J. Phys. B: Atom. Molec. Phys., Vol. 10, No. 7, 1977. Printed in Great Britain. © 1977

Elastic scattering of electrons by molecular and atomic hydrogen

B van Wingerden, E Weigold†, F J de Heer and K J Nygaard‡
FOM Institute for Atomic and Molecular Physics, Kruislaan 407, Amsterdam, The Netherlands

Received 28 September 1976, in final form 22 November 1976

Abstract. Absolute experimental cross sections are presented for elastic differential scattering of electrons by molecular hydrogen at impact energies between 100 and 2000 eV and at scattering angles between 5 and 50°. The results are compared with the relative experimental cross sections of previous experiments and with the data of different theoretical calculations. Total elastic cross sections are considered as well. The theoretical cross sections of Khare and Shoba, including the effects of exchange and polarization, are the closest to our experimental data. The present absolute molecular hydrogen cross sections, together with the 100 and 200 eV ratio measurements of the differential elastic cross sections of H_2 and H of Lloyd and co-workers, were used to obtain a new set of absolute elastic cross sections for atomic hydrogen. These experimental data are compared with the absolute experimental cross sections obtained by Williams and with theory.

1. Introduction

Elastic scattering of electrons by molecular hydrogen is one of the simplest electron–molecule scattering processes, and it is therefore of importance to obtain accurate absolute differential cross sections for this process. The present work concerns itself with experiments in the energy range of 100–2000 eV and in the angular range of 5–55° where a number of calculations have been reported. The Born approximation has been used most extensively (Ford and Browne 1973 and references therein) with some calculations allowing for the effects of exchange (Khare and Moiseiwitsch 1965, Massey and Mohr 1932) as well as polarization (Khare and Shoba 1974, Truhlar and Rice 1974 and references therein). The eikonal approximation has been used recently by Bhattacharyya and Ghosh (1975, 1976 private communication) at electron impact energies between 9·4 and 100 eV. The more recent Born calculations of Ford and Browne (1973) and Liu and Smith (1973) concern themselves primarily with the dependence of the cross section on the accuracy of the molecular hydrogen wavefunction used in the calculations. The differential cross sections are found to be quite sensitive to the details of the molecular wavefunction for small values of the momentum transfer K. Polarization phenomena are also particularly important in this region (i.e. small scattering angles) and the various calculations differ significantly. Bonham

† School of Physical Sciences, The Flinders University of South Australia, Bedford Park, SA, Australia 5042.
‡ Department of Physics, University of Missouri–Rolla, Rolla, Missouri 65401, USA.

and Iijima (1963) have carried out Born calculations for elastic and total scattering with both the Wang (1928) and Weinbaum (1933) molecular wavefunctions, and they discussed the effect of the chemical bond on these calculations (see also §4.3). Although Srivastava *et al* (1975) recently reported some absolute differential elastic cross sections for electrons on molecular hydrogen at 3–75 eV and 20–135°, no absolute measurements have been published at 100 eV and above. The recent data of Fink *et al* (1975) at 100–1000 eV and 3–130° were normalized at 90° to their theoretical $\sigma(\theta)$ values calculated by means of the static-potential theory. Williams (1969) and Lloyd *et al* (1974) obtained relative differential cross sections at 100 and 200 eV and 20–130°. Lloyd *et al* normalized their data to the Born exchange calculations of Khare and Moiseiwitsch (1965) at 60°. The angular dependences of the differential cross sections of Williams (1969), Lloyd *et al* (1974) and Fink *et al* (1975), all using crossed-beam techniques, are in good agreement. However, they disagree significantly with the older measurements of Webb (1935) taken at 30–912 eV and 5–150° and of Hughes and McMillen (1932) at 35–200 eV and 50–170°. Arnot (1931) was the first to determine relative elastic cross sections for electrons on H_2 at 29–820 eV and 10–120°. The latter three experiments were performed with a static gas target. Both techniques should lead to equal results but, probably due to systematic errors, the older measurements give relatively too large cross sections at larger angles (see §4.1). In the work of Srivastava *et al* (1975) in the energy range of 3–75 eV a crossed-beam scattering geometry was used.

In addition to its fundamental importance in the field of electron–molecule scattering, accurate absolute elastic e–H_2 cross sections are needed to normalize elastic e–H cross sections. Lloyd *et al* (1974) measured ratios for the elastic scattering from atomic hydrogen to that from molecular hydrogen. Part of the motivation of the present e–H_2 work was, therefore, to obtain absolute elastic e–H cross sections using the relevant ratios of Lloyd *et al* (1974).

In §2 we give a brief outline of the experimental apparatus and procedure used, which is largely identical to that described in detail by Jansen *et al* (1976 to be referred to as I). The results for H_2 are summarized in §3 and compared with the experimental results of other authors as well as the most relevant theoretical calculations in §4. Section 5 contains the atomic hydrogen cross sections, derived from the cross section ratios for atomic and molecular hydrogen and the present absolute molecular hydrogen cross sections. They are compared with the recent absolute measurements of Williams (1975) as well as with the predictions of several theoretical models.

2. Experimental

The experimental apparatus, method and calibration procedure for the cross sections are identical to those discussed in detail by Jansen *et al* (1976) and only a brief outline will be given here.

The apparatus used is a conventional-type electron spectrometer. An electron gun provides an electron beam (energy between 100 and 3000 eV, current between 10^{-10} and 10^{-7} A) which, after collimation (divergence half angle 0·5°), enters a differentially pumped collision chamber. After collision the electrons are differentially selected as a function of the scattering angle by a rotatable analysing system (angular resolution 0·5° and reproducibility 10′). In this Kuyatt–Simpson-type analysing system the accepted electrons are energy-analysed by a double hemispherical electrostatic energy analyser with an energy resolution of a few electronvolts and are finally counted with a channeltron. All rotational, as well as final vibrational, states are therefore summed over in the measurements, the energy resolution function being essentially flat over several electronvolts. The gun, collision chamber and analysing system are situated in a high-vacuum chamber pumped by a liquid-air-baffled oil diffusion pump. The residual gas pressure in this chamber is 10^{-7} Torr. The target gas pressure P in the collision chamber is usually 10^{-3} Torr, which raises the pressure in the high-vacuum chamber to $0{\cdot}005P$. The primary current is measured inside the collision chamber by a Faraday cup which can be moved into and out of the primary beam. The absolute target gas pressure is measured by a Baratron membrane manometer. The earth's magnetic field is reduced by a mu-metal shielding inside the high-vacuum chamber and outside by an additional pair of Helmholtz coils resulting in a residual magnetic field of less than 1 mG in the direction perpendicular to the plane of detection and less than 5 mG in this plane.

The experimental procedure consists of measuring relative differential cross sections as a function of angle θ at fixed primary electron energies E. These relative cross sections are put on an absolute scale by measuring the energy dependence at a fixed angle and using an experimental apparatus calibration factor. The relative cross section is given by

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}(E, \theta) \propto \frac{S(E, \theta) \sin \theta}{I_{\mathrm{b}} P} \tag{1}$$

where $S(E, \theta)$ is the count rate of scattered electrons detected by the multiplier, I_{b} the primary beam current and P the target pressure. Here $\sin \theta$ accounts for the variation of the scattering path length viewed by the analyser system. Two corrections have to be made: (i) a background correction for the residual gas and (ii) a correction factor $F(E, \theta)$ related to the absorption of electrons due to total scattering in the target gas. $F(E, \theta)$ is larger for smaller E and varies over the range 1·02–1·05.

The experiment has been fully controlled by a PDP-15 computer via a CAMAC system. This enables automatic change and monitoring of external variables and direct statistical tests of the data and cross sections to be obtained. To calculate the relative differential cross section (see equation (1)) from the measured variables the same computer program is used as in I.

As described in I an apparatus calibration factor f_{c} has been determined by carrying out absolute differential cross section measurements for N_2 at $\theta = 5$–$9°$ and $E = 500$ eV. The factor is defined as

$$f_{\mathrm{c}} = \frac{1}{5} \sum_{\theta} \left(\frac{\sigma_{\mathrm{abs}}(500, \theta)}{\sigma_{\mathrm{rel}}(500)_{\theta} F(500, \theta)} \right)_{\mathrm{N}_2}, \qquad \theta = 5, 6, 7, 8 \text{ and } 9° \tag{2}$$

where $\sigma_{\mathrm{abs}}(500, \theta)$ is the measured absolute differential cross section for N_2 at 500 eV and angle θ, $\sigma_{\mathrm{rel}}(500)_{\theta}$ is the relative differential cross section for N_2 at 500 eV and angle θ as derived from the energy-dependent measurement, and $F(500, \theta)$ is the corresponding absorption correction factor.

The energy dependence of the relative cross section at 10°, i.e. $\sigma_{\mathrm{rel}}(E)_{10}$, for H_2 was measured under experimental conditions identical to those for N_2. The absolute cross section at 10°, i.e. $\sigma_{\mathrm{abs}}(E)_{10}$, for H_2 then follows from the relative one by

$$\sigma_{\mathrm{abs}}(E)_{10} = f_{\mathrm{c}} \sigma_{\mathrm{rel}}(E)_{10} F(E, 10). \tag{3}$$

Table 1. Estimated errors (%) in the absolute differential elastic cross sections.

E(eV)	$\Delta\sigma_{abs}(\theta)$	E(eV)	$\Delta\sigma_{abs}(\theta)$
100	6·6–8·1	500	6·8–8·4
150	6·3–8·0	700	6·8–8·4
200	6·8–8·4	1000	7·7–8·7
300	6·8–8·4	2000	7·7–8·7
400	6·8–8·4		

The absolute differential cross section at an energy E is then given by

$$\sigma_{abs}(\theta)_E = f_c \frac{\sigma_{rel}(E)_{10}}{\sigma_{rel}(10)_E} \sigma_{rel}(\theta)_E F(E, \theta) \tag{4}$$

where $\sigma_{rel}(E)_{10}$ is the relative cross section in the energy-dependent measurement for H_2 at $\theta = 10°$ and $\sigma_{rel}(10)_E$ is the relative cross section in the angular-dependent measurement at different preset primary electron energies. The total relative error in the absolute cross section (see equation (4)) is a combination of fractional errors. For $\sigma_{rel}(\theta)_E F(E, \theta)$ this is caused by the uncertainties in the current, gas pressure, count-rate measurements and the interpolation procedure to get the cross sections at integer degree angles. Furthermore, we have the fractional errors in f_c equal to 0·049, and in the ratio $\sigma_{rel}(E)_{10}/\sigma_{rel}(10)_E$, the latter varying between 0·034 and 0·071. In general, the error increases as a function of angle and in table 1 the minimum and maximum errors at each energy are given as a percentage. Detailed considerations have been given in I.

3. Summary of the H_2 results

The absolute elastic differential cross sections obtained for electron scattering by molecular hydrogen are summarized in table 2. The data, which are available in 1° intervals upon request, for convenience are not listed at all angles in the table. The errors have been discussed in the previous section.

4. Discussion of the results

4.1. Comparison with previous experiments

In tables 3–11 we compare our experimental results with those obtained by other workers and with the results of various calculations. Since none of the other experimental cross sections were measured absolutely, we have normalized them all to the present results. This was carried out as follows. Firstly, the average normalization factor was determined for the data of Fink *et al* (1975) at angles between 5 and 50° in table 2. Then, because the resulting normalized data of Fink *et al* (1975) had many more overlapping angles with the other experimental groups, these data were used for further normalization of the data of Lloyd *et al* (1974), Williams (1969), Webb (1935) and Arnot (1931) in a similar way between 20 and 150°. We did not consider the data of Hughes and McMillen (1932), because they 'did not make an

Table 2. Absolute differential cross sections of electrons elastically scattered by molecular hydrogen (in units of a_0^2).

θ(deg) \ E(eV)	100	150	200	300	400	500	700	1000	2000 $\times 10^2$
5	9·46	6·52	5·02	3·82	2·59	2·26	1·58	1·44	104
6	8·68	5·61	4·30	3·39	2·26	1·93	1·36	1·21	81·3
7	7·86	4·91	3·75	2·86	1·99	1·66	1·18	0·984	61·4
8	6·98	4·33	3·28	2·42	1·75	1·44	1·00	0·800	44·9
9	6·16	3·84	2·87	2·00	1·55	1·24	0·850	0·642	31·9
10	5·45	3·42	2·51	1·76	1·33	1·08	0·714	0·510	21·7
12	4·39	2·68	1·95	1·34	0·997	0·795	0·492	0·315	10·9
14	3·55	2·11	1·55	1·03	0·743	0·572	0·332	0·195	6·37
15	3·15	1·90	1·39	0·895	0·643	0·480	0·273	0·157	5·23
16	2·79	1·74	1·23	0·791	0·556	0·406	0·225	0·128	4·35
18	2·30	1·44	0·976	0·617	0·403	0·289	0·153	0·0884	3·21
20	1·92	1·17	0·800	0·478	0·303	0·211	0·108	0·0625	2·31
25	1·24	0·716	0·458	0·249	0·149	0·100	0·0537	0·0315	1·12
30	0·820	0·443	0·276	0·136	0·0797	0·0556	0·0316	0·0183	0·523
35	0·552	0·278	0·161	0·0805	0·0483	0·0348	0·0207	0·0113	0·279
40	0·372	0·175	0·101	0·0530	0·0328	0·0244	0·0137	0·0062	0·169
45	0·254	0·117	0·0692	0·0375	0·0242	0·0180	0·0088	0·0037	0·115
50	0·158	0·083	0·0474	0·0278	0·0171		0·0064	0·0025	0·069
55									

extensive study of the elastic scattering' and their results cannot be well reproduced in tabular form by using their graph.

At 100 and 200 eV (tables 3 and 5) most experiments can be compared. For these two energies there is generally good agreement between the results of this work, Fink *et al*, Lloyd *et al* and Williams, except that at 20 and 30° the cross sections of Williams are smaller than those in the present work and those of Fink *et al*. Also, at 20° the data of Lloyd *et al* are too small. The measurements of Webb (1935) and Arnot (1931) disagree with those just mentioned. In their work the relative cross section is too large at larger angles. Even at 100 eV, Webb's cross sections start to rise above 100°. The deviations may be due to back-scattering effects.

At the other overlapping energies (400 eV, table 7 and 1000 eV, table 10) there is also generally good agreement between the present work and that of Fink *et al* (1975) who normalized their data at 90° to the static-potential theory. The data of Fink *et al* given here were obtained by normalization to ours as described previously, the multiplication factor being 0·834 at 100 eV, 1·02 at 200 eV, 0·968 at 400 eV and 0·914 at 1000 eV. The relatively low factor of 0·834 at 100 eV reflects the relatively high cross sections of Fink *et al* (1975) at 100 eV (see figure 6 in their article). The internal consistency of the present set of data is demonstrated better when all data are plotted as a function of momentum transfer K (see below).

4.2. *Comparison with theory*

Our absolute data for differential scattering are generally in good agreement with the normalized ones of Fink *et al* (1975), and therefore comparison with theory generally leads to the same conclusions. In figure 1 we have given our data as a function of the momentum transfer K up to 5 a_0^{-1}. We know that when the first Born approximation

Table 3. Comparison of experimental and theoretical differential cross sections (in units a_0^2) for electrons elastically scattered by H_2 at impact energy $E = 100$ eV.

θ (deg)	This work	Fink *et al* (1975)	Lloyd *et al* (1974)	Williams (1969)	Webb (1935)	Ford and Browne (1973)		Khare and Shoba (1974)			Truhlar and Rice (1970, 1971, 1974)	Khare and Moiseiwitsch (1965)	Bhattacharyya and Ghosh (1976)
						Born	Born vibr	Born	Born E	Born EP	DS_1 EP	Born E	Eikonal EP
0						1·95				8·25		2·97	
5	9·46	11·3				1·87		1·94	2·75	5·58	12·6		9·11
10	5·45	5·42				1·66		1·72	2·42	3·97	7·49	2·45	5·85
20	1·92	1·94	1·68	1·56	1·28	1·07		1·10	1·53	1·76	2·43	1·60	2·43
30	0·820		0·832	0·735	0·547	0·580		0·592	0·808	0·813	0·750	0·859	1·02
40	0·372	0·348	0·381	0·344	0·253	0·288		0·298	0·395	0·381	0·290	0·422	0·433
50	0·158	0·167	0·185	0·180	0·132	0·146	0·149	0·152	0·194	0·187	0·135	0·207	0·196
60		0·0918	0·0940	0·0970	0·0808	0·0816	0·0840	0·0835	0·103	0·0962	0·0806	0·109	0·0984
70		0·0560	0·0557	0·0610	0·0588	0·0516	0·0537	0·0520	0·0617	0·0589	0·0322	0·0653	0·0569
80		0·0393	0·0359	0·0422	0·0417	0·0367	0·0382	0·0365	0·0420	0·0411	0·0352	0·0445	0·0376
90		0·0304	0·0287	0·0312	0·0315	0·0281	0·0294	0·0281	0·0316	0·0313	0·0253	0·0335	0·0276
100		0·0253	0·0244	0·0255	0·0261	0·0225	0·0234	0·0227	0·0252	0·0252	0·0195	0·0268	0·0217
110		0·0209	0·0207	0·0206	0·0266	0·0185	0·0192	0·0190	0·0208	0·0209	0·0160	0·0223	0·0177
120		0·0182	0·0189	0·0180	0·0281	0·0156	0·0162	0·0163	0·0176	0·0177	0·0136	0·0190	0·0148
130		0·0161	0·0185	0·0161	0·0348	0·0135	0·0140	0·0142	0·0153	0·0154	0·0117	0·0165	0·0126

Table 4. As table 3 except E = 150 eV.

θ (deg)	This work	Ford and Browne (1973) Born	Ford and Browne (1973) Born, vibr	Gupta and Khare (1976) Born	Gupta and Khare (1976) Born E	Gupta and Khare (1976) Born EP	Truhlar and Rice (1970, 1971, 1974) DS_1 EP
0		1·95				7·66	
5	6·52	1·83		1·90	2·41	4·71	11·2
10	3·42	1·54		1·58	2·00	2·91	5·89
20	1·17	0·823		0·840	1·05	1·12	1·42
30	0·413	0·356		0·368	0·448	0·435	0·358
40	0·175	0·150	0·152	0·156	0·185	0·178	0·140
50	0·083	0·072	0·0745	0·0739	0·0845	0·0832	0·079

is valid all data must lie on a common curve. We note that such a universal dependence exists for the experimental points at K larger than about three atomic units and that these points almost coincide with the first Born calculation of Ford and Browne (1973) and of Liu and Smith (1973). Both theoretical groups used very accurate molecular wavefunctions for H_2 and their results agree well with each other. Their calculations have also been rather well verified by the experiments of Ulsh *et al* (1974) at 25 keV and 1–10°. However, in figure 1 we observe that at small K values, the experimental points deviate from the common first Born curve. As found before in the case of helium (see for instance Jansen *et al* 1976) the discrepancy is caused by the polarizability of the target and by the exchange of the incoming electron with the target electrons. Because these effects become more important at low impact energies, the elastic cross sections are the largest at these energies and have the largest deviation from the Born curve as seen in figure 1. In tables 3–11, the Born results of Ford and Browne (1973) were obtained at the quoted angles by interpolation of their original data which was given as a function of K. Ford and Browne (1973) have also calculated the cross sections for vibrational excitation. Because our data do not correspond to pure elastic scattering, but include vibrational excitations, we have to compare with (Born) calculations including that excitation. As can be seen from tables 3–11, the calculations of Ford and Browne (1973) show that the only effect of including vibrational excitation is to increase the cross sections marginally at large K. The calculations do not extend further than $K = 5{\cdot}8\ a_0^{-1}$ where the increase is 5·8%. None of the other calculations presented in tables 3–11 include the effect of vibrational excitation, so that we have neglected it in the comparison of the other calculations with our experimental data. In tables 3–11, where we compare the experimental data with different theoretical calculations, we can also see the influence of the effect of exchange of electrons and of polarization of the target by considering the different plane-wave approximations of Khare and Shoba (1974) at E = 100 and 200 eV (see also figure 3 of their paper) and S N Gupta and S P Khare (1976 unpublished) who have extended the work of this group at other impact energies. It is clear that their approximation, including the effects of exchange and polarization, is closest to our experiment (see 100 and 200 eV data, tables 3 and 5). The results of other calculations including exchange and polarization in tables 3–11 are presented by the polarized Born (DS_1) data of Truhlar and Rice (1970, 1971, 1974) and by the eikonal data of P K Bhattacharyya and A S Ghosh (1976 private communication).

Table 5. As table 3 except $E = 200$ eV.

θ (deg)	This work	Fink *et al* (1975)	Lloyd *et al* (1974)	Williams (1969)	Webb (1935)	Arnot (1931) 205 eV	Ford and Browne (1973) Born	Ford and Browne (1973) Born, vibr	Khare and Shoba (1974) Born	Khare and Shoba (1974) Born E	Khare and Shoba (1974) Born EP	Truhlar and Rice (1970, 1971, 1974) DS_1 EP	Khare and Moiseiwitsch (1965) Born E
0							1·95				7·37		2·43
5	5·02	5·42					1·80		1·86	2·23	4·18	10·2	
10	2·51	2·53				2·18	1·42		1·47	1·75	2·39	4·77	1·77
20	0·800	0·778	0·505	0·647	0·423	0·619	0·638		0·657	0·773	0·790	0·898	0·806
30	0·276		0·255	0·243	0·169	0·204	0·235	0·238	0·243	0·280	0·269	0·214	0·291
40	0·101	0·0916	0·0941	0·102	0·0651	0·0814	0·0915	0·0938	0·0940	0·105	0·103	0·095	0·107
50	0·0474	0·0497	0·0544	0·0485	0·0399	0·0529	0·0455	0·0473	0·0455	0·0494	0·0494	0·046	0·0491
60		0·0296	0·0290	0·0296	0·0280	0·0354	0·0281	0·0292	0·0281	0·0298	0·0300	0·0252	0·0294
70		0·0206	0·0192	0·0211	0·0190	0·0256	0·0191	0·0199	0·0195	0·0205	0·0210	0·0164	0·0204
80		0·0143	0·0144	0·0151	0·0151	0·0167	0·0133	0·0138	0·0140	0·0146	0·0147	0·0116	0·0147
90		0·0103	0·0100	0·0107	0·0127	0·0154	0·00921	0·00967	0·0101	0·0104	0·0105	0·00809	0·0107
100		0·00743	0·00887	0·00783	0·0116		0·00665	0·00704	0·0073	0·0075	0·0075	0·00564	0·00776
110		0·00567	0·00552	0·00582	0·0112				0·0054	0·0055	0·0055	0·00403	0·00574
120		0·00458		0·00459	0·0106				0·0041	0·0042	0·0042	0·00302	0·00439
130		0·00377		0·00378	0·00938				0·0033	0·0036	0·0036	0·00238	0·00350

Table 6. As table 3 except E = 300 eV.

θ (deg)	This work	Ford and Browne (1973) Born	Ford and Browne (1973) Born, vibr	Gupta and Khare (1976) Born	Gupta and Khare (1976) Born E	Gupta and Khare (1976) Born EP
0		1·95				7·09
5	3·82	1·73		1·79	2·02	2·52
10	1·76	1·23		1·26	1·42	1·77
20	0·478	0·415		0·421	0·467	0·456
30	0·136	0·120	0·122	0·123	0·134	0·129
40	0·0530	0·0467	0·0489	0·0468	0·0495	0·0495
50	0·0278	0·0256	0·0269	0·0256	0·0266	0·0268

Table 7. As table 3 except E = 400 eV.

θ (deg)	This work	Fink *et al* (1975)	Webb (1935) 412 eV	Ford and Browne (1973) Born	Ford and Browne (1973) Born, vibr	Gupta and Khare (1976) Born	Gupta and Khare (1976) Born E	Gupta and Khare (1976) Born EP	Truhlar and Rice (1970, 1971, 1974) 412 eV DS_1 EP
0				1·95				6·95	
5	2·59	2·63		1·66		1·71	1·88	3·09	7·40
10	1·33	1·32	1·04	1·07		1·09	1·19	1·39	2·33
20	0·303	0·295	0·226	0·275	0·278	0·285	0·306	0·295	0·244
30	0·0797		0·0931	0·0724	0·0753	0·0739	0·0777	0·0765	0·0695
40	0·0328	0·0329	0·0422	0·0308	0·0320	0·0307	0·0317	0·0319	0·026
50	0·0171	0·0177	0·0223	0·0169	0·0176	0·0174	0·0178	0·0179	0·0138
60		0·00970		0·00921	0·00958	0·0101	0·0103	0·0103	0·00760
70		0·00544				0·0056	0·0057	0·0057	0·00393
80		0·00343				0·0032	0·0033	0·0033	0·00216
90		0·00236				0·00209	0·0021	0·0021	0·00131
100		0·00173				0·0015	0·0015	0·0015	0·000837
110		0·00135				0·0013	0·0013	0·0013	0·000552
120		0·00111				0·00107	0·00107	0·00107	0·000381
130		0·000936				0·0009	0·0009	0·0009	0·000280

Table 8. As table 3 except E = 500 eV.

θ (deg)	This work	Ford and Browne (1973) Born	Ford and Browne (1973) Born, vibr	Gupta and Khare (1976) Born	Gupta and Khare (1976) Born E	Gupta and Khare (1976) Born EP
0		1·95				
5	2·26	1·60		1·65	1·77	2·77
10	1·08	0·939		0·953	1·02	1·14
20	0·211	0·194	0·197	0·201	0·213	0·204
30	0·0556	0·0502	0·522	0·0505	0·0523	0·0522
40	0·0244	0·0227	0·236	0·0228	0·0233	0·0235
50		0·0115	0·0120	0·0124	0·0126	0·0126

Table 9. As table 3 except E = 700 eV.

θ (deg)	This work	Ford and Browne (1973) Born	Born, vibr	Gupta and Khare (1976) Born	Born E	Born EP
0		1·95				6·77
5	1·58	1·48		1·52	1·60	2·31
10	0·714	0·72		0·736	0·773	0·808
20	0·108	0·110	0·113	0·113	0·117	0·113
30	0·0316	0·0306	0·319	0·0306	0·0312	0·0314
40	0·0137	0·0136	0·0141	0·0143	0·0144	0·0144
50	0·0064			0·0063	0·0064	0·0064

Table 10. As table 3 except E = 1000 eV.

θ (deg)	This work	Fink *et al* (1975)	Ford and Browne (1973) Born	Born, vibr	Gupta and Khare (1976) Born	Born E	Born EP
0			1·95				6·70
5	1·44	1·43	1·32		1·36	1·41	1·85
10	0·510	0·559	0·511		0·517	0·535	0·531
20	0·0625	0·0572	0·0594	0·0618	0·0602	0·0613	0·0609
30	0·0183		0·0186	0·0193	0·0191	0·0193	0·0194
40	0·0062	0·0062	0·00668	0·00694	0·0074		
50	0·0025	0·0025			0·0027		
60		0·00129			0·00141	0·00141	0·00141
70		0·000817			0·000912	0·000913	0·000913
80		0·000523			0·000552	0·000552	0·000552
90		0·000340			0·000349	0·000349	0·000349
100		0·000258			0·000262	0·000262	0·000262
110		0·000206			0·000213	0·000213	0·000213
120		0·000160			0·000172	0·000172	0·000172
130		0·000129			0·000139	0·000139	0·000139

Table 11. As table 3 except E = 2000 eV.

θ (deg)	This work	Ford and Browne (1973) Born	Born, vibr	Gupta and Khare (1976) Born	Born E	Born EP
0		1·95				6·62
5	1·04	0·93		0·952	0·969	1·08
10	0·217	0·192	0·0195	0·199	0·202	0·193
20	0·0231	0·0217	0·0226	0·0220	0·0221	0·0222
30	0·00523			0·0054		
40	0·00169			0·0026		
50	0·00069			0·0016		

The latter eikonal data were obtained by Bhattacharyya and Ghosh (1976) by taking into account all orientations of the target molecule, while in their earlier paper (Bhattacharyya and Ghosh 1975) only considered three orientations to average the molecular angles. On considering all the 'exchange–polarization' calculations, it can be seen that the overall best agreement with experiment is given by the calculations of Khare and co-workers. However, at 5 and 10°, the difference between their calculation and

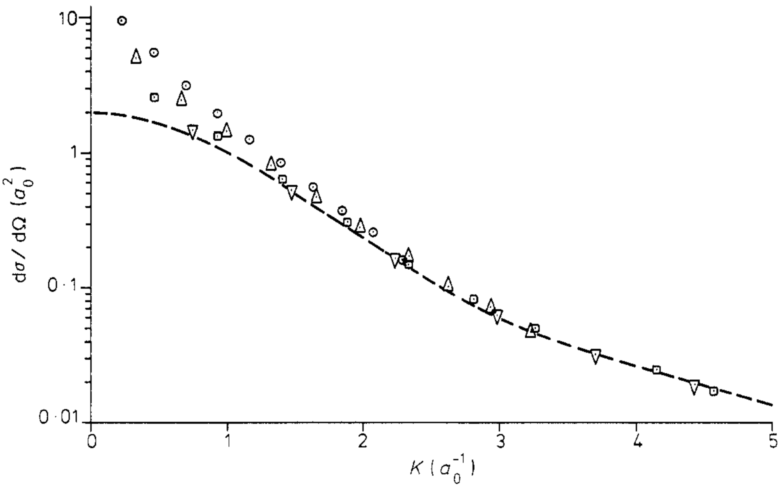

Figure 1. Absolute differential cross sections for electrons elastically scattered by H_2 plotted against momentum transfer K at impact energies of 100 (○), 200 (△), 400 (□) and 1000 eV (▽); broken curve, first Born approximation.

experiment is often very large. At 100 eV and these angles the calculation of Bhattacharyya and Ghosh gives better results.

4.3. The independent-atom model (IAM)

Very often the experimental cross sections of molecules are compared with calculations based on the independent-atom model (IAM); see for instance Massey *et al* (1969), Bonham and Fink (1974). In such a model the scattering is described by a coherent superposition of the scattering on the atoms, in which the contribution of the molecular bond is improperly treated. In this model the differential elastic cross sections for H_2 can be presented by

$$\frac{d\sigma}{d\Omega} = \frac{8(8Z^2 + K^2)^2}{(4Z^2 + K^2)^4} \left(1 + \frac{\sin Kd}{Kd}\right) a_0^2. \tag{5}$$

In the IAM the first factor on the right-hand side corresponds to the Born elastic scattering from two atomic hydrogen atoms ($Z = a_0^{-1}$) and the second factor accounts for the interference effect. The quantity d is the most probable internuclear distance, equal to 1·401 a_0. However, due to the improper treatment of the binding effect, the IAM cross sections differ from experiment, as has been first shown by Geiger (1964) for elastic scattering studying the angular distribution of 25 keV electrons scattered by H_2. Roscoe (1938) has calculated the Born differential elastic cross section for H_2 by means of eigenfunctions of Wang (1928), Rosen (1931) and Weinbaum (1933), and Bonham and Iijima (1963) have improved these calculations to study the binding effect. From the theoretical and experimental work mentioned before it follows that equation (5) leads to good approximate results compared to the Born approximation, except at the smaller angles, when Z is taken equal to 1·166 a_0^{-1} (corresponding to Wang 1928), or to 1·193 a_0^{-1} (corresponding to Weinbaum 1933). In table 12 we compare the IAM and modified IAM results with the Born results of Liu and Smith (1973). We see that for most K values (not near zero) there is good agreement between Born and IAM with $Z = 1{\cdot}193\ a_0^{-1}$, that is within about

Table 12. Comparison of differential elastic scattering cross sections (in units a_0^2) obtained by the Born approximation (Liu and Smith 1973) with those of the (modified) independent-atom model (see equation (5)) taking Z equal to $1\,a_0^{-1}$, $1{\cdot}166\,a_0^{-1}$ and $1{\cdot}193\,a_0^{-1}$ respectively and $d = 1{\cdot}401\,a_0$.

		(Modified) independent-atom model		
$K(a_0^{-1})$	Born	$Z = 1\,a_0^{-1}$	$Z = 1{\cdot}166\,a_0^{-1}$	$Z = 1{\cdot}193\,a_0^{-1}$
0	1·90	4·00	2·16	1·98
0·143	1·88	3·93	2·13	1·95
0·428	1·60	3·40	1·90	1·74
0·890	1·11	2·07	1·27	1·18
1·14	0·831	1·42	0·933	0·873
1·43	0·561	0·883	0·622	0·587
2·00	0·234	0·315	0·250	0·240
2·57	0·100	0·119	0·102	0·0994
2·85	0·0690	0·0777	0·0689	0·0675
4·28	0·0209	0·0213	0·0204	0·0202
5·71	0·00819	0·00826	0·00812	0·00809
7·14	0·00287	0·00289	0·00286	0·00286
10·7	0·00063	0·00063	0·00063	0·00063
14·3	0·00020	0·00020	0·00020	0·00020

5%. For $Z = 1{\cdot}166\,a_0^{-1}$, the agreement starts above $K = 2\,a_0^{-1}$. All results are close to each other above $K = 4\,a_0^{-1}$. In figure 1 we have seen that the experimental elastic scattering data for e–H_2 almost agree with the Born approximation above about $K = 3\,a_0^{-1}$. This means that for $K = 4\,a_0^{-1}$, the IAM with $Z = a_0^{-1}$ gives a good description for the elastic scattering from H_2. As K increases the first factor on the right-hand side of equation (5) obviously approaches the formula for Rutherford scattering for the two hydrogen nuclei,

$$\left(\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\right)_{\mathrm{R}} = 2\frac{4}{K^4}. \tag{6}$$

In that case the screening effect of the electrons becomes negligible.

4.4. *Total elastic cross sections*

In order to obtain experimental total elastic cross sections, the differential elastic cross sections were integrated according to

$$\sigma_{\mathrm{el}} = 2\pi \int_0^{\pi} \sigma_{\mathrm{el}}(\theta) \sin\theta\, \mathrm{d}\theta. \tag{6}$$

Since the present data were restricted to angles between 5 and 50°, we used the sets of Fink *et al* (1975) normalized to our data for angles between 50 and 130° (the largest angle in their experiment). At energies of 150, 300, 700 and 2000 eV, where Fink *et al* (1975) had no data, we constructed additional cross sections at larger angles by using the fact that at large K values these cross sections are approximately a unique function of K, independent of impact energy. For the largest angles we extrapolated our data by means of the IAM formula with $Z = 1{\cdot}193$ (see §4.3). Between 0 and 5° we extrapolated the integrand $\sigma_{\mathrm{el}}(\theta)\sin\theta$ by a parabolic function.

Table 13. Integrated elastic cross sections (in units of a_0^2) for electron scattering by molecular hydrogen.

Energy (eV)	This work	Ford and Browne (1973) Born	Gupta and Khare (1976) Born	Born E	Born EP	Truhlar and Rice (1970, 1971, 1974) DS_1 EP	Bhattacharyya and Ghosh (1975) Eikonal EP
100	3·17	1·68	1·73†	2·30†	2·72†	3·65	3·83
150	1·85	1·15	1·16	1·42	1·69	2·45	
200	1·28	0·872	0·89†	1·04†	1·22†	1·85	
300	0·809	0·587	0·60	0·66	0·79		
400	0·543	0·443	0·45	0·49	0·58		
412						0·899	
500	0·420	0·355	0·36	0·39	0·46		
600						0·452	
700	0·260	0·255	0·26	0·27	0·32		
1000	0·186	0·179	0·18	0·19	0·22		
2000	0·097	0·0895	0·09	0·09	0·10		

† Calculated by Khare and Shoba (1974).

We obtained σ_{el} of Ford and Browne (1973) by using their Born values for differential elastic scattering, given up to $K = 5{\cdot}8\ a_0^{-1}$, and extrapolating at larger K values again by means of the IAM formula with $Z = 1{\cdot}193$. Our experimental results, which have errors within about $\pm 10\%$, are given in table 13 and compared with theoretical calculations of different groups. The best agreement is obtained with the Born EP calculations of Gupta and Khare (1976), although differences are present up to a factor of about 1·30 at 700 eV. Calculations show that at 1000 and 2000 eV the contribution to the integrand comes for a large part from angles between about 0 and 10°. Thus we need very accurate measurements at small angles to get reliable σ_{el} values at high energies.

In figure 2 we illustrate some of the data in a plot of $\sigma_{el}E$ against E. Inokuti and McDowell (1974) show that such a plot is useful, because in the Born approximation the cross section can be given by

$$\sigma_{el} = \pi k^{-2}(A + Bk^{-2} + Ck^{-4} + Dk^{-6} + \ldots)\, a_0^2 \tag{7}$$

where k^2 is the energy in rydbergs. The constants in equation (7) have been given by Inokuti and McDowell (1974) for electron–atom scattering. It is clear that our experimental results approach the Born values near 2000 eV. The σ_{el} value of Ulsh *et al* (1974) at 25 keV is equal to $0{\cdot}00789\, a_0^2$, corresponding to $\sigma_{el}E = 197\, a_0^2$ eV; using the Born values of $\sigma_{el}(K)$ of Ford and Browne (1973) and extrapolating for larger K values as mentioned before, we find at 25 keV that $\sigma_{el} = 0{\cdot}00719\, a_0^2$ and $\sigma_{el}E = 180\, a_0^2$ eV.

5. Elastic electron–atomic-hydrogen scattering cross sections

The elastic scattering of electrons by atomic hydrogen is the simplest non-trivial atomic elastic scattering process, and it has therefore attracted a great deal of theoretical attention. Unfortunately, due to the difficulty of producing pure ground-state atomic hydrogen beams, there have been only two experimental investigations of

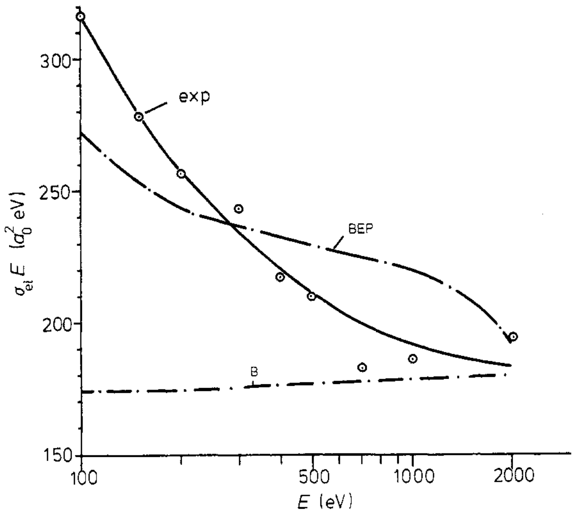

Figure 2. Total elastic cross sections multiplied by impact energy E plotted against E for electrons elastically scattered by H_2. —○— present experiment (error smaller than about 10%); –·–·– (B) Born approximation of Gupta and Khare (1976); —·—·— BEP) Born–exchange–polarization approximation of Gupta and Khare (1976).

the elastic scattering of electrons by atomic hydrogen in the intermediate-energy range, both using a modulated atom beam in their crossed-beam technique.

Lloyd *et al* (1974) measured the ratios of the atomic hydrogen to molecular hydrogen scattering cross sections over the angular range 15–130° at a number of energies. They also measured the elastic molecular hydrogen angular distributions, and by normalizing these distributions to the calculated cross sections of Khare and Moiseiwitsch at 60°, they obtained values of the atomic hydrogen elastic differential cross sections.

Absolute atomic differential cross sections were obtained by Williams (1975) using a quite different procedure. Firstly, absolute cross section values in helium were calculated by making a phaseshift analysis of the elastic scattering from helium around the $1s2s^2\ ^2S$ resonance. From measurements of relative beam flux densities for helium and molecular hydrogen beams, and of the dissociation fraction of 3000 °C molecular hydrogen beams, absolute cross section values in atomic hydrogen were then determined. The measurements also required accurate determination of electron beam optics, atomic beam profiles, transmission of scattered electrons in the energy analyser and lenses as a function of energy, detector efficiency as a function of angle and energy, and variation of the analyser solid angle with change of scattering angle. This is discussed in more detail by Williams and Willis (1975). Williams claims an accuracy of $\pm 11\%$ for his measurements.

In the present paper we use the 100 and 200 eV ratio measurements of Lloyd *et al* (1974) together with the present absolute molecular hydrogen cross sections to obtain another set of absolute elastic atomic hydrogen cross sections.

The molecular hydrogen cross sections were obtained from tables 3–11 by taking our data at 50° and below, and taking the weighted average of the normalized data of Fink *et al* (1975), Lloyd *et al* (1974) and Williams (1969) at angles larger than 50°. The resulting elastic cross sections for atomic hydrogen at 100 and 200 eV are shown in table 14. The errors quoted in parentheses are evaluated by combining the errors in the H_2 cross sections and those in the ratios given by Lloyd *et al* 1974). Also included in table 14 are the measurements of Williams (1975) with his reported errors and the cross sections calculated in various theoretical approximations. At 100 eV the agreement between the two sets of experimental results is generally very good; on average the present cross sections are larger by a factor 1·05. At 200 eV the largest differences occur at 20° (factor 1·38), at 60° (factor 1·27) and at 50° (factor 1·20). On average the present data are larger by a factor 1·16. In figure 3 we have plotted the cross sections against momentum transfer K and compared with the Born approximation (see Byron and Joachain 1975). We have not included those data of Williams (1975) which fall close to the present cross sections (within 10%). Since we expect that the 100 eV cross sections should lie higher than the 200 eV cross sections at small K ($K \leqslant 1{\cdot}5$ au), it seems probable that the present 200 eV cross sections are somewhat too high ($\sim 10\%$) as compared to the 100 eV cross sections (below 90°). In particular our cross sections seem to be too large at the 200 eV angles mentioned above. In table 14 the tabulated theoretical results are those of the eikonal Born series (EBS) the Glauber and Born approximation of Byron and Joachain (1973, 1975, 1977b), the full eikonal approximation calculations of Foster and Williamson (1976a), the second-order potential calculations of Winters *et al* (1974), the impact-parameter formalism four-state coupled-channel second-order potential calculations of Bransden and Noble (1976), the optical-model calculation of Vanderpoorten (1975) and the Born E and Born EP calculations of Jhanwar *et al* (1975) and B L Jhanwar and S P Khare (1976 unpublished). We have also included in the table the recent calculations of Foster and Williamson (1976b) which correct their earlier direct scattering amplitudes for exchange effects. The EBS theory is closest to the experimental data, followed by the BEP calculations of Jhanwar and Khare (1976), and generally in better agreement with the cross sections of Williams than our cross sections which are often larger. It is interesting to note that all the other calculations fall significantly below the experimental values. Numerical studies on dispersion relations by one of us for e^-–H scattering strongly suggest that in the forward direction the EBS approximation gives very good results above 200 eV and seems to overestimate the cross section at lower energies. This implies that the experimental cross sections may be somewhat too high, particularly at small angles. At large angles it would be desirable to have theoretical data with the static approximation which appears to be rather reliable (see Byron and Joachain 1974a, b, 1977a, b). Although the full eikonal approximation of Foster and Williamson (1976a, b) fails quite badly at large angles, the calculations do show the importance of exchange effects. That effect is also shown by the BE (Jhanwar and Khare 1976) and Born calculations. It is not surprising that the full eikonal approximation of Foster and Williamson (1976a, b) gives poor results at large angles since the straight-line eikonal trajectory is a poor approximation to the actual trajectory of an electron scattered through a large angle. The calculations of Bransden and Noble (1976) are similarly only expected to yield good results at small angles.

Table 14 also lists the integrated elastic atomic hydrogen cross sections. In order to obtain the experimental total elastic cross sections, we used equation (6) in §4.4. The experimental data of this work and of Williams (1975) were extrapolated to 10 and 180° by normalizing theoretical EBS data to the experimental ones at the smallest and largest angles used in the experiment. Between 0 and 10° we extrapolated the integrand $\sigma_{\mathrm{el}}(\theta)\sin\theta$ by a parabolic function. We see that the experimental cross sections are closest to the EBS results, which are expected to be good above 200 eV,

Table 14. Comparison of absolute experimental and theoretical differential and total cross sections (in units a_0^2) for the elastic scattering of electrons by atomic hydrogen. The numbers in parentheses are the total errors in the last significant digits.

E (eV)	θ (deg)	This work[a]	Williams (1975)	Byron and Joachain (1973, 1975, 1977b)			Vander-poorten (1975)	Foster and Williamson (1976a, b)		Winters *et al* (1974)	Bransden and Noble (1976)	Jhanwar *et al* (1975)	Jhanwar and Khare (1976)	
100	15	1·59(11)		1·45[b]	0·834[c]	0·704[d]	1·22[e]	0·925[f]	1·11[g]	1·24[h]		1·14[i]	0·931[j]	1·21[i]
	20	1·17(8)	1·10(10)	0·915	0·546	0·554	0·774	0·587	0·722	0·812	0·689[h]	0·693	0·723	0·819
	30	0·525(35)	0·509(49)	0·407	0·251	0·313	0·346			0·366	0·295	0·288	0·396	0·393
	40	0·257(21)	0·288(27)	0·199	0·124	0·171	0·167	0·121	0·139	0·180		0·146	0·210	0·201
	50	0·131(10)	0·132(12)	0·106	0·0667	0·0959	0·0879			0·0966	0·0743	0·0858	0·114	0·109
	60	0·074(8)	0·072(7)	0·0613	0·0387	0·0568	0·0501	0·0299	0·0307	0·0572		0·0548	0·0660	0·0640
	70	0·048(5)	0·049(5)	0·0385	0·0242	0·0358	0·0312			0·0350		0·0368	0·0407	0·0399
	80	0·0319(34)	0·0295(30)	0·0260	0·0161	0·0239	0·0204	0·0102	0·00905	0·0228		0·0257	0·0267	0·0264
	90	0·0227(20)	0·0209(20)	0·0188	0·0114	0·0169	0·0148			0·0161		0·0186	0·0186	0·0185
	100	0·0162(20)	0·0155(15)	0·0143	0·00848	0·0125	0·0110	0·00475	0·00423	0·0121				
	110	0·0130(15)	0·0115(12)	0·0114	0·00660	0·00970	0·00843					0·0109	0·0105	0·0105
	120	0·0107(12)	0·0092(9)	0·00948	0·00535	0·00784	0·00682	0·00280	0·00241	0·00753				
	130	0·0084(9)	0·0078(7)	0·00816	0·00451	0·00658	0·00580					0·00746	0·00706	0·00705
	σ_{el}	1·83	1·75	1·57		0·938	1·31	1·23	1·35	1·40		1·21		1·37
200	20	0·577(48)	0·419(40)	0·400	0·311	0·344	0·371	0·344	0·391	0·385	0·339	0·280	0·387	0·379
	30	0·200(15)	0·172(17)	0·154	0·121	0·144	0·142			0·150	0·132	0·109	0·158	0·156
	40	0·0774(73)	0·0706(68)	0·0657	0·0522	0·0632	0·0602	0·0459	0·0490	0·0621		0·0549	0·0682	0·0680
	50	0·0379(32)	0·0314(32)	0·0318	0·0254	0·0310	0·0290			0·0298	0·0271	0·0303	0·0329	0·0329
	60	0·0237(23)	0·0187(19)	0·0174	0·0138	0·0169	0·0159	0·00959	0·00966	0·0164		0·0177	0·0177	0·0177
	70	0·0145(13)	0·0125(14)	0·0105	0·00827	0·0101	0·00939			0·00969		0·0109	0·0105	0·0105
	80	0·0100(10)	0·0086(9)	0·00689	0·00536	0·00651	0·00612	0·00331	0·00321	0·00625		0·00713	0·00674	0·00674
	90	0·0062(8)	0·0058(6)	0·00485	0·00371	0·00450	0·00421			0·00420		0·00493	0·00463	0·00463
	100	0·00411(51)	0·00412(41)	0·00361	0·00272	0·00329	0·00309	0·00157	0·00149	0·00312				
	110	0·00347(60)	0·00323(31)	0·00282	0·00209	0·00253	0·00239					0·00274	0·00259	0·00259
	σ_{el}	0·789	0·669	0·634		0·484	0·581	0·691	0·75	0·581		0·56		0·57

[a] Also using Lloyd *et al* (1974), see text.
[b] EBS results.
[c] Glauber results.
[d] Born results.
[e] Optical-model results.
[f] Full eikonal results.
[g] 'Post' exchange-corrected eikonal results.
[h] Second-order potential results.
[i] BEP results.
[j] BE results.

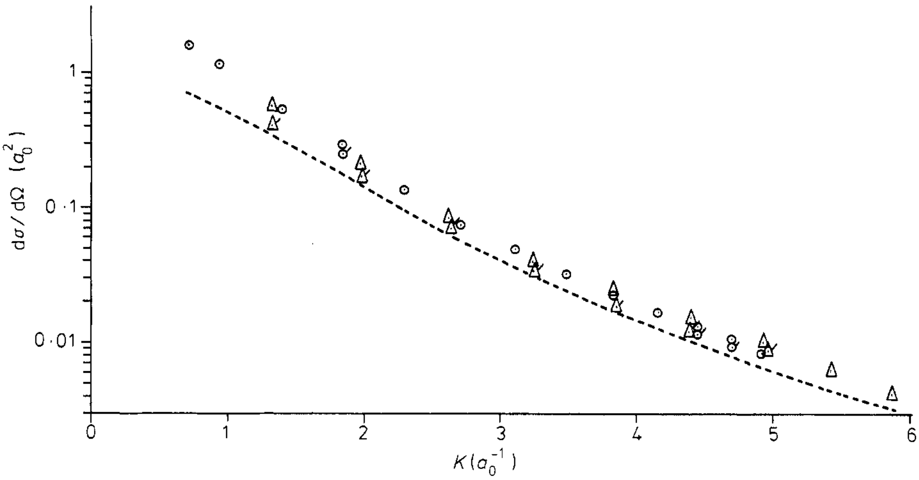

Figure 3. Absolute differential cross sections for electrons elastically scattered by H plotted against momentum transfer K at impact energies of 100 and 200 eV. Experimental points are: ○ present work, 100 eV; ○ Williams (1975), 100 eV; △ present work, 200 eV; △ Williams (1975), 200 eV. Broken curve: first Born approximation.

but are probably too large at lower energies. This conclusion is based on the analysis carried out for elastic scattering of electrons from helium by de Heer and Jansen (1975).

Acknowledgments

We are indebted to all those investigators who sent us their data in tabular form and in particular to Professor S P Khare and co-workers who carried out additional theoretical calculations. We thank Mr W van der Kaay for help with the computer programs.

This work is part of the research program of the Stichting voor Fundamenteel Onderzoek der Materie (Foundation for Fundamental Research on Matter) and was made possible by financial support from the Nederlandse Organisatie voor Zuiver-Wetenschappelijk Onderzoek (Netherlands Organisation for the Advancement of Pure Research).

References

Arnot F L 1931 *Proc. R. Soc.* **133** 615–36

Bhattacharyya P K and Ghosh A S 1975 *Phys. Rev.* A **12** 480–5

Bonham R A and Fink M 1974 *High Energy Electron Scattering, ACS Monograph 169* (New York: Van Nostrand Reinhold) chap IV

Bonham R A and Iijima T 1963 *J. Phys. Chem.* **67** 2266–72

Bransden B H and Noble C J 1976 *J. Phys. B: Atom. Molec. Phys.* **9** 2461–8

Byron F W and Joachain C J 1973 *Phys. Rev.* **8** 1267–82

——1974a *J. Phys. B: Atom. Molec. Phys.* **7** L212–5

——1974b *Phys. Lett.* **49A** 306–8

——1975 *FOM Report No* 37521

——1977a *Phys. Rev.* A **15** 128–46

——1977b *J. Phys. B: Atom. Molec. Phys.* **10** 207–26

Fink M, Jost K and Herrmann D 1975 *Phys. Rev.* A **12** 1374–82
Ford A L and Browne J C 1973 *Chem. Phys. Lett.* **20** 284–90
Foster G and Williamson W Jr 1976a *Phys. Rev.* A **13** 936–40
——1976b *Phys. Rev.* A **13** 2023–7
Geiger J 1964 *Z. Phys.* **181** 413–25
de Heer F J and Jansen R H J 1975 *FOM Report No* 37173
Hughes A L and McMillen J H 1932 *Phys. Rev.* **41** 39–48
Inokuti M and McDowell M R C 1974 *J. Phys. B: Atom. Molec. Phys.* **7** 2382–95
Jansen R H J, de Heer F J, Luyken H J, van Wingerden B and Blaauw H J 1976 *J. Phys. B: Atom. Molec. Phys.* **9** 185–212
Jhanwar B L, Khare S P and Shoba P 1975 *J. Phys. B: Atom. Molec. Phys.* **8** 1228–35
Khare S P and Moiseiwitsch B L 1965 *Proc. Phys. Soc.* **85** 821–39
Khare S P and Shoba P 1974 *J. Phys. B: Atom. Molec. Phys.* **5** 420–7
Liu J W and Smith V H 1973 *J. Phys. B: Atom. Molec. Phys.* **6** L275–9
Lloyd C R, Teubner P J O, Weigold E and Lewis B R 1974 *Phys. Rev.* A **10** 175–81
Massey H S W, Burhop E H S and Gilbody H B 1969 *Electronic and Ionic Impact Phenomena* vol 2 (Oxford: Clarendon)
Massey H S W and Mohr C B O 1932 *Proc. R. Soc.* **135** 258–75
Roscoe R 1938 *Phil. Mag.* **26** 32–41
Rosen B 1931 *Phys. Rev.* **38** 2099–114
Srivastava S K, Chutjian A and Trajmar S 1975 *J. Chem. Phys.* **63** 2659–65
Truhlar D G and Rice J K 1970 *J. Chem. Phys.* **52** 4480–501
——1971 *J. Chem. Phys.* **55** 2005
——1974 *Phys. Lett.* **47A** 372–4
Ulsh R C, Wellenstein H F and Bonham R A 1974 *J. Chem. Phys.* **60** 103–11
Vanderpoorten R 1975 *J. Phys. B: Atom. Molec. Phys.* **8** 926–39
Wang S C 1928 *Phys. Rev.* **31** 579–86
Webb G M 1935 *Phys. Rev.* **47** 384–8
Weinbaum S 1933 *J. Chem. Phys.* **1** 593–6
Williams J F 1975 *J. Phys. B: Atom. Molec. Phys.* **8** 2191–9
Williams J F and Willis B A 1975 *J. Phys. B: Atom. Molec. Phys.* **8** 1641–69
Williams K 1969 *Proc. 6th Int. Conf. on Physics of Electronic and Atomic Collisions* (Cambridge, Mass: MIT Press) p 735
Winters K H, Clark C D, Bransden B H and Coleman J P 1974 *J. Phys. B: Atom. Molec. Phys.* **7** 788–98