Born Cross Sections for Inelastic Scattering of Electrons by Hydrogen Atoms. III. 5*s*, 5*p*, 5*d*, 5*f*, 5*g* States*†

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Born total cross sections are computed for the strong optically allowed transitions from $n=5$ to $n'=6$, at incident energies between 0.2 ev and 1361 ev. Thirty energy values are considered for the 5*s* to 6*p* and 5*g* to 6*h* cases, and nine for the other transitions. The cross sections obtained are larger than those of comparable transitions for lower *n*. The Bethe (dipole) approximation is also used, and is found to give good agreement with the Born results down to relatively low energies (≈ 3 ev).

INTRODUCTION

THIS paper extends the previous computations[1,2] of the Born cross sections, for inelastic scattering of electrons by hydrogen atoms, to the 5*s*, 5*p*, 5*d*, 5*f*, and 5*g* states. The five strong optically allowed transitions from $n=5$ to $n'=6$ are considered.

FORMULATION

The Born total cross section for the transition from the state nl to the state $n'l'$ was shown in Paper I to be of the form

$$\sigma_{nl,n'l'}(k)/\pi a_0^2 = B_{nl,n'l'}(ka_0)^{-2}(a_{-1}I_{2(n+n')}^{-1} + a_1 I_{2(n+n')}^1 + a_3 I_{2(n+n')}^3 + \cdots + a_t I_{2(n+n')}^t),$$

where

$$I_q^{-1} = \left[\frac{1}{2}\sum_{\nu=1}^{q-1}\{(q-\nu)(1+\gamma^2)^{q-\nu}\}^{-1} - \frac{1}{2}\ln(1+1/\gamma^2)\right]_{\gamma_1}^{\gamma_2},$$

$$I_q^r(r\geq 1) = \left[\frac{1}{2}\sum_{\nu=0}^{\frac{1}{2}[r-1]}(-1)^{\nu+1}\binom{\frac{1}{2}[r-1]}{\nu}\{(q-1-\tfrac{1}{2}[r-1]+\nu)(1+\gamma^2)^{q-1-\frac{1}{2}[r-1]+\nu}\}^{-1}\right]_{\gamma_1}^{\gamma_2}.$$

The γ limits are related to the momentum $\hbar\mathbf{k}$ and energy E of the incident electron by[3]

$$\gamma_2\gamma_1 = (n'-n)/(n'+n), \quad ka_0 = (\gamma_2+\gamma_1)(n'+n)/2n'n,$$
$$E = 13.6050(ka_0)^2 \text{ ev}.$$

The constants B and a_r are determined by the particular transition; a_0 is the Bohr radius. For $n=5$ to $n'=6$ transitions, $t=31$. The cross section represents an average over the initial, and sum over the final, magnetic quantum numbers.

RESULTS

The total cross sections for the 5*s* to 6*p* and the 5*g* to 6*h* transitions were calculated at thirty incident energies between 0.196 ev and 1361 ev. For the 5*p* to 6*d*, 5*d* to 6*f*, and 5*f* to 6*g* transitions, nine energies were considered. Threshold is at 0.166 ev. Computations were performed at the lower energies, where the Born approximation is invalid, for use in the development of simpler approximation formulas for the cross section.[4]

The coefficients in $\sigma(k)$ for the various transitions are listed in Table I.

Strong cancellation occurs both in the I_q^r and in the summation in $\sigma(k)$, particularly for the lower l values, and appears to increase with n. In a few instances, though the calculations were begun with eleven figures, no digits are reportable for the total cross section in Table II. Much of the repetitive portions of the calculations was performed on a Burroughs E101 digital computer. Each value in the tables is believed to be accurate to an error of no more than one in the last digit.

The cross sections are plotted in Fig. 1.

DISCUSSION

Previous work[5,1] on the $n=2$ to $n'=3$ and $n=3$ to $n'=4$ transitions indicated that the largest cross sec-

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‡ On sabbatical leave from St. John's University from January to August, 1960.

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[2] L. Fisher, S. N. Milford, and F. R. Pomilla, Phys. Rev. **119**, 153 (1960). Hereafter referred to as Paper II.

[3] H. Bethe and E. Salpeter, *Quantum Mechanics of One- and Two-Electron Atoms* (Springer-Verlag, Berlin, Germany, 1957), p. 1.

[4] S. N. Milford, Astrophys. J. **131**, 407 (1960).

[5] H. S. W. Massey and E. H. S. Burhop, *Electronic and Ionic Impact Phenomena* (Oxford University Press, New York, 1952), pp. 170–171.

TABLE I. Born cross-section coefficients.[a]

	$5s$-$6p$	$5p$-$6d$	$5d$-$6f$	$5f$-$6g$	$5g$-$6h$
B	3.9780866254(2)	4.0887388712(2)	5.5264350352(2)	7.7589636832(2)	1.0972271875(3)
a_{-1}	1.0000000000(0)	1.0000000000(0)	1.0000000000(0)	1.0000000000(0)	1.0000000000(0)
a_1	−1.0240000000(2)	−8.0400000000(1)	−5.8400000000(1)	−3.6400000000(1)	−1.4400000000(1)
a_3	3.6595303110(3)	2.6570943694(3)	1.4121643611(3)	5.7767948051(2)	9.8400000000(1)
a_5	−5.7230077718(4)	−4.1278829771(4)	−1.6761170916(4)	−4.5813956709(3)	−2.8000000000(2)
a_7	4.8548074630(5)	3.5165666529(5)	1.1355221015(5)	2.0000720587(4)	5.2498181818(2)
a_9	−2.4914736053(6)	−1.7826961481(6)	−4.7288896046(5)	−4.9916157208(4)	−4.6618181818(2)
a_{11}	8.2001519318(6)	5.6593387991(6)	1.2568581020(6)	8.0400716473(4)	6.7556363636(2)
a_{13}	−1.7892761494(7)	−1.1603535305(7)	−2.1565447393(6)	−9.7605384756(4)	−2.0058181818(2)
a_{15}	2.6385623835(7)	1.5607917101(7)	2.3801066094(6)	9.1218577226(4)	1.3135818181(3)
a_{17}	−2.6531569956(7)	−1.3809389874(7)	−1.6604754139(6)	−5.2221335064(4)	
a_{19}	1.8187343637(7)	7.9550297232(6)	7.0326572042(5)	1.2905228571(4)	
a_{21}	−8.4211925696(6)	−2.9044990593(6)	−1.6425962687(5)		
a_{23}	2.5822640676(6)	6.3726228874(5)	1.6348482156(4)		
a_{25}	−5.0606951675(5)	−7.5600096916(4)			
a_{27}	5.9510361106(4)	3.7381132623(3)			
a_{29}	−3.7274453051(3)				
a_{31}	9.4171954745(1)				

[a] The numbers in parenthesis are scale factors. E.g., $-1.024(2) = -1.024\times 10^2$.

tions would be for optically allowed transitions in which n and l change in the same sense; these are the ones investigated for the $n=5$ to $n'=6$ case. The cross sections are considerably larger than for comparable transitions of lower n, in agreement with the trend noted in Papers I and II.

For allowed transitions the Bethe (dipole) approximation was given in Paper I as

$$\sigma_{nl,n'l'}(k)/\pi a_0^2 = g_{nl,n'l'}(ka_0)^{-2}\ln[b_{nl,n'l'}(ka_0)^2],$$

TABLE II. Born total cross sections (units of πa_0^2).

Energy (ev)	$5s$-$6p$	$5p$-$6d$	$5d$-$6f$	$5f$-$6g$	$5g$-$6h$
0.196					469(1)
0.351					1174(1)
0.443		1(3)	2(3)	527(1)	1260(1)
0.537		2(3)	3(3)	568(1)	1274(1)
0.800	14(2)	19(2)	31(2)	587(1)	1193(1)
1.06	15(2)	20(2)	31(2)	561(1)	1084(1)
1.22	15(2)	19(2)	31(2)	542(1)	1026(1)
1.67	15(2)				8833
2.16	14(2)				7690
3.67	11(2)	14(2)	20(2)	327(1)	5585
4.92	10(2)				4607
8.73	73(1)				3081
13.3	56(1)	63(1)	91(1)	140(1)	2257
19.7	43(1)				1671
26.9	35(1)				1311
34.8	29(1)				1067
43.5	24(1)				892.5
53.0	21(1)	23(1)	33(1)	489	761.0
65.5	18(1)				640.1
78.7	16(1)				549.9
92.2	14(1)				482.2
107.8	12(1)				423.2
121.0	11(1)				384.1
139.9	99				340.0
165.6	86				294.8
217.4	69				233.9
276.7	57				190.3
340.2	48				159.3
680.3	27				87.26
1360.6	15	16	22	31.6	47.44

where

$$g_{nl,n'l'} = (4/3)[(l+1)/(2l+1)]\,|J_{nl,n'l'}/a_0|^2,$$

$$b_{nl,n'l'} = 4(\kappa_c a_0)^2(nn')^4/(n'^2-n^2)^2.$$

The radial integrals $|J/a_0|^2$ are tabulated by Green *et al.*[6] The cutoff momentum κ_c for each transition was obtained by equating the Bethe expression to the Born cross section at the highest energy calculated. Values for $\kappa_c a_0$ are given in Table III, together with the estimated energies $E(1\%)$ and $E(10\%)$ at which the Bethe and Born cross sections differ by 1% and 10%, re-

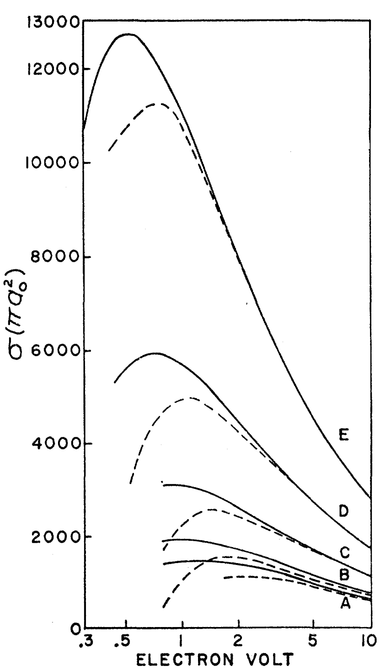

FIG. 1. Born (solid curves) and Bethe (broken curves) total cross sections for the 5–6 transitions of H atoms. (A) $5s$-$6p$. (B) $5p$-$6d$. (C) $5d$-$6f$. (D) $5f$-$6g$. (E) $5g$-$6h$.

[6] L. C. Green, P. P. Rush, and C. D. Chandler, Astrophys. J. Suppl. **3**, 37 (1957).

TABLE III. Momentum cutoff values and estimated energies at which the Born and Bethe cross sections differ by 1% and 10%.

	$\kappa_c a_0$	$E(1\%)$ (ev)	$E(10\%)$ (ev)
5s-6p	0.024	19	3
5p-6d	0.027	13	2.3
5d-6f	0.030	9	1.8
5f-6g	0.0360	5	1.2
5g-6h	0.04611	2.5	0.7

spectively. It will be noted that the Bethe formula reproduces the Born results to relatively low energies. It should be emphasized that $E(1\%)$ and $E(10\%)$ in this paper and in Papers I and II are rough estimates only.

Current work at St. John's University is aimed at extending these cross section results to large values of n by more approximate methods, and also to testing the range of validity of Born's approximation for the calculations to date.

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High-Frequency Region of the Bremsstrahlung Spectrum*

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The McVoy-Fano theory of the connection between the atomic photoelectric effect and the high-frequency region of the bremsstrahlung spectrum has been extended to next order in αZ. The contribution from p states is determined and is important in heavy elements. Predictions for the high-frequency limit are in reasonable agreement with experiment. Information is also obtained concerning angular distributions and polarization correlations.

I. INTRODUCTION

IN the high-frequency region of the bremsstrahlung spectrum almost all the energy of the incident electron is radiated. Since the outgoing electron is of low energy, the process cannot be treated with the Bethe-Maximon[1] methods. In contrast to the Born-approximation prediction of the Bethe-Heitler formula,[2] the bremsstrahlung cross section remains finite in the high-frequency limit, when the photon energy achieves its maximum value and the electron velocity $\beta=0$. Fano, Koch, and Motz[3] have noted that in this limit bremsstrahlung is an approximate inverse of the atomic photoelectric effect, and that a prediction for its cross section follows from the theoretical work on the photoeffect. Using Nagasaka's results[4] for the photoeffect, they obtain fairly good agreement with experiments on the bremsstrahlung "tip." A more rigorous, but limited, derivation of the relationship has been given by McVoy and Fano[5]: To lowest order in $a\equiv Ze^2$ the matrix elements for inverse photoeffect from the K shell and for the high-frequency limit of bremsstrahlung are identical, apart from normalization factors.[6]

It is now known that Nagasaka's expression for the high-energy limit of the photoeffect, which corrected the Hall formula[7] in order a, is itself incorrect in order a^2.[8–10] For all a the total cross section for the K shell in the high-energy limit is fairly well represented by[8]

$$\sigma=(4\pi e^2a^5/k)(1-4\pi a/15)\times\exp\{2[-1+(1-a^2)^{\frac{1}{2}}]\ln a-2a\cos^{-1}a\},\quad(1)$$

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[5] K. W. McVoy and U. Fano, Phys. Rev. **116**, 1168 (1959), hereafter referred to as MF, also U. Fano, Phys. Rev. **116**, 1156 (1959).

[6] We use unrationalized units and set $\hbar=c=m_e=1$; $O(x)$ shall mean "of order x" and $y=O(x)$ shall mean "y is of order x."

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