J. Phys. B: Atom. Molec. Phys., Vol. 12, No. 6, 1979. Printed in Great Britain

Total cross sections for electron scattering by Ne, Ar, Kr and Xe

F J de Heer, R H J Jansen† and W van der Kaay

FOM-Institute for Atomic and Molecular Physics, Kruislaan 407, Amsterdam/Wgm, The Netherlands

Received 8 September 1978

Abstract. A set of total cross sections for scattering of electrons by Ne, Ar, Kr and Xe has been evaluated over the energy range of about 20 to 3000 eV by means of the analysis of experiments and theories on total cross sections for elastic scattering, ionisation and excitation, and on differential cross sections for elastic and inelastic scattering. The total cross sections for scattering of electrons are evaluated by adding those for ionisation, excitation and elastic scattering and they are accurate to about 5–10%. They appear to be in very good agreement with the recent experimental results on total electron scattering of Wagenaar *et al.*

1. Introduction

The analysis and evaluation of cross sections for total scattering by noble gases over a large energy range was started by de Heer and Jansen (1975a, b) in connection with the theoretical work of Bransden and McDowell (see for instance Bransden and McDowell 1970) on the phaseshift and dispersion-relation analysis of electron–atom scattering. In our previous work (de Heer and Jansen 1977) a set of total cross sections of electron scattering by He, σ_{tot}, has been evaluated by adding experimental data of total cross sections for elastic scattering (σ_{el}), ionisation (σ_{ion}) and excitation (σ_{exc}). In the present article this work is extended to the other noble gas atoms Ne, Ar, Kr and Xe and must be considered as a re-consideration and extension of our previous results (de Heer and Jansen 1975b).

It is not our intention to give a review of the theoretical work on elastic and total cross sections, with which we compare our results. For that we refer the reader to an article of de Heer (1975). For convenience we have given a survey of theoretical calculations in the appendix, partly taken from Jansen (1975).

One of the best reviews of the different experiments on σ_{tot} has been given by Bederson and Kieffer (1971). In these experiments a simple beam attenuation method (see Ramsauer 1921) has been used. Recently interest in this field has been renewed (see for instance Blaauw *et al* 1977).

In the following sections we shall show how we come to our σ_{ion}, σ_{exc}, σ_{el} and σ_{tot} values successively, for Ne, Ar, Kr and Xe respectively. In the case of Ne our description of the procedure is relatively more extended for the sake of an introduction to our method of calculation.

† Present address: Waterloopkundig Laboratorium, Postbus 177, Delft, The Netherlands.

0022-3700/79/060979+24$01.00

2. Ionisation of Ne

Absolute ionisation cross sections were derived by using the experimental values of Rapp and Englander-Golden (1965), error 7%; Smith (1930), error about 7%; Asundi and Kurepa (1963), error 8%; Schram *et al* (1964, 1966b), error 7%; Gaudin and Hageman (1967), error 10%; and Fletcher and Cowling (1973), error 4%. The errors given here are those quoted by the authors. Some data are given in the compilation of Kieffer (1965) and the addendum (Kieffer 1966); see also Kieffer and Dunn (1966).

The average experimental values given in column 2 of table 1 have been derived by a procedure given by Langenberg and van Eck (1976). This procedure also allows us to use data for which the absolute scale is not known. We had to consider the data of Smith (1930) and Asundi and Kurepa (1963) in this way, because no correction is made in these data for the so called Ishii effect (Ishii and Nakayama 1961, see also de Vries and Rol 1965) in the gas pressure measurement. In the first step of the averaging procedure a weighted average of the data was derived with an absolute scale taking into account the errors given above (for Fletcher and Cowling we took 7% instead of 4%). We then fitted the data of Smith (1930) and Asundi and Kurepa (1963) to this weighted average by a kind of least-square method (see Langenberg and van Eck 1976). Then we restarted the weighted averaging procedure with all the original absolute data, including the fitted data of Smith (1930) and Asundi and Kurepa (1963). The calculations led to an external and an internal error of which the larger is given in table 1. The external error was evaluated by considering only the average experimental values with respect to

Table 1. Total cross sections for ionisation, excitation and inelastic scattering (in units of a_0^2) for electrons incident on Ne. The numbers in parentheses are the total errors in the last significant digits.

E(eV)	$\sigma_{\text{gross ion}}$ experimental average	$\sigma_{\text{count ion}}/\sigma_{\text{gross ion}}$	$\sigma_{\text{count ion}}$ experimental	$\sigma_{\text{count ion}}$ theory Saxon (1973)	σ_{exc} semi-empirical	σ_{inel} semi-empirical	σ_{inel} theory Saxon (1973)
30	0·3951 (390)	1	0·3951 (390)		0·3588 (718)	0·7539 (817)	
40	0·8647 (522)	1	0·8647 (522)		0·4836 (885)	1·348 (103)	
50	1·284 (70)	1	1·284 (70)		0·5694 (951)	1·853 (137)	
60	1·634 (74)	1	1·634 (74)		0·6084 (912)	2·242 (117)	
70	1·920 (82)	1	1·920 (82)		0·6084 (809)	2·528 (115)	
80	2·135 (76)	0·9927	2·119 (78)		0·5928 (693)	2·712 (104)	
90	2·307 (82)	0·9851	2·273 (84)		0·5772 (577)	2·850 (101)	
100	2·409 (72)	0·9771	2·354 (74)	6·852	0·5694 (474)	2·923 (88)	7·205
150	2·644 (89)	0·9646	2·550 (90)	5·340	0·5023 (334)	3·052 (96)	5·697
200	2·636 (102)	0·9548	2·517 (101)	4·414	0·4675 (233)	2·985 (104)	4·746
300	2·400 (106)	0·9416	2·260 (102)	3·328	0·3610 (180)	2·621 (104)	3·606
400	2·124 (91)	0·9420	2·001 (88)	2·702	0·2968 (148)	2·298 (89)	2·942
500	1·901 (102)	0·9450	1·796 (98)	2·289	0·2539 (127)	2·050 (99)	2·500
600	1·699 (109)	0·9524	1·618 (105)	1·995	0·2227 (114)	1·841 (106)	2·184
700	1·548 (101)	0·9527	1·475 (97)	1·772	0·1980 (99)	1·673 (98)	1·944
800	1·419 (92)	0·9548	1·355 (89)	1·598	0·1803 (90)	1·535 (89)	1·756
900	1·305 (91)	0·9553	1·247 (88)	1·458	0·1649 (82)	1·412 (88)	1·604
1000	1·216 (85)	0·9556	1·162 (82)	1·342	0·1522 (76)	1·314 (82)	1·478
2000	0·7025 (332)	0·9526	0·6692 (323)	0·7698	0·08874 (148)	0·7579 (323)	0·8528
3000	0·5107 (254)	0·9493	0·4848 (246)	0·5518	0·06412 (321)	0·5489 (248)	0·6129
4000	0·4041 (201)	0·9586	0·3874 (197)	0·4342	0·05075 (254)	0·4382 (199)	0·4832

the data for which the absolute scale was originally known. The data thus obtained contain errors of about 4%. The average experimental ionisation cross sections discussed so far are so called gross ionisation cross sections, that is

$$\sigma_{\text{gross ion}} = \sigma_i(\text{Ne}^+) + 2\sigma_i(\text{Ne}^{2+}) + \ldots. \tag{1}$$

In fact what we need are counting ionisation cross sections defined by

$$\sigma_{\text{count ion}} = \sigma_i(\text{Ne}^+) + \sigma_i(\text{Ne}^{2+}) + \ldots. \tag{2}$$

A number of investigations have been carried out on the partial ionisation cross sections (see for instance Schram *et al* 1966a, Gaudin and Hageman 1967, van der Wiel *et al* 1969, and Bleakney 1930) $\sigma_i(\text{Ne}^+)$, $\sigma_i(\text{Ne}^{2+})$ and so on. From these data, by averaging, we have calculated $\sigma_{\text{count ion}}/\sigma_{\text{gross ion}}$. These values are given in column 3 of table 1. The accuracy is estimated to be 1% or better. Now it is possible to arrive at the $\sigma_{\text{count ion}}$ values in column 4 of table 1, which can be compared with the theoretical Bethe cross sections of Saxon (1973). It is clear that at lower energies the Bethe cross sections are much larger than the experimental ones, approaching a factor of 1·12 at 4000 eV.

3. Excitation of Ne above 200 eV

A simplified Ne I level scheme is given in figure 1. On the left-hand side the electronic configuration is given and on the right-hand side the levels are indicated by the Paschen notation. To get the cross sections for excitation to discrete states of the neutral Ne atom we have to consider 2p–*n*s, 2p–*n*d and 2p–*n*p transitions ($n \geqslant 3$). The first two series are optically allowed and the latter series is optically forbidden in the excitation process.

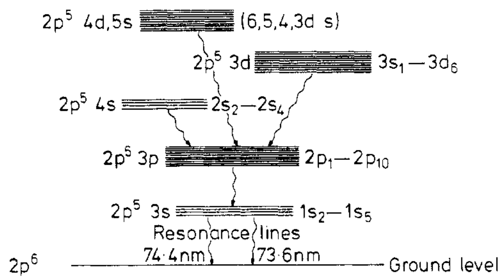

Figure 1. Simplified diagram of Ne I.

In the evaluation of the total cross section for excitation, σ_{exc}, including all excited states, the procedure followed differed above and below 200 eV. We shall first discuss the region above 200 eV. From the experimental work of de Jongh (1971) or de Jongh and van Eck (1971), of van Raan (1973) and of Sharpton *et al* (1970), all measuring emission of radiation, it follows that for our purpose it is a very good approximation to take the theoretical Bethe cross sections for the excitation cross sections. Saxon (1973) has calculated the sum of the cross sections of all relevant excitation processes in this approximation. Albat and Gruen (1974, 1975) have limited their work to a few relevant transitions using rather accurate wavefunctions. According to the Bethe approximation the cross section for an optically allowed transition is given by

$$\sigma_n = \frac{4\pi a_0^2}{E/R} M_n^2 \ln\left(4c_n \frac{E}{R}\right) \tag{3}$$

where a_0 is the first Bohr radius, R the Rydberg energy, E the kinetic energy of the incident electrons corrected for relativistic effects and c_n a constant dependent on the properties of the excited state: c_n, according to Albat and Gruen, is not very sensitive to the accuracy of the wavefunctions used in the calculation. For excitation to a discrete state with energy E_n, M_n^2 is related to the optical oscillator strength f_n by:

$$M_n^2 = f_n R/E_n. \tag{4}$$

For symmetry forbidden excitation processes, the excitation cross section is given by:

$$\sigma_n = \frac{4\pi a_0^2}{E/R} b_n. \tag{5}$$

The quantities c_n and b_n are independent of E and can be found from the generalised oscillator strength $f_n(K)$, where K is the momentum transfer (for details see Saxon 1973, or Kim and Inokuti 1971). They were evaluated by Saxon (1973) for the transitions 2p→3s, 4s, 5s, 3d, 4d, 3p and 4p, where fine structure has been ignored, by numerical integration of $f_n(K)$, as given by a calculation of McGuire (1971), who used an approximation to the Herman–Skillman central potential. Then Saxon fitted the values of $M_n^2 \ln c_n$ and b_n to a functional form $D_1(n-\delta)^{-3}+D_2(n-\delta)^{-5}$ using the quantum defect constants as given in table 3 of her work, in order to extend the results to higher principal quantum numbers. The absolute scale of M_n^2 was fitted to experiment, because f_n derived from the McGuire data differed by as much as 30% from the experimental value. Thus Saxon (1973) arrived at the following Bethe parameters (see table 6 of her article) given in table 2.

Using more accurate wavefunctions Albat and Gruen (1975) showed that Σb_n in this table is too high. They found a value of 0·0503 for b_3, which is a factor 0·4898 smaller than the b_3 value of Saxon. Therefore we took

$$\sum_{n\geqslant 3} b_n = 0{\cdot}4898 \times 0{\cdot}1748 = 0{\cdot}0856.$$

Applying the Bethe formulae (see equations (3) and (4)) for optically allowed transitions (2p–ns and 2p–nd, $n \geqslant 3$) and (see equation (5)) for symmetry forbidden transitions (2p–np, $n \geqslant 3$), we arrive at the semi-empirical Bethe cross sections for total excitation, σ_{exc}, as given in column 6 of table 1 for $E \geqslant 200$ eV. In this calculation we use the parameters of Saxon for excitation to s and d states (see table 2) and the parameter $\Sigma_{n\geqslant 3}\, b_n = 0{\cdot}0856$ for excitation to p states.

Table 2. Parameters for Bethe cross sections for discrete excitation in Ne, from Saxon (1973).

State	$\sum_{n\geqslant 3} M_n^2$	$\sum_{n\geqslant 3} M_n^2 \ln c_n$	$\sum_{n\geqslant 3} b_n$
s	0·1745	−0·3184	
d	0·0393	−0·0912	
p			0·1748

4. Inelastic scattering of electrons by Ne above 200 eV

Adding $\sigma_{\text{count ion}}$ (experimental) and σ_{exc} (semi-empirical), we get σ_{inel} (semi-empirical). These numbers can be compared with the purely theoretical σ_{inel} values of Saxon (1973) as is done in columns 7 and 8 of table 1. The differences between these two sets of numbers are similar to the differences between experimental and theoretical $\sigma_{\text{count ion}}$ cross sections. We see that between 1000 and 4000 eV the semi-empirical values are 13–10% smaller than the purely theoretical values for σ_{inel}. At lower energies it is clear that the theoretical cross sections become relatively much larger than the experimental ones. The error in σ_{exc} has been taken to be equal to 5% in this energy range.

5. Inelastic scattering of electrons by Ne below 200 eV

In order to obtain values of σ_{exc} (column 6 in table 1) for impact energies below 200 eV, where the Bethe approximation is no longer valid, we take an energy dependence for σ_{exc} similar to the measured $3s'[1\frac{1}{2}]^0$ excitation cross section including cascade of de Jongh (1971) or of de Jongh and van Eck (1971). For extrapolation towards smaller energies we normalise the data of de Jongh (1971) at 200 eV to the Bethe cross section for total excitation calculated before (see § 3). This procedure is justified to some extent, because above 200 eV the energy dependence of de Jongh's experimental cross sections appears to be the same as that of the semi-empirical total excitation cross section of Saxon (see column 6 of table 1). Below 200 eV the σ_{exc} values thus obtained may not be so accurate, but their contribution to σ_{tot} becomes relatively smaller with decreasing impact energy.

We have neglected pure triplet excitation to the metastable $1s_5$ and $1s_3$ states which do not decay by dipole radiation. From the calculations of Sharpton *et al* (1970) it is evident that the metastable states contribute very little (less than about one per cent) in our energy range.

In the same way as in § 4, σ_{inel} can be calculated by adding $\sigma_{\text{count ion}}$ and σ_{exc} (see column 7 of table 1). The error in σ_{exc} has been taken between 20% at 30 eV and 5% at 200 eV.

6. Elastic scattering of electrons by Ne

In this section we present the results for σ_{el} by integrating the differential elastic cross section $\sigma_{\text{el}}(\theta)$ according to the formula

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

The procedure is the same as that carried out before for He (see Jansen 1975 and de Heer and Jansen 1977). We have used the data of different groups and carried out the integration of $\sigma_{\text{el}}(\theta) \sin\theta$ for each of these groups when this had not previously been done by themselves. For an explanation of our procedure we first discuss how we have handled the data of Jansen *et al* (1976) who measured $\sigma_{\text{el}}(\theta)$ only for $5° < \theta < 55°$ in the energy range 100–3000 eV. In order to cover a larger angular range, these data were extended using the absolute data of other authors normalised to the data of Jansen *et al*

(1976). The following data were used for the extension of the angular range. At 100 and 150 eV, for $55° \leq \theta \leq 150°$: Kurepa *et al* (1975)†. At 200 eV for $2° \leq \theta < 5°$: Bromberg (1974); for $55° \leq \theta \leq 110°$: J P Bromberg (1975, private communication), supplemented by Kurepa *et al* (1975)†; and for $110° < \theta \leq 150°$: Kurepa *et al* (1975)†. Between 300 and 500 eV, for $2° \leq \theta < 5°$: Bromberg (1974); for $55° \leq \theta \leq 110°$: J P Bromberg (1975, private communication); and for $110° \leq \theta \leq 150°$: Gupta and Rees (1975).

At higher energies no suitable experimental data were available for extension. Because it is experimentally difficult to measure at angles close to zero and π, $\sigma_{el}(\theta)$ is only available in an angular range between a lower limit $\theta_m \neq 0$ and an upper limit $\theta_M \neq \pi$. This leads to a splitting of equation (6) into three terms

$$\begin{aligned} \sigma_{el} &= 2\pi[I(0, \theta_m) + I(\theta_m, \theta_M) + I(\theta_M, \pi)] \\ I(x, y) &= \int_x^y \sigma_{el}(\theta) \sin\theta \, d\theta \qquad 0 < \theta_m < \theta_M < \pi. \end{aligned} \tag{7}$$

$I(\theta_m, \theta_M)$ was calculated by numerical integration. $I(0, \theta_m)$ and $I(\theta_M, \pi)$ were obtained by extrapolation of the integrand $\sigma_{el}(\theta) \sin\theta$. The latter is zero at $\theta = 0, \pi$. Just as in our previous work (see Jansen 1975 and de Heer and Jansen 1977) we have extrapolated the integrand for $0 \leq \theta < \theta_m$ by a parabolic function and for $\theta_M < \theta \leq \pi$ by a linear function of θ. In many cases this extrapolation procedure will lead to relatively small additional errors in θ_{el} if θ_m is not too large and θ_M is not too small.

Above 1000 eV we had the experimental $\sigma_{el}(\theta)$ values of Jansen *et al* (1976) only up to about $\theta_M = 55°$. Therefore the error in σ_{el} might be relatively large here due to the extrapolation over a large angular range. We checked this at 1000 eV by extending Jansen's data with the theoretical ones of Fink and Yates (1970) up to 150°. The value of σ_{el} derived from the extended data is 0·918 times smaller than the value originally quoted by de Heer and Jansen (1975b) and is used later. For 2000 and 3000 eV we had no theoretical data available for extension beyond 55°.

Considering the integration procedure with $\theta_M = 150°$ more critically at lower impact energies and using the theoretical $\sigma_{el}(\theta)$ RSE data of Walker (1971, 1974, private communication), it appeared that it made sense to extend θ_M up to 180° for energies smaller than 200 eV. This extension was made for both the $\sigma_{el}(\theta)$ data of Jansen *et al* (1976) and those of other groups considered later. This is important because $\sigma_{el}(\theta)$ rises steeply above 150° up to 180°. Consequently this resulted in an increase of σ_{el} with a factor of 1·03 at 20 eV, 1·05 at 40 eV and 1·01 at 200 eV and values in between at other energies compared to the method of linear extrapolation of $\sigma_{el}(\theta) \sin\theta$ above 150° used before.

The total elastic cross sections corresponding to Jansen *et al* (1976), including all those corrections to the method used by de Heer and Jansen (1975b), are given in the second column of table 3.

Also data of other groups are given in this table which have been obtained in a similar way from their own $\sigma_{el}(\theta)$, extended with those of other experimental groups and the RSE data of Walker. In particular for the data of Williams and Crowe (1975), at low energies between about 30° and 150° it was important to use the RSE data of Walker (1971, 1974, private communication) for extension up to 180°.

† M V Kurepa, L D Vušković and S Kalezić (1975, private communication).

Table 3. Total elastic cross sections (in units of a_0^2) obtained from experimental $\sigma_{el}(\theta)$ data for electrons incident on Ne. The numbers in parentheses are the total errors in the last significant digits.

E(eV)	Jansen *et al* (1976) 7%	Bromberg (1974, 1975†) 3%	Gupta and Rees (1975), Gupta (1975) 10%	Kurepa *et al* (1975†) 17·5%	Dubois and Rudd (1976) 12%	Williams and Crowe (1975) 11%	Semi-empirical (average)	
20						13·40	12·30	(135)
30						12·34	11·32	(124)
40						11·68	10·71	(117)
50					11·0	11·79	10·82	(92)
60							10·40‡	(92)
70							9·987‡	(787)
80							9·570‡	(658)
90							9·154‡	(537)
100	8·78		8·77	8·999	7·90	9·820	8·737	(406)
150	6·03		6·71	4·897			6·196	(357)
200	5·04	4·962	4·97	4·090	5·40	5·642	4·994	(125)
300	4·015	4·007	3·88				4·000	(107)
400	3·21	3·213	3·24				3·215	(86)
500	2·75	2·730	2·55		2·82		2·721	(71)
700		2·211					2·211	(66)
1000	1·627						1·627	(120)
2000	1·02						1·02	(7)
3000	0·748						0·748	(52)

† Private communication.
‡ Interpolated.

The σ_{el} values of Dubois and Rudd (1976) and of Gupta and Rees (1975) or Gupta (1975) have been obtained by themselves. We corrected those of Gupta and Rees (1975), who used a linear extrapolation above 150°, by extension of $\sigma_{el}(\theta)\sin\theta$ up to 180°. The average values in column 8 of table 3 have been obtained by the procedure of Langenberg and van Eck (1976) mentioned before. Values at 60, 70, 80 and 90 eV have been interpolated. Because of the relatively large errors in the low-energy data, the structure around 50 eV in σ_{el} is probably not real and within the error limit.

In table 4 we compare the averaged semi-empirical σ_{el} data of Ne with the theoretical results. It is clear that in our energy range the first Born approximation does not hold as the conditions for its validity are not fulfilled (see van Wingerden *et al* 1976). At higher energies, over 200 eV, the best agreement is obtained with the static exchange approach of Dewangan and Walters (1977). In this approach, absorption and polarisation effects, which are not considered, may cancel each other (see Byron and Joachain 1977). When we look at the more sophisticated calculations, which consider absorption, polarisation and exchange effects, the best overall agreement is obtained above 200 eV with the distorted-wave second Born approximation of Dewangan and Walters (1977). The R-matrix calculations of Blum and Burke (1975), which also include these effects, differ from the empirical values by 14% at 20 eV down to 8% at 200 eV. Below 100 eV our semi-empirical data also come close to the relativistic exchange (RSE) cross sections of Walker (1971, 1974, private communication) and the polarised orbital (SEP) values of Thompson (1971).

Table 4. Total elastic cross sections (in units of a_0^2) for electrons incident on Ne. Comparison of semi-empirical and theoretical data. The numbers in parentheses are the total errors in the significant digits.

E(eV)	Semi-empirical	First Born[a]	First Born[b]	(DWSBA)[b]	Static potential (SE)[6]	R matrix[c]	OM[d]	Static potential (RS)[e]	Polarised orbital (SEP)[f]	Static potential (S)[g]	(SP)[g]	(SEP)[g]	(RSE)[h]	(RSEP)[h]
20	12·30 (135)					14·04			13·16				14·63	13·15
30	11·32 (124)					13·15			13·28				13·34	13·16
40	10·71 (117)					12·10			12·91				12·18	12·98
50	10·82 (92)					11·58			12·30				11·19	12·35
60	10·40 (92)								11·62				10·36	11·65
70	9·987 (787)								10·95				9·629	
80	9·570 (658)								10·29					
90	9·154 (537)								9·708					
100	8·737 (400)	23·12				7·878	6·444	6·693	9·178	5·979	12·11	12·97	7·942	9·162
150	6·196 (357)					6·293		5·217		4·455	7·733	8·722	6·208	7·189
200	4·994 (125)	12·48	12·32	5·498	5·184	5·394	4·385	4·431		3·788	5·532	6·263	5·167	5·979
300	4·000 (107)	8·567	8·451	4·115	3·990		3·460	3·570		3·044	3·699	4·112		5·179
400	3·215 (86)	6·521	6·440	3·362	3·330		2·940	3·045		2·622	2·932	3·199		3·817
500	2·721 (71)	5·265	5·184	2·893	2·884		2·589	2·677		2·318	2·494	2·683		
700	2·211 (66)	3·553	3·378	2·300	2·315		2·122							2·632
1000	1·627 (120)	2·681	2·642	1·794	1·813			1·733		1·515	1·546	1·614		
2000	1·02 (7)	1·354	1·332	1·065	1·071									
3000	0·748 (52)	0·9051	0·8922	0·7571	0·7634									

[a] Inokuti and McDowell (1974).
[b] Dewangan and Walters (1977).
[c] Blum and Burke (1975).
[d] Byron and Joachain (1977).
[e] Fink and Yates (1970).
[f] Thompson (1971).
[g] Jhanwar *et al* (1978).
[h] Walker (1971, 1974 private communication).

7. Total scattering of electrons by Ne

The semi-empirical total cross sections for scattering, given in the second column of table 5, have been obtained by addition of the semi-empirical data for elastic and inelastic cross sections in tables 1 and 3. The structure in σ_{tot} at low energy (50 eV) is probably not real and in fact due to inaccuracies in the σ_{el} values used (see also table 3). Comparison is made with the experimental data of Wagenaar (1978) and except at low energies, good agreement is obtained. In this paper we do not intend to review the older experimental work, but this will be done in a forthcoming paper by Wagenaar *et al.* Again the first Born approximation overestimates the cross section. Both the distorted-wave second Born approximation of Dewangan and Walters (1977) and the optical model of Byron and Joachain (1977) lead to σ_{tot} values which are about 10–20% larger than the semi-empirical or experimental ones.

Table 5. Total scattering cross sections (in units of a_0^2) for electrons incident on Ne. The numbers in parentheses are the total errors in the last significant digits.

E(eV)	Semi-empirical	Experimental Wagenaar (1978)	First Born Inokuti and McDowell (1974)	DWSBA Dewangan and Walters (1977)	OM Byron and Joachain (1975)
20	12·30 (135)				
30	12·07 (124)	13·45			
40	12·06 (117)	13·18			
50	12·67 (93)	12·81			
60	12·64 (93)	12·48			
70	12·52 (80)	12·08			
80	12·28 (67)	11·67			
90	12·00 (55)	11·25			
100	11·66 (41)	10·81	29·5		14·2
150	9·248 (370)	9·312			
200	7·979 (163)	8·289	16·8	9·770	9·64
300	6·621 (150)	6·671	11·9	7·634	7·53
400	5·513 (124)	5·649	9·27	6·346	6·29
500	4·771 (121)	4·920	7·57	5·466	5·45
700	3·884 (118)	3·948	5·66	4·367	4·40
1000	2·941 (145)			3·393	
2000	1·778 (74)			1·998	
3000	1·297 (56)			1·433	

8. Ionisation of Ar

Absolute gross ionisation cross sections were derived by using the experimental data of Rapp and Englander-Golden (1965), error 7%; Schram *et al* (1964), error 7%; Gaudin and Hageman (1967), error 10%; Fletcher and Cowling (1973), error 4%; Srinivasan and Rees (1967), error about 7%; Kurepa *et al* (1974), error 9%; Smith (1930), error about 7%; Tozer and Craggs (1960), error about 7%; and Asundi and Kurepa (1963), error 8%. The procedure for averaging has been described in § 1. Because of the Ishii effect (see § 2) the data of the last three groups just mentioned were used on a relative scale. The results are given in column 2 of table 6.

Table 6. Total cross sections for ionisation, excitation and inelastic scattering (in units of a_0^2) for electrons incident on Ar. The numbers in parentheses are the total errors in the last significant digits.

E(eV)	$\sigma_{\text{gross ion}}$ experimental average	$\dfrac{\sigma_{\text{count ion}}}{\sigma_{\text{gross ion}}}$	$\sigma_{\text{count ion}}$ experimental	$\sigma_{\text{count ion}}$ theory Kim *et al* (1973)	σ_{exc} semi-empirical	σ_{inel} semi-empirical	σ_{inel} theory Kim *et al* (1973)
20	2·299 (63)	1	2·299 (63)		1·816 (363)	4·115 (368)	
30	6·565 (174)	1	6·565 (174)		2·659 (495)	9·224 (525)	
40	8·797 (252)	1	8·797 (252)		2·815 (487)	11·61 (55)	
50	9·471 (304)	0·995	9·424 (304)		2·750 (437)	12·17 (53)	
60	9·756 (278)	0·986	9·619 (290)		2·698 (391)	12·32 (49)	
70	10·32 (30)	0·977	10·08 (31)		2·633 (348)	12·71 (47)	
80	10·31 (32)	0·968	9·980 (326)		2·568 (303)	12·55 (45)	
90	10·50 (30)	0·959	10·07 (31)		2·529 (256)	12·60 (40)	
100	10·21 (26)	0·9498	9·697 (265)	18·72	2·503 (228)	12·20 (35)	21·64
150	9·468 (283)	0·9396	8·896 (280)	14·09	2·310 (178)	11·21 (33)	16·40
200	8·566 (256)	0·9353	8·012 (252)	11·43	1·920 (123)	9·932 (28)	13·35
300	6·999 (255)	0·9342	6·538 (247)	8·427	1·458 (73)	7·996 (77)	9·885
400	5·942 (232)	0·9305	5·529 (223)	6·751	1·187 (59)	6·716 (230)	7·938
500	5·126 (222)	0·9297	4·766 (212)	5·668	1·009 (50)	5·775 (218)	6·677
600	4·380 (164)	0·9280	4·065 (159)	4·906	0·881 (44)	4·946 (165)	5·787
700	3·926 (147)	0·9278	3·643 (141)	4·337	0·783 (39)	4·426 (146)	5·120
800	3·573 (138)	0·9275	3·314 (132)	3·894	0·708 (35)	4·022 (137)	4·602
900	3·297 (134)	0·9277	3·059 (128)	3·539	0·646 (32)	3·705 (132)	4·185
1000	3·036 (130)	0·9269	2·814 (124)	3·248	0·596 (30)	3·410 (128)	3·844
2000	1·741 (77)	0·9225	1·606 (73)	1·831	0·344 (17)	1·950 (75)	2·175
3000	1·267 (63)	0·9216	1·168 (59)	1·301	0·247 (12)	1·415 (60)	1·548
4000	0·9854 (488)	0·9197	0·9063 (458)	1·019	0·195 (10)	1·101 (47)	1·214

In § 2 we have given the formulae for gross and count ionisation cross sections and in order to calculate the latter we needed partial ionisation cross sections. A lot of the previous work has been discussed by van der Wiel *et al* (1969) and Schram (1966). The data of Schram and Gaudin and Hageman (1967) lead to almost equal ratios of $\sigma_{\text{count ion}}/\sigma_{\text{gross ion}}$ and are affirmed by more recent data of Schmidt *et al* (1976a, b), Shchemelinin and Andreev (1976) and Wight and van der Wiel (1976). The numbers in column 3 of table 6 have been evaluated using the data of Gaudin and Hageman (1967) between 100 and 2000 eV, those of Schram (1966) at 3000 and 4000 eV and fitting those of Bleakney (1930) to these at lower energies. The accuracy of these ratios is generally estimated to be about 1%. Then we calculated $\sigma_{\text{count ion}}$ as given in column 4 of table 6 and compared these with the theoretical Bethe cross sections of Kim *et al* (1973). It is clear that at low energies the Bethe cross sections become much larger than the experimental ones.

9. Excitation of Ar and inelastic scattering of electrons by Ar

The simplified level scheme of Ar I is similar to that given for Ne in figure 1 of § 3, only the outer electron shell is connected with principal quantum number 3 for Ar instead of 2 for Ne.

The evaluation of total excitation cross sections, including all excited states, has been performed by the Argonne group (see Kim *et al* 1973) using the Bethe approximation (see also § 3). Although the results have not been given explicitly, they can be derived from the results presented by Kim *et al* (1973) by subtracting their σ_{inel} and $\sigma_{\text{count ion}}$ cross sections. Thus we get the semi-empirical σ_{exc} cross sections of the Argonne group, presented in column 6 of table 6 above 100 eV. In order to obtain values of σ_{exc} for impact energies below 150 eV, where the Bethe approximation is no longer valid, our procedure is similar to the one used for Ne (see § 5). We assume that σ_{exc} exhibits an energy dependence similar to the measured $4s'[1\frac{1}{2}]^0$ excitation cross sections including cascade of de Jongh (1971) or de Jongh and van Eck (1971). For the extrapolation towards smaller energies we normalise the data of de Jongh (1971) at 150 eV to the Bethe cross section for total excitation by multiplying them by 3·63. Just as in § 5 we have neglected pure triplet excitation to the $1s_5$ and $1s_3$ states.

In the same way as given in § 4 and § 5, σ_{inel} can be calculated by adding $\sigma_{\text{count ion}}$ and σ_{exc} (see column 7 of table 6). Compared to the theoretical σ_{inel} values of Kim *et al* (1973), between 2000 eV and 4000 eV, the σ_{inel} data calculated by us are 12–9% smaller. This difference becomes much larger at smaller energies.

For reasons of completeness we mention the analysis of Ar collision data by Eggarter (1975).

10. Elastic scattering of electrons by Ar

The procedure for obtaining the total elastic cross section, σ_{el}, from experimental differential cross sections, $\sigma_{\text{el}}(\theta)$, has been described in § 6. In order to extend the angular range beyond 55°, the $\sigma_{\text{el}}(\theta)$ data of Jansen *et al* (1976) have been continued up to 150° by using the corresponding cross sections (normalised to Jansen *et al*) of Dubois and Rudd (1976) at 100, 200 and 500 eV, and Williams and Willis (1975) at 150 and 300 eV. Data for extension at 400 eV were estimated by interpolation between 300 and 500 eV. For extension of the angular range to 180° we used the RSE data of Walker (1971, 1974, private communication) at 100 and 200 eV and the RS data of Walker (1971, 1974, private communication) at 300 and 400 eV. Compared to a linear extrapolation of $\sigma(\theta)\sin\theta$ from 150° to 180°, the inclusion of Walker's data changed the total elastic cross section by a factor of 1·064, 1·037, 1·022 and 1·011 at 100, 200, 300 and 400 eV respectively. At 150 eV we took σ_{el} to be 1·05 times larger than the value obtained with the linear extrapolation of $\sigma(\theta)\sin\theta$ between 150° and 180°.

Similar procedures were applied to the data of Bromberg (1974, 1975, private communication) between 200 and 500 eV to extend above angles of 25° and Williams and Willis (1975) between 20 and 400 eV to extend both at small and large angles (above 150°). For the extension above 150° at energies below 100 eV we used the best fitting values (RSE) of Walker (1971, 1974, private communication). The σ_{el} data of Jansen *et al* (1976) at 750–3000 eV have been obtained originally by means of $\sigma_{\text{el}}(\theta)$ data only up to 55° and could therefore be less accurate than the ones at lower impact energy. On the other hand at higher impact energies we have relatively smaller contributions to σ_{el} from the larger angles. As a test we carried out the integration at 500 and 1000 eV using Jansen's $\sigma_{\text{el}}(\theta)$ data only up to 55° and compared it with the integration for $\sigma_{\text{el}}(\theta)$ up to 150°, where at 1000 eV we extended Jansen's data with the RS data of Fink and Yates (1970). The σ_{el} values for extended $\sigma_{\text{el}}(\theta)$ integration are a factor of 0·962 and 0·973 smaller than for $\sigma_{\text{el}}(\theta)$ integration up to 55° respectively at

500 and 1000 eV. Therefore we corrected Jansen's previous σ_{el} value at 1000 eV by this factor and at 750 eV by a factor of 0·968.

The total σ_{el} data of Gupta and Rees (1975) or Gupta (1975), of Vusković and Kurepa (1976) and of Dubois and Rudd (1976) were provided by themselves. The semi-empirical average values (last column of table 7) have been obtained by the method explained previously.

Table 7. Total elastic cross sections (in units of a_0^2) obtained from experimental $\sigma_{el}(\theta)$ data for electrons incident on Ar. The numbers in parentheses are the total errors in the last significant digits.

E(eV)	Jansen *et al* (1976) 7%	Bromberg (1974, 1975†) 3%	Gupta and Rees (1975), Gupta (1975) 10%	Vusković and Kurepa (1976) 17·5%	Dubois and Rudd (1976) 12%	Williams and Willis (1975) 11%	Semi-empirical (average)
20					68·4	71·31	74·15 (665)
30						47·21	49·80 (547)
40						32·28	33·96 (373)
50					25·6	26·48	27·65 (247)
60				26·98			24·28 (243)
70				24·41			21·95 (219)
80			20·12	21·87			19·60 (194)
90				18·87			17·89 (179)
100	16·51		18·04	17·33	17·1	18·66	17·36 (85)
150	13·21		14·83	13·33		11·86	13·55 (70)
200	11·09	11·51	12·68		10·9	9·809	11·43 (29)
300	8·810	8·742	10·19			7·820	8·809 (230)
400	7·555	7·560	8·46			6·156	7·555 (230)
500	6·727	6·739	6·81		7·23		6·734 (177)
750	5·33						5·33 (39)
800					4·83		
1000	4·55						4·55 (33)
2000	2·87						2·87 (20)
3000	2·05						2·05 (14)

† Private communication.

In table 8 they are compared with different theoretical calculations and the phaseshift analysis of experiments by Gibson and Rees (1976). Although the optical model (OM) calculations are the only ones which fulfil the so called unitary relations, because of the complex potential for the effect of the absorption of the particles into inelastic channels, we see in table 8 that, often, results closer to our semi-empirical values are obtained with all the different approaches using a real potential. In particular at many impact energies good results have been obtained by Pindzola and Kelly (1974) in the static-potential method. Also the phaseshift analysis of Gibson and Rees (1976) is done with a real potential, which is not justified above the inelastic threshold. At 25, 50 and 100 eV their values are given as a result of analysis of the combined data of Gupta and Rees (1975), Dubois and Rudd (1975), Williams and Willis (1975) and Vusković and Kurepa (1976). Compared to our semi-empirical data the agreement is reasonably good.

Table 8. Total elastic cross sections (in units of a_0^2) for electrons incident on Ar. Comparison of semi-empirical and theoretical data. The numbers in parentheses are the total errors in the last significant digits.

E(eV)	Semi-empirical	First Born[a]	Static potential (s)[a]	OM[a]	Static potential (s)[b]	(SEP)[b]	(RS)[c]	(s)[d]	(RS)[e]	(RSE)[c]	(RSEP)[e]	Polarised orbital (SEP)[f]	OM[g] I	OM[g] II	OM[h]	Phaseshift analysis[i]
20	74·15 (665)		68·5	68·7						69·02	69·72	71·3				69·5
30	49·10 (547)		49·0	42·4						50·10	51·22	52·2				
40	33·96 (373)		37·7	31·6						38·08	41·66	41·6				
50	27·65 (247)		31·1	26·7						30·90	35·66	35·1			25·59	24·4
60	24·28 (243)		26·4	22·6						26·31	31·41	30·8			23·66	
70	21·95 (219)	110	22·8	19·7						23·16		27·4				
80	19·60 (194)	101	20·6	18·0						20·87		25·0			19·94	
90	17·89 (179)	92·1	18·9	16·5						19·13		23·1				
100	17·36 (85)	85·0	17·3	15·3	14·08	22·97	15·41	21·49		17·77	22·26	21·5	13·7	15·2	16·62	16·7
150	13·55 (70)	59·3	13·0		11·41	15·64	12·44	17·07		13·74	17·26	16·6				
200	11·43 (29)	44·6	10·2		10·03	12·34	10·90	14·77		11·70	14·56		9·96	10·8	11·01	
300	8·809 (230)	30·3	7·16		8·376	9·348	9·041		7·799		11·62		8·35	8·80		
400	7·555 (230)	23·2			7·319	7·867	7·897				9·911		7·35	7·65	6·146	
500	6·734 (177)				6·552	6·915	7·040						6·63	6·85		
700											7·168		5·61			
750	5·33 (39)															
800					5·092	5·261	5·432						5·23	5·35		
1000	4·55 (33)				4·478	4·600	4·788						4·62	4·71		
2000	2·87 (20)															
3000	2·05 (14)															

[a] Pindzola and Kelly (1974).
[b] Khare and Ashak Kumar (1978).
[c] Fink and Yates (1970).
[d] Berg *et al* (1971).
[e] Walker (1971, 1974 private communication).
[f] Thompson (1971).
[g] Joachain *et al* (1977).
[h] Furness and McCarthy (1973).
[i] Gibson and Rees (1976).

11. Total scattering of electrons by Ar

In table 9 we see that there is very good agreement between our semi-empirical data and the experimental results of Wagenaar (1978). As far as the OM calculations of Joachain *et al* (1977) are concerned, the best agreement is with his data labelled by I. Data with labels I and II differ in the way in which the second-order potential has been derived (see Joachain *et al* 1977).

Table 9. Total scattering cross sections (in units of a_0^2) for electrons incident on Ar. The numbers in parentheses are the total errors in the last significant digits.

E(eV)	Semi-empirical	Experimental Wagenaar (1978)	OM Joachain *et al* (1977)	
			I	II
20	78·27 (666)	72·25		
30	58·32 (550)	49·74		
40	45·57 (373)	42·35		
50	39·82 (253)	36·57		
60	36·60 (249)	33·87		
70	34·66 (224)	32·58		
80	32·15 (199)	31·18		
90	30·49 (183)	30·03		
100	29·56 (92)	29·02	31·5	33·3
150	24·75 (77)	24·64		
200	21·36 (40)	20·91	22·6	23·0
300	16·81 (80)	17·13	18·3	18·2
400	14·27 (33)	14·62	15·6	15·4
500	12·51 (28)	12·82	13·7	13·4
700		10·41	11·0	
1000	7·96 (35)		8·64	8·65
2000	4·82 (21)			
3000	3·47 (15)			

12. Ionisation of Kr

Absolute gross ionisation cross sections were derived by using the experimental data of Rapp and Englander-Golden (1965), error 7%; Schram *et al* (1964), error 7%; Srinivasan and Rees (1967), error about 7%; Tozer and Craggs (1960), error about 7%; and Asundi and Kurepa (1963), error 8%. The procedure for averaging has been described in § 2. Because of the Ishii effect (see § 2) the data of the last two groups just mentioned were used on a relative scale. The results are given in column 2 of table 10. For calculation of the count ionisation cross sections we use the partial ionisation cross sections of Schram (1966) and of Tate and Smith (1934), which fit very well with each other as far as $\sigma_{\text{count ion}}/\sigma_{\text{gross ion}}$ is concerned and in this way they also coincide with the data of Fiquet-Fayard and Ziesel (1963). We estimate that our values of $\sigma_{\text{count ion}}/\sigma_{\text{gross ion}}$ are generally accurate to about 5%.

Table 10. Total cross sections for ionisation, excitation and inelastic scattering (in units of a_0^2) for electrons incident on Kr. The numbers in parentheses are the total errors in the last significant digits.

E(eV)	$\sigma_{\text{gross ion}}$ experimental average	$\frac{\sigma_{\text{count ion}}}{\sigma_{\text{gross ion}}}$	$\sigma_{\text{count ion}}$ experimental	σ_{exc} semi-empirical	σ_{inel} semi-empirical
20	4·174 (159)		4·174 (159)	2·6 (5)	6·774 (525)
30	9·627 (340)		9·627 (340)	3·51 (70)	13·14 (78)
40	11·92 (45)	1·0	11·92 (45)	3·57 (71)	15·49 (84)
50	13·14 (70)	0·972	12·77 (73)	3·49 (70)	16·26 (101)
60	14·05 (74)	0·924	12·98 (94)	3·39 (68)	16·37 (116)
70	14·66 (52)	0·905	13·27 (81)	3·31 (66)	16·58 (104)
80	14·90 (53)	0·90	13·41 (82)	3·24 (65)	16·65 (105)
90	14·79 (52)	0·89	13·16 (80)	3·21 (64)	16·37 (102)
100	14·74 (65)	0·8817	13·00 (87)	3·15 (63)	16·15 (102)
150	13·59 (67)	0·887	12·05 (85)	2·70 (54)	14·75 (101)
200	12·17 (60)	0·88	10·71 (75)	2·22 (44)	12·93 (87)
300	9·994 (496)	0·869	8·685 (611)	1·71 (34)	10·40 (70)
400	8·631 (428)	0·875	7·552 (532)	1·42 (28)	8·972 (601)
500	7·454 (370)	0·86	6·410 (452)	1·18 (24)	7·590 (512)
600	6·735 (334)	0·8667	5·837 (411)	1·04 (21)	6·877 (462)
700	6·093 (302)	0·8662	5·278 (372)	0·91 (18)	6·188 (413)
800	5·561 (276)	0·8478	4·715 (332)	0·82 (16)	5·535 (369)
900	5·121 (254)	0·8629	4·419 (311)	0·76 (15)	5·179 (345)
1000	4·792 (238)	0·8612	4·127 (291)	0·71 (14)	4·837 (323)
2000	2·826 (198)	0·8519	2·407 (207)	0·40 (8)	2·807 (222)
3000	2·095 (147)	0·8416	1·763 (152)	0·29 (6)	2·053 (163)
4000	1·657 (116)	0·8299	1·375 (118)	0·228 (46)	1·603 (127)

13. Excitation of Kr and inelastic scattering of electrons by Kr

For Kr we do not have sufficient experimental and theoretical data to evaluate the excitation cross sections. Here we use the Ar excitation cross sections and the fact that σU^2 is a universal function of E/U, where U is the excitation energy. In our approximation we take the average excitation energy of the resonance levels for U. Then we get the excitation cross sections for Kr (see column 5 of table 10) by using the semi-empirical excitation cross sections of table 6. We can only give a rough estimate for the error in these Kr excitation cross sections. Then the cross section for total inelastic scattering, σ_{inel}, is obtained by adding σ_{ion} and σ_{exc} (see column 6 of table 10).

14. Elastic scattering of electrons by Kr

To obtain the semi-empirical σ_{el} values (see table 11) the $\sigma_{\text{el}}(\theta)$ data of Jansen and de Heer (1976) were extended first beyond 55° up to 150° by using the corresponding cross sections (normalised to Jansen *et al*) of K Jost and D Hermann (private communication) and Mehr (1967) at 100 eV, of Mehr (1967) at 150, 200, 300 eV and 500 eV and of Williams and Crowe (1975) at 400 eV. The data of Mehr extended to about 158° and those of Williams and Crowe to about 150°. Because the cross section often rises

Table 11. Total elastic cross sections (in units of a_0^2) obtained from experimental $\sigma_{el}(\theta)$ and theoretical ones for electrons incident on Kr. The numbers in parentheses are the total errors in the last significant digits.

E(eV)	Jansen and de Heer (1976) 7%	Bromberg (1974, 1975†) 3%	Williams and Crowe (1975) 11%	Semi-empirical (average)	Static potential (S) Berg *et al* (1971)	Static potential (RS) Fink and Yates (1970)	Static potential Walker (1971, 1974†)		
							(RS)	(RSE)	(RSEP)
20			71·80	71·80 (790)				68·94	82·05
30			49·08	49·08 (540)				49·75	63·47
40			37·79	37·79 (416)				39·50	52·43
50			32·46	32·46 (357)				33·60	45·00
60									39·50
70									
80									
90									
100	22·91		27·09	22·10 (155)	20·47	20·04		21·42	27·52
150	16·26			15·68 (110)	17·02	16·97			20·85
200	13·72	13·03	19·69	13·13 (36)		14·99	16·64	14·60	17·44
300	11·68	11·32		11·37 (32)		12·61	14·01	12·12	14·10
400	10·06	9·658	10·01	9·717 (270)		11·18	12·32	10·60	12·08
500	8·618	8·446		8·473 (235)		10·15			
700									9·160
1000	6·275			6·053 (424)		7·290			
2000	4·168			4·021 (281)					
3000	3·486			3·363 (235)					

† Private communication.

steeply in the backward direction the experimental data were extended with normalised theoretical data of Walker (1971, 1974, private communication) in the RS or RSE approach. Including these data led to a change of the relevant σ_{el} data by a factor of between 0·99 and 1·04. At 1000 eV the $\sigma_{el}(\theta)$ data of Jansen and de Heer (1976) were extended with the theoretical RS data of Walker up to 180°, normalised on experiment near 55°. At 2000 eV and 3000 eV no data were available to extend $\sigma_{el}(\theta)$ of Jansen and de Heer (1976) beyond 55°. In order to estimate the extra uncertainty in σ_{el} due to this, we compared σ_{el} at 1000 eV obtained from experimental $\sigma_{el}(\theta)$ data only up to 55° with the number in table 11, getting respectively 6·010 and 6·275 for σ_{el}. So at 2000 and 3000 eV we estimate the extra uncertainty to be about a factor of 1·04.

Bromberg (1974) has measured $\sigma_{el}(\theta)$ for e–Kr only between 3° and 25°. The σ_{el} data of Bromberg in table 11 have been derived from those of Jansen and de Heer by multiplying the latter by a factor equal to the average quotient of the $\sigma_{el}(\theta)$ data of Bromberg and Jansen and de Heer at the relevant impact energies.

Williams and Crowe's (1975) σ_{el} data were obtained from their $\sigma_{el}(\theta)$ values between 20° and 150°. At small angles we extended their data in the usual manner with those of Jansen and de Heer (1976) down to 5° at 100, 200 and 400 eV, and with those of Walker (1971, 1974, private communication) in the RSE approach down to 0° at 20–50 eV. For large angles their $\sigma_{el}(\theta)$ values were also extended with those of Walker (1971, 1974, private communication) in the RSE approach up to 180°.

When we compare the σ_{el} data of the three experimental groups in table 11, those of Williams and Crowe (1975) deviate from the others outside the error limits quoted. Because at high energies the σ_{el} data of Williams depend heavily on their $\sigma_{el}(\theta)$ cross sections at their smallest angle 20° and the extrapolation between 0° and 20°, we have not averaged all the σ_{el} data in the usual manner. For the semi-empirical average values we took the average of Jansen and de Heer (1976) and Bromberg (1974) between 100 and 3000 eV, and the data of Williams and Crowe between 20 and 50 eV.

The values thus obtained are compared with results of different kinds of static-potential calculation of Fink and Yates (1970), Walker (1971, 1974, private communication) and Berg *et al* (1971). The overall agreement between the semi-empirical values and theory is relatively the best for the RSE approach of Walker (1974, private communication) and the RS approach of Fink and Yates (1970) with differences of a factor of 0·97–1·11 and 0·91–1·20 respectively.

15. Ionisation of Xe

Absolute gross ionisation cross sections were derived by using the experimental data of Rapp and Englander-Golden (1965), error 7%; Schram *et al* (1964), error 7%; Tozer and Craggs (1960), error around 7%; and Asundi and Kurepa (1963), error around 8%. The data of the last two groups were again used on a relative scale. The average data are given in column 2 of table 12. For calculations of the count ionisation cross sections we use the partial ionisation cross section of Schram (1966) from 500 to 4000 eV. Below 500 eV the data of Tate and Smith (1934) are available, but they deviate from Schram (1966) when comparing the ratio $\sigma_{\text{count ion}}/\sigma_{\text{gross ion}}$. We adjusted the data of Tate and Smith to those of Schram, increasing their $\sigma_{\text{count ion}}/\sigma_{\text{gross ion}}$ values. All the values used for $\sigma_{\text{count ion}}/\sigma_{\text{gross ion}}$ are given in column 3 of table 12. There may be a large error in these data, estimated to be up to about 10% at 4 keV. New data on partial ionisation cross sections are necessary for better accuracy.

Table 12. Total cross sections for ionisation, excitation and inelastic scattering (in units of a_0^2) for electrons incident on Xe. The numbers in parentheses are the total errors in the last significant digits.

E(eV)	$\sigma_{\text{gross ion}}$ experimental average	$\sigma_{\text{count ion}}/\sigma_{\text{gross ion}}$	$\sigma_{\text{count ion}}$ experimental	σ_{exc} semi-empirical	σ_{inel} semi-empirical
15	3·414 (148)		3·414 (148)		
20	8·462 (345)		8·462 (345)	3·0 (6)	11·46 (69)
30	13·95 (57)	1·0	13·95 (57)	4·80 (96)	18·75 (112)
40	15·99 (65)	0·97	15·51 (70)	4·72 (94)	20·23 (117)
50	17·31 (71)	0·93	16·10 (92)	4·55 (91)	20·65 (129)
60	18·13 (74)	0·886	16·06 (104)	4·41 (88)	20·47 (136)
70	18·52 (76)	0·873	16·16 (117)	4·31 (46)	20·47 (126)
80	18·84 (77)	0·86	16·20 (131)	4·23 (85)	20·43 (156)
90	19·21 (78)	0·85	16·33 (147)	4·14 (83)	20·47 (169)
100	19·89 (158)	0·846	16·83 (202)	4·04 (81)	20·87 (218)
150	19·45 (95)	0·8510	16·55 (184)	3·30 (66)	19·85 (195)
200	17·32 (100)	0·8443	14·62 (169)	2·75 (55)	17·37 (178)
300	14·49 (60)	0·8337	12·08 (131)	2·03 (41)	14·11 (137)
400	12·51 (56)	0·8395	10·50 (115)	1·66 (33)	12·16 (120)
500	10·91 (41)	0·8276	9·029 (965)	1·41 (28)	10·44 (100)
600	9·737 (392)	0·8195	7·979 (860)	1·23 (25)	9·209 (896)
700	8·918 (423)	0·8068	7·195 (796)	1·08 (21)	8·275 (823)
800	8·030 (251)	0·7914	6·355 (666)	0·99 (20)	7·345 (695)
900	7·464 (282)	0·7925	5·915 (632)	0·90 (18)	6·815 (657)
1000	6·932 (220)	0·7937	5·502 (577)	0·825 (165)	6·327 (600)
2000	4·139 (290)	0·7814	3·234 (395)	0·47 (9)	3·704 (405)
3000	3·049 (213)	0·7704	2·349 (287)	0·34 (7)	2·689 (295)
4000	2·418 (169)	0·7582	1·833 (224)	0·266 (53)	2·099 (230)

16. Excitation of Xe and inelastic scattering of electrons by Xe

The excitation data for Xe have been obtained in the same way as for Kr, namely by application of the scaling formula using excitation data for Ar. After that σ_{inel} is obtained in the usual way (see table 12).

17. Elastic scattering of electrons by Xe

To obtain the semi-empirical σ_{el} values (see table 13) the $\sigma_{\text{el}}(\theta)$ data of Jansen and de Heer (1976) were first extended beyond 55° up to 140° by using the corresponding cross sections (normalised to Jansen and de Heer) of K Jost and D Hermann (private communication) at 100–500 eV and up to 158° at 1000 eV by using Mehr's (1967) data. Because of the rise of the cross section towards 180° theoretical RE data of Walker (1971, 1974, private communication) were used to extend the angular range. This was not possible at 1000 eV, because of a lack of theoretical data. The latter extension increased the σ_{el} data by a factor of between 1·03 and 1·11. At 2000 eV and 3000 eV no data were available to extend $\sigma_{\text{el}}(\theta)$ of Jansen and de Heer (1976) beyond 55°. In order to estimate the extra uncertainty in σ_{el} due to this, we compared σ_{el} at 1000 eV obtained from experimental $\sigma_{\text{el}}(\theta)$ data only up to 55° with the number in table 13 for

Table 13. Total elastic cross sections (in units of a_0^2) obtained from experimental $\sigma_{el}(\theta)$ and theoretical ones for electrons incident on Xe. The numbers in parentheses are the total errors in the last significant digits.

E(eV)	Jansen and de Heer (1976) 7%	Bromberg (1974, 1975†) 3%	Williams and Crowe (1975) 11%	Semi-empirical (average)	Static potential (S) Berg *et al* (1971)	Static potential (RS) Fink and Yates (1970)	Static potential Walker (1971, 1974†)		
							(RS)	(RSE)	(RSEP)
20			98·77	98·77 (1086)				82·17	137·8
30			95·52	95·52 (1051)				74·11	53·74
40								35·17	36·99
50								19·79	29·93
60			16·38	16·38 (180)				14·69	26·28
70									
80									
90									
100	18·04			17·23 (121)	26·64	15·62		14·06	22·53
150	16·40			15·66 (110)	25·93	17·11	15·91	16·50	22·09
200	17·67		18·06	16·87 (118)		17·78	20·46	17·09	21·23
300	15·15	13·47		13·69 (54)	23·15	17·01	19·11	16·42	19·07
400	14·07	13·28	14·48	13·40 (38)		15·58	17·38	14·97	17·26
500	12·45	11·82		11·92 (33)		14·30			
700		10·03		10·12 (30)			13·71	11·88	13·60
1000	8·935			8·551 (599)		10·47			
2000	6·166			5·889 (412)					
3000	5·157			4·925 (345)					

† Private communication.

σ_{el} data up to 158°, getting 8·825 and 8·935 respectively for σ_{el}. So at 2000 and 3000 eV we estimate the extra uncertainty to be about a factor of 1·01.

Bromberg (1974) has measured $\sigma_{el}(\theta)$ for e–Xe only between 3° and 25°. The σ_{el} data of Bromberg (1974) at 300–500 eV in table 13 have been derived from those of Jansen and de Heer (1976) by multiplying the latter by a factor equal to the average quotient of $\sigma_{el}(\theta)$ of both groups at the relevant impact energies. At 700 eV Bromberg's data have been extended with those of Mehr (1967) up to 157°. Williams and Crowe's (1975) σ_{el} data were obtained from their $\sigma_{el}(\theta)$ values between 20° and 150° in the same way as described for electrons incident on Kr (see § 14). The extension of $\sigma_{el}(\theta)$ to 180° was done with the RSE data of Walker at 200 and 400 eV and the RSEP data of Walker at 20, 30 and 60 eV. When we compare the σ_{el} data of the three experimental groups given in table 13, there is good agreement between them. Notwithstanding, we took the same averaging procedure as that given in § 14, because Williams and Crowe's σ_{el} values at 200 and 400 eV depend heavily on their $\sigma_{el}(\theta)$ cross sections at their smallest angle and the extrapolation between 0° and 20°.

Comparison of our semi-empirical σ_{el} data with theory shows that the best overall agreement is with the RSE calculations of Walker, although relatively large deviations are present below 100 eV and the structure in the energy dependence is not quite the same for the semi-empirical and the theoretical RSE data. For a more definite conclusion more $\sigma_{el}(\theta)$ data are needed between 20 and 100 eV.

18. Total scattering of electrons by Kr and Xe

In table 14 we see that within the combined error limits there is good agreement between our semi-empirical values and the cross sections of Wagenaar (1978), measured experimentally above 100 eV. At low energies the differences are larger, in particular for Xe. Because in this energy region in our empirical cross sections a large contribution comes from σ_{el} data based on Williams and Crowe's (1975) data only, more experimental data for $\sigma_{el}(\theta)$ are needed. Although the total cross section data of Wagenaar (1978) appear very reliable, it would be useful to have a second set of data of another experimental group in the energy range from about 20 to 100 eV with about the same accuracy (around 5%).

19. Conclusion

By analysis of different experiments on ionisation, excitation and elastic scattering, total cross sections have been evaluated for ionisation, excitation, inelastic scattering, elastic scattering and total scattering in the case of electrons incident on Ne, Ar, Kr and Xe between 20 and 3000 eV. The error in the cross sections derived generally varies between about 2 and 10%.

As far as the ionisation and inelastic cross sections are concerned, a comparison with the Born approximation is possible for Ne and Ar. At the highest impact energies up to 4 keV, our semi-empirical data are still about 10% lower than the corresponding Born values, which is beyond our error limit of about 4%. For elastic scattering the Born approximation does not hold. The most sophisticated calculations for elastic scattering have been applied to Ne and Ar considering the effects of exchange, absorption of electrons into inelastic channels and polarisation effects. For Ne these calculations

Table 14. Total scattering cross sections (in units of a_0^2) for electrons incident on Kr and Xe. The numbers in parentheses are the total errors in the last significant digits.

E(eV)	Kr		Xe	
	Semi-empirical	Experimental Wagenaar (1978)	Semi-empirical	Experimental Wagenaar (1978)
20	78·57 (792)		110·2 (109)	130·4
30	62·22 (546)	71·21	114·3 (106)	78·29
40	53·28 (424)	61·76		57·47
50	48·72 (371)	55·60		52·06
60		51·31	36·85 (226)	47·30
70		47·80		45·28
80		44·16		44·74
90		41·01		43·76
100	38·25 (186)	38·27	38·10 (229)	42·66
150	31·01 (149)	30·08	35·51 (224)	38·63
200	26·06 (94)	27·14	34·24 (214)	35·31
300	21·77 (77)	22·36	27·80 (147)	30·34
400	18·69 (66)	18·87	25·56 (126)	26·78
500	16·06 (56)	16·78	22·36 (105)	24·05
700		14·01	18·40 (88)	20·16
1000	10·89 (533)		14·88 (85)	
2000	6·828 (358)		9·593 (578)	
3000	5·416 (286)		7·614 (454)	

extend between 20 and 3000 eV. The agreement with our semi-empirical σ_{el} values varies between 0 and 14%. For Ar the OM calculations extend from 20 to 1000 eV. The agreement with our semi-empirical σ_{el} values for the OM II of Joachain *et al* (1977) above 200 eV is better than about 6%, while for the OM of Pindzola and Kelly below 100 eV it is generally better than about 10%.

For all the targets considered theoretical approaches have been applied for calculations of $\sigma_{el}(\theta)$ or σ_{el}, which do not fulfil the unitary relations. These models contain real potentials, sometimes considering relativistic, exchange and polarisation effects, but do not consider the absorption of particles into an inelastic channel. Notwithstanding they often provide σ_{el} values in good agreement with our semi-empirical values. For Ne the SE of Dewangen and Walters (200–3000 eV) differs by less than 4% and the RSE of Walker from 20% at 20 eV down to 3% at 200 eV. For Ar and Kr the RSE calculations of Walker give σ_{el} values generally within about 10% of the semi-empirical ones, over a large energy range starting at 20 eV. For Xe the agreement between the different static-potential approaches and our semi-empirical σ_{el} values is often not better than about 20%, which is outside the error claimed by us. For total scattering comparison with theory is only possible for Ne and Ar with DWSBA and OM calculations. For Ne the semi-empirical values are lower than those of theory, from 20% at 100 eV to 13% at 700 eV, and for Ar by between 6 and 10% over the energy range 100–1000 eV.

Finally the total scattering cross sections obtained by the addition of σ_{el}, σ_{ion} and σ_{exc} are generally in very good agreement with the recent direct experimental data of Wagenaar (1978) between 15 and 750 eV, who claims an accuracy of about 4%.

Acknowledgments

We are thankful to all who provided numerical data for use in this article including Dr C B Lucas, who calculated a number of total elastic cross sections from his data bank of phaseshifts.

This work is part of the research programme 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).

Appendix

Survey of the theoretical calculations on elastic and total scattering of electrons by Ne, Ar, Kr and Xe (partly copied from Jansen 1975).

A.1. Flane-wave approximations

Authors	Method	Gas
Inokuti and McDowell (1974)	S	Ne
Dewangan and Walters (1977)	S	Ne
Pindzola and Kelly (1974)	S	Ar
Khare and Shoba (1974)	S	Ne, Ar
Khare and Shoba (1974)	SE	Ne, Ar
Khare and Shoba (1974)	SEP	Ne, Ar

A.2. Phaseshifts (partial waves)

Symbol	Authors	Method	Gas
(SF)	Jhanwar *et al* (1978)	S	Ne
(SF)	Khare and Ashak Kumar (1978)	S	Ar
	Walker (1971)	RS	Ar
	Berg *et al* (1971)	S	Ar, Kr, Xe
	Fink and Yates (1970)	RS	Ne, Ar, Kr, Xe
	Dewangan and Walters (1977)	SE	Ne
	Thompson (1971)	SEP	Ne, Ar
	Walker (1974)	RS	Xe
	Walker (1971)	RSE	Ne, Ar, Kr, Xe
	Walker (1974)	RSEP	Ne, Ar, Kr, Xe
R matrix	Blum and Burke (1975)	SEPA	Ne

A.3. Second-order potential

Symbol	Authors	Method	Gas
(DWSBA)	Dewangan and Walters (1974)	SEPA	Ne
(SFP)	Jhanwar *et al* (1978)	SP	Ne
(SFPE)	Jhanwar *et al* (1978)	SEP	Ne
(SFPE)	Khare and Ashak Kumar (1978)	SEP	Ar

Symbol	Authors	Method	Gas
Ab initio OM	Byron and Joachain (1975)	SEPA	Ne
Ab initio OM	Joachain *et al* (1977)	SEPA	Ar
Ab initio OM	Pindzola and Kelly (1974)	SEPA	Ar
Semi-phenomenological OM	Lewis *et al* (1974a)	SEPA	Ar
Semi-phenomenological OM	Lewis *et al* (1974b)	SEPA	Ne
Semi-phenomenological OM	Furness and McCarthy (1973)	SEPA	Ar

A.4. Symbols on the right-hand side

S—static potential.
E—including exchange effects.
P—including polarisation effects.
A—including absorption effects.
R—including relativistic effects.

Abbreviations on the left-hand side refer to symbols used by the authors.

Note added in proof

With regard to total and partial ionisation cross section measurements, some new information has become available which has been included in the reference list but has no direct impact on the results of the present study: namely Egger and Märk (1978), Skutlartz (1978) and P Nagy, A Skutlartz and V Schmidt (private communication).

References

Albat R and Gruen N 1974 *J. Phys. B: Atom. Molec. Phys.* **7** L9–13
—— 1975 *J. Phys. B: Atom. Molec. Phys.* **8** 959–64
Asundi R K and Kurepa M V 1963 *J. Electron. Control* **15** 41–50
Bederson B and Kieffer L J 1971 *Rev. Mod. Phys.* **43** 601–40
Berg R A, Purcell J E and Green A E S 1971 *Phys. Rev.* A **3** 508–10
Blaauw H J, de Heer F J, Wagenaar R W and Barends D 1977 *J. Phys. B: Atom. Molec. Phys.* **10** L299–303
Bleakney W 1930 *Phys. Rev.* **36** 1303–8
Blum K and Burke P G 1975 *J. Phys. B: Atom. Molec. Phys.* **8** L410–3
Bransden B H and McDowell M R C 1970 *J. Phys. B: Atom. Molec. Phys.* **3** 29–33
Bromberg J P 1974 *J. Chem. Phys.* **61** 963–9
Byron F W and Joachain C J 1977 *Phys. Rev.* A **15** 128–46
Dewangan D P and Walters H J 1977 *J. Phys. B: Atom. Molec. Phys.* **10** 637–61
Dubois R D and Rudd M E 1976 *J. Phys. B: Atom. Molec. Phys.* **9** 2657–67
Eggarter E 1975 *J. Chem. Phys.* **62** 833–47 (Erratum: 1976 *J. Chem. Phys.* **65** 1044)
Egger F and Märk T D 1978 *Z. Naturf.* **33a** 1111–3
Fiquet-Fayard F and Ziesel J P 1963 *Proc. 6th Int. Conf. on Ionisation Phenomena in Gases, Paris* ed P Hubert and E Cremieu-Alcan, vol. 1, A **12** 37–40
Fink M and Yates A C 1970 *Atom. Data* **1** 385–456
Fletcher J and Cowling I R 1973 *J. Phys. B: Atom. Molec. Phys.* **6** L258–61
Furness J B and McCarthy I E 1973 *J. Phys. B: Atom. Molec. Phys.* **6** 2280–91
Gaudin A and Hageman R 1967 *J. Chim. Phys.* **64** 1209–21
Gibson J R and Rees J A 1976 *J. Phys. B: Atom. Molec. Phys.* **9** L105–9
Gupta S C 1975 *PhD Thesis* University of Liverpool
Gupta S C and Rees J A 1975 *J. Phys. B: Atom. Molec. Phys.* **8** 1267–73
de Heer F J 1975 *Proc. 9th Int. Conf. on Physics of Electronic and Atomic Collisions* ed J S Risley and R Geballe (Seattle and London: University of Washington Press) Invited Lectures, Review Papers and Progress Reports pp 79–97

de Heer F J and Jansen R H J 1975a *FOM-Report* No 37173
—— 1975b *FOM-Report* No 37174
—— 1977 *J. Phys. B: Atom. Molec. Phys.* **10** 3741–58
Ishii H and Nakayama K 1961 *Trans. 8th National Vacuum Symp.* (Oxford: Pergamon) p 519
Jansen R H J 1975 *PhD Thesis* University of Amsterdam, The Netherlands
Jansen R H J and de Heer F J 1976 *J. Phys. B: Atom. Molec. Phys.* **9** 213–26
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 Ashok Kumar Jr 1978 *J. Phys. B: Atom. Molec. Phys.* **11** 887–94
Joachain C J, Vanderpoorten R, Winters K H and Byron F W 1977 *J. Phys. B: Atom. Molec. Phys.* **10** 227–38
de Jongh J P 1971 *PhD Thesis* University of Utrecht, The Netherlands
de Jongh J P and van Eck J 1971 *Proc. 7th Int. Conf. on Physics of Electronic and Atomic Collisions* (Amsterdam: North-Holland) Abstracts pp 701–3
Khare S P and Ashok Kumar Jr 1978 *Pramana* **10** 63–73
Khare S P and Shoba P 1974 *J. Phys. B: Atom. Molec. Phys,* **3** 420–7
Kim Y K and Inokuti M 1971 *Phys. Rev.* A **3** 665–78
Kim Y K, Naon M and Cornille M 1973 *Argonne National Laboratory Radiological and Environment Research Division Report* ANL-8060, part I, pp 14–23
Kieffer L J 1965 *A Compilation of Critically Evaluated Electron Impact Ionization Cross Section Data for Atoms and Diatomic Molecules*; *JILA Report* No 30 (Boulder: University of Colorado)
—— 1966 *JILA Report* No 30 addendum (see above)
Kieffer L J and Dunn G H 1966 *Rev. Mod. Phys.* **38** 1–35
Kurepa M V, Cadez I M and Pejcev V M 1974 *Fizika* **6** 185–209
Langenberg A and van Eck J 1976 *J. Phys. B: Atom. Molec. Phys.* **9** 2421–33
Lewis B R, Furness J B, Teubner P J O and Weigold E 1974a *J. Phys. B: Atom. Molec. Phys.* **7** 1083–90
Lewis B R, McCarthy I E, Teubner P J O and Weigold E 1974b *J. Phys. B: Atom. Molec. Phys.* **7** 2549–56
McGuire E J 1971 *Phys. Rev.* A **3** 267–79
Mehr J 1967 *Z. Phys.* **198** 345–50
Pindzola M S and Kelly H P 1974 *Phys. Rev.* A **9** 323–31
van Raan A F J 1973 *Physica* **65** 566–78
Ramsauer C 1921 *Ann. Phys., Lpz.* **66** 546
Rapp D and Englander-Golden P 1965 *J. Chem. Phys.* **43** 1464–79
Saxon R P 1973 *Phys. Rev.* **8** 839–49
Schmidt V, Sandner N and Kuntzemüller H 1976a *Phys. Rev.* A **13** 1743–7
Schmidt V, Sandner N, Kuntzemüller H, Dhez P, Wuilleumier F and Källne E 1976b *Phys. Rev.* A **13** 1748–55
Schram B L 1966 *Physica* **32** 197–208
Schram B L, Boerboom A J H and Kistemaker J 1966a *Physica* **32** 185–96
Schram B L, de Heer F J, van der Wiel M J and Kistemaker J 1964 *Physica* **31** 94–112
Schram B L, Moustafa H R, Schutten J and de Heer F J 1966b *Physica* **32** 734–40
Sharpton F A, St John R M, Lin C C and Fayen F E 1970 *Phys. Rev.* 1305–22
Shchemelinin S G and Andreev E P 1976 *Sov. Phys.-JETP* **44** 261–8
Skutlartz A 1978 *PhD Thesis* University of Freiburg, West Germany
Smith P T 1930 *Phys. Rev.* **36** 1293–302
Srinivasan V and Rees J A 1967 *Br. J. Appl. Phys.* **18** 59–64
Tate J T and Smith P T 1934 *Phys. Rev.* **46** 773–6
Thompson D G 1971 *J. Phys. B: Atom. Molec. Phys.* **4** 468–82
Tozer B A and Craggs J D 1960 *J. Electron. Control* **8** 103
Vusković L and Kurepa M V 1976 *J. Phys. B: Atom. Molec. Phys.* **9** 837–42
Wagenaar R W 1978 *FOM-Report* No 43948
Walker D W 1971 *Adv. Phys.* **20** 257–323
van der Wiel M J, El-Sherbini Th M and Vriens L 1969 *Physica* **42** 411–20
Wight G R and van der Wiel M J 1976 *J. Phys. B: Atom. Molec. Phys.* **9** 1319–27
Williams J F and Crowe A 1975 *J. Phys. B: Atom. Molec. Phys.* **8** 2233–48
Williams J F and Willis B A 1975 *J. Phys. B: Atom. Molec. Phys.* **8** 1670–82
van Wingerden B, de Heer F J, Jansen R H J and Los J 1976 *Electron and Photon Interactions with Atoms* ed. H Kleinpoppen and M R C McDowell (New York and London: Plenum) pp 185–9