p) basis to calculate the 1s → 3s, 3p cross sections. Very recently Morgan¹⁷ and Edmunds and McDowell¹⁸ have carried out thirteen and ten state non-exchange close coupling calculations at energies of 35 and 54.4 eV. In addition there is an important Unitarised Born Approximation (UBA) by Somerville²².

The only extensive experimental results are those of Mahan et al²³. We have used the graphs in Mahan's thesis to extract numerical values.

(a) 1s → 3p. The near threshold values of Hata et al² of $\Omega_{1s,3p} = 0.116$ at X = 1.01 and 0.179 at X = 1.04 should be accurate to ± 10%. For X > 1.6 the UBA, MCE and DWPO values are in close agreement and may be represented by

$$\Omega_{1s,3p}(X) = 0.759 \ln X - 0.331 X^{-1} + 0.485 X^{-2} \quad (10)$$

for this range (see Fig. 4). The experimental values we obtain from Mahan's work lie about 30% below this curve, but that is within the large experimental uncertainty. Notice that eqn (10)

gives a result 6% below the Bethe model even at 200 times threshold. The theoretical position appears satisfactory, but it would be of great interest to have an absolute experiment, preferably at more than one energy. Brouillard (private communication) has obtained a beam of H(3p) by laser excitation of H(2s); a super-elastic experiment $H(3p) + e \rightarrow H(1s) + e$ might be possible.

(b) $\Omega_{1s,3s}$. This is a small cross section and $\Omega_{1s,3s} \leq 0.176$ (the Born limit). The threshold value is 0.065^2 rising to 0.103 at $X = 1.04$. The UB values appear accurate at small X and are bracketed by experiment. The 12/13 NECC results of Morgan seem anomalous in decreasing from 0.14 to 0.087 between 35 and 54.4 eV. At larger X the MCE and DWPO values are in

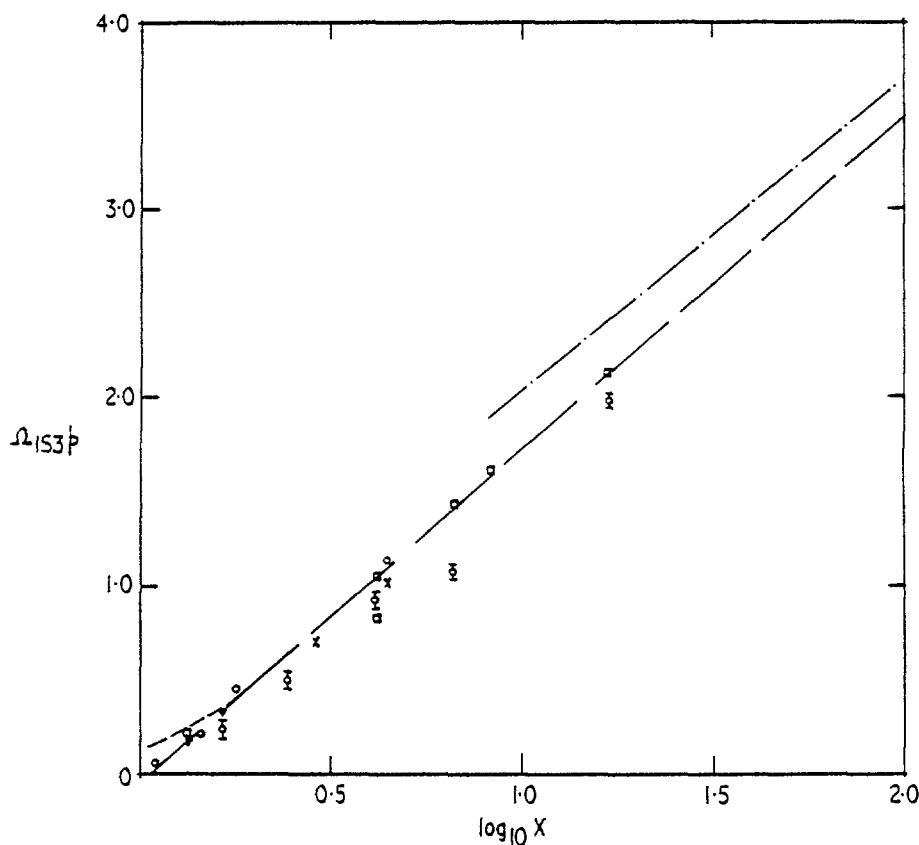


Fig. 4 As for Fig. 1 but $\Omega_{1s,3p}$. The experimental values (δ) are those of Mahan et al.²³ The theoretical values are \square Hata et al.²; \circ UB²²; \times 12/13 NECC¹⁷, DWPO¹⁹, ∇ MCE²¹. The --- line is eqn (10) and the upper - o - o - line the Bethe approximation.

reasonable agreement though the experimental value at $X = 16.5$ (200 eV) may be as much as 10% too high. There are no results above this energy except for the FBA and we have assumed a smooth extrapolation from the DWPO values to the FBA. A reasonable fit over the whole range is provided by

$$\Omega_{1s,3s}(X) = 0.176 - 0.487 X^{-1} + 0.367 X^{-2} \quad (11)$$

with an accuracy of better than $\pm 15\%$.

(c) $\Omega_{1s,3d}$. This is a much more difficult case. The cross section is larger than $\sigma_{1s,3s}$. The Glauber values²⁰ of Bhadra and Gosh are in good agreement with the DWPO I results of Syms et al¹⁹ above 200 eV ($X = 16.5$) and suggest that in the FBA limit $\Omega_{1s,3d} \approx 0.14$. However, the DWPO II results which include distortion effects in the target wave function lie a factor of two lower up to 200 eV. The threshold and near threshold values² of 0.067 at $X = 1.01$, 0.087 at $X = 1.04$ should be accurate and together with the UB values²² show a rapid rise to a maximum of $\Omega \approx 0.18$ at 54.4 eV in good agreement with Morgan's¹⁷ 13 NECC result. Her 12 NECC result at 35 eV is anomalously high, probably because of the increased importance of exchange at that energy.

The Mahan et al experimental values shown in Fig. 5 were obtained by normalising to the FBA at 500 eV. The measurement at 200 eV ($X = 16.5$) is in close agreement with the Glauber and DWPO I calculations as a consequence. A reasonable fit is

$$\Omega_{1s,3d} = 0.120 + 0.388 X^{-1} - 0.441 X^{-2} \quad (12)$$

though the accuracy is not high.

The relative large values of $\sigma_{1s,3d}$ compared with $\sigma_{1s,3s}$ are probably due to the strong 3p - 3d dipole coupling: Ω_{3p} is about ten times larger than Ω_{3s} or Ω_{3d} and while only the 3sL channel can be pumped from 3p, 3pL ± 1 connects to 3dL and 3dL ± 2 . A seven channel calculation with only these channels would be of interest.

We can now use (10), (11), (12) to give an estimate of σ_{13} , for $X \geq 2$, using the Hata et al values² near threshold. The results are shown in Fig. 6. The minimum of our quantal estimates near $X = 1.4$ (~ 17 eV) may be spurious; more accurate calculations and new experimental measurements to test it are urgently required. The FBA overestimates below 100 times threshold and at its worst is about 75% high. We again show the classical result (with the usual reservations that n, n' are too small for it to be strictly applicable) and the Johnson semi-empirical formula. We have again used the form given by Gee et al³ claimed to be valid for $n, n' \geq 5$. The classical result is somewhat more accurate than the FBA below $X = 4.5$ though it approaches the FBA from above for larger X .

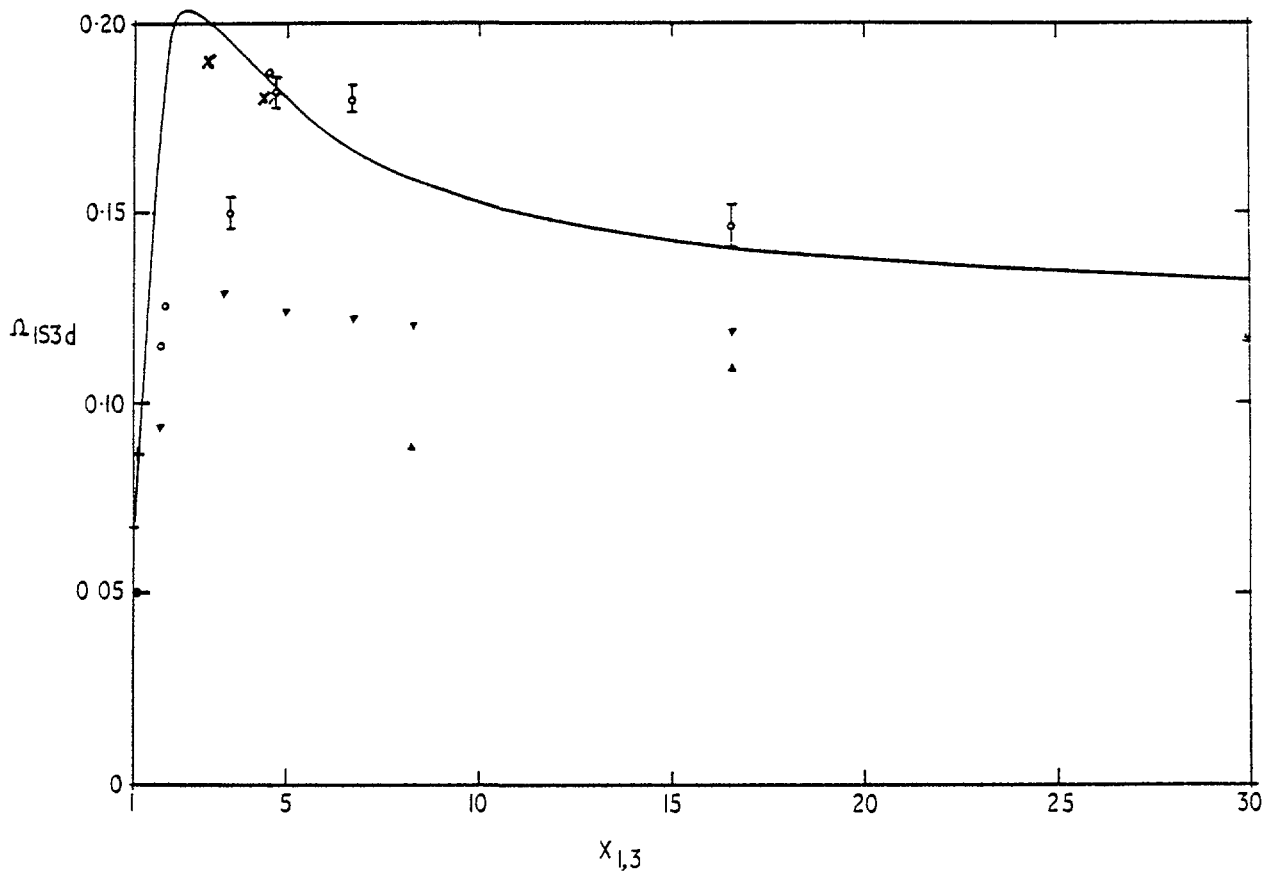


Fig. 5 As for Fig. 1 but $\Omega_{1s,3d}$. The experimental points are shown as \circ . Theoretical values are +, 18CC²; \circ UB²²; \times 12/13 NECC¹⁷; \blacktriangle DWPO II¹⁹; ∇ Glauber²⁰. The solid line is eqn (11).

Quite surprisingly both it and the FBA tend to the accurate CC calculations near threshold. Johnson's formula is poor in the threshold region but is a better approximation to the quantal result for $4.0 < X < 15$ than is the FBA. It suggests that the minimum near $X = 1.4$ may possibly be real. For the present we recommend the Hata et al values for $X < 1.04$ and our quantal curve for $X > 2$, but cannot recommend values for the intermediate range.

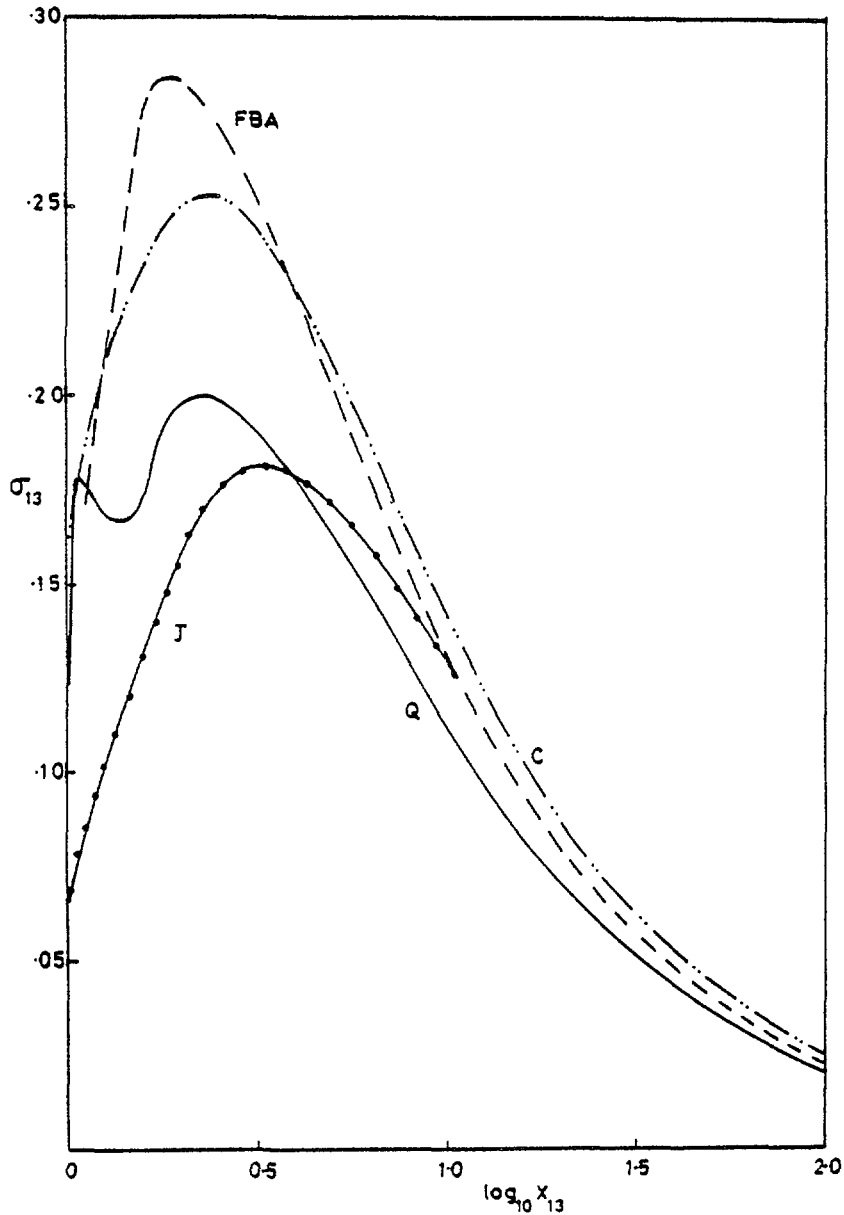


Fig. 6 $\sigma_{13} (\pi a_0^2)$. The solid curve Q is our best estimate. The minimum near $X = 1.4$ may not be real. FBA is the Born, C the Classical and J the Johnson semi-empirical result.

Results for $(n, n') = (2, 3), (2, 4), (3, 4), (1, 4)$

(a) σ_{23} . There are no experimental measurements. We suggest these should be a high priority. The value of σ_{23} is a vital parameter in estimating the ionisation state of atomic hydrogen in plasmas. Johnson and Hinno²⁴ give tables based on Johnson's¹ semi-empirical formula. The classical³, semi-empirical¹ and FBA values of σ_{23} are shown in Fig. 7, together with the accurate quantal calculations of Hata et al². These however extend only from $X = 1.07$ to $X = 1.3$, but confirm that the semi-empirical result which was filled to earlier 6CC calculations is about 75% too high near threshold. Both semi-empirical and classical calculations tend to the FBA at high energies.

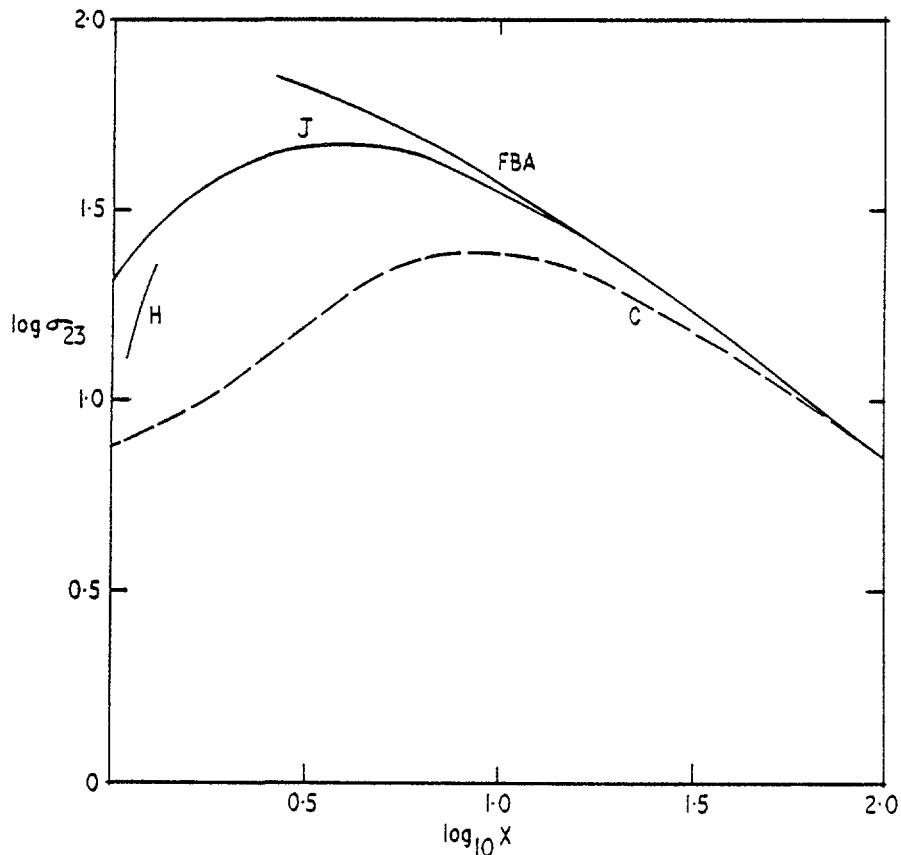


Fig. 7 σ_{23} (πa_0^2). As Fig. 6, but curve H is the Hata et al² quantal calculation.

We have also carried out 10 NECC calculations¹⁸ at two energies, $X = 12.1$ and $X = 22.4$. These results cannot be given great reliance since they do not include exchange effects and omit coupling to states higher than $n = 4$. Further work including these effects is in progress. We do not recommend any values except those of Hata et al in the range $1.07 \leq X \leq 1.30$ which should be reliable to within $\pm 10\%$. Improved quantal calculations are urgently required for $1.3 < X < 10$. We are intending to improve the 10 NECC results at $X = 12.1, 22.4$ by including localised exchange and a closed second Born approximation to the states with $n > 4$. We also propose, in collaboration with others, to extend Somerville's early work on the Unitarised FBA to a wide range of (n, n') cross sections.

(b) Other (n, n') transitions. Apart from the FBA semi-empirical and classical results there is little information. Edmunds and McDowell¹⁸ have reported 10 NECC values at two energies (corresponding to impact energies of 35 and 54.4 eV for $(1, n')$) for all (n, n') with $n, n' \leq 4$. We see no point in retabulating these values as until exchange effects and higher state couplings are included we have no way of assessing their reliability. Other, independent, calculations would be welcome.

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