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Absolute electron impact ionization cross-sections and polarisability volumes for C_2 to C_4 aldehydes, C_4 and C_6 symmetric ethers and C_3 to C_6 ketones

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ABSTRACT

Absolute total electron impact ionization cross-sections from 15 to 285 eV are reported for the C_2 to C_4 aldehydes, the C_{2v} symmetric C_4 and C_6 ethers and C_3 to C_6 ketones. The reproducibility of the measured cross-sections over the full energy range is better than ±4%, and absolute cross-sections measured for N_2 and SF_6 as reference species are in excellent agreement with values reported by several other groups claiming accuracies of around ±5%. Monotonic relationships previously shown to exist between maximum ionization cross-section and polarisability volume and between maximum ionization cross-section and the total number of carbon atoms in the skeletal chain are shown to apply to the aldehydes, ethers and ketones reported here. These relationships provide useful means for estimating unknown cross-sections with available literature polarisability volumes in good accord with values estimated from the measured maximum ionization cross-sections. The experimental data were also compared with calculations carried out using the binary encounter Bethe (BEB) method for the calculation of total ionization cross-sections.

1. Introduction

We have previously reported on the influence of functional group, molecular shape and size, molecular orientation and three-dimensional structure on ionization efficiency. This has revealed some interesting and useful correlations between the maximum electron impact ionization cross-section and other fundamental molecular parameters, such as molecular polarisability volume and ionization potential [1–9]. Accurate measurements of the absolute total ionization cross-section may be used together with empirical and theoretical relationships to estimate unknown values for other molecular parameters, such as molecular polarisability volume, and may also be used to test theoretical predictions [10,11]. In the present work we report absolute total electron impact ionization cross-sections for C_2 to C_4 aldehydes, C_4 and C_6 symmetric ethers and C_3 to C_6 ketones, including several isomers, from a few electron volts above threshold to 285 eV. Experimental values for the maximum ionization cross-section are compared with values calculated using the binary encounter Bethe (BEB) method of Kim and Rudd [12–16].

2. Experimental

The ionization cell used for these measurements has been described previously [3,17]. Briefly, the ionization cell is housed in a vacuum chamber with a typical background pressure of $\sim 10^{-7}$ Torr. A magnetically constrained electron beam of variable energy and regulated to 75 nA trap current passes through a heated cylindrical brass ionization cell and terminates at a positively biased electron trap. The inner wall of the collision cell is coated with colloidal graphite in order to prevent surface scattering of charged particles, an important consideration since the cell wall serves as the ion collector. Analar grade chemicals obtained from Aldrich were ≥99% and were dried over $MgSO_4$ before use.

Absolute electron ionization cross-sections, σ_i, are calculated from the following equation:

$$\frac{I^+}{I^-} = n\sigma_i x \quad (1)$$

where I^+ and I^- are the measured ion and electron currents, n is the number density of the target gas and x is the path length through the collision cell. Assuming ideal gas behaviour, the above expression can be rewritten as

$$\frac{I^+}{I^-} = \frac{P\sigma_i x}{k_B T} \quad (2)$$

where P and T are the pressure and temperature of the target gas and k_B is Boltzmann's constant. Temperature is measured with a thermocouple embedded in the collision cell wall, sample vapour pressure, typically 5×10^{-4} Torr, is measured using an absolute MKS Baratron Model 627 with 0.1 Torr full scale and the electron and ion currents are measured using Keithley Model 486 picoammeters.

Ionization efficiency curves are highly reproducible from run to run, even for experiments carried out several weeks apart. The

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Table 1
Data table for molecules studied

Molecule	Letter used in Figs. 1–3	IUPAC	# C's	$\sigma_{\max}$expt (Å^2)	$\sigma_{\max}$BEB (Å^2)	α(lit) (Å^3)	α(eq (3)) (Å^2)
Nitrogen				2.5	2.58	1.7403	1.7
Sulfur hexaflouride				7.1	7.64		4.8
Acetaldehyde	a	Ethanal	2	6.7	5.89	4.6	4.5
Propionaldehyde	b	Propanal	3	9.7	8.32	6.5	6.5
Butyraldehyde	c	Butanal	4	12.4	10.7	8.2	8.4
Isobutryaldehyde	d	2-Methylpropanal	4	11.9	10.49		8.1
Diethyl ether	a	Ethoxyethane	4	14.2	12.22	8.73	9.6
Dipropyl ether	b	Propoxypropane	6	17.8	17.2		12.0
Diisopropyl ether	c	2-Isopropoxypropane	6	19.6	17.17	12.5	13.3
Acetone	a	Propanone	3	9.0	8.54	6.4	6.1
Methyl ethyl ketone	b	Butanone	4	12.3	10.98	8.12	8.3
Methyl propyl ketone	c	Pentan-2-one	5	13.9	13.48	9.93	9.4
Diethyl ketone	d	Pentan-3-one	5	15.4	13.52	9.93	10.4
Methyl isopropyl ketone	e	3-Methylbutan-2-one	5	16.1	13.33		10.9
Ethyl propyl ketone	f	Hexan-3-one	6	16.9	15.97		11.4
Methyl butyl ketone	g	Hexan-2-one	6	17.1	15.96		11.6
Methyl *tert*-butyl ketone	h	3,3-Dimethylbutan-2-one	6	16.9	15.84		11.4
Methyl *sec*-butyl ketone	i	3-Methylpentan-2-one	6	17.0	15.9		11.5
Methyl *iso*-butyl ketone	j	4-Methylpentan-2-one	6	18.1	15.97		12.2

1 Å^2 = 1 × 10^{-20} m^2 and 1 Å^3 = 1 × 10^{-30} m^2.

results reported here are the averages of between 5 and 10 repeated determinations for each target gas, made over a period of several months. Before and after each data run, three to five measurements were made of the ionization efficiency curve for N_2. These were compared with the data recommended in the compilation by Lindsay and Mangan [9] as an independent assessment of the accuracy of the data. The "recommended" maximum cross-section for N_2 is given as 2.51 Å^2 (±5%) and the absolute values measured in this work always fall within the range of 2.50–2.52 Å^2. Measurements for SF_6 were also made as a cross-check on accuracy with a mean value of 7.05 Å^2 (±4%) recorded in this work. A review of electron interactions with SF_6 by Christophorou and Olthoff [18] recommends a $\sigma_{\max}$ value of 6.97 Å^2 (±7%) based on the measurements of Rapp and Englander-Golden [19] between threshold and 300 eV, in good accord with the absolute values measured in this instrument.

3. Results and discussion

Table 1 lists the molecules studied and the maximum cross-section values measured. Cross-section data for the aldehydes, ketones and ethers measured over the electron energy range from 15 to 285 eV are shown graphically in Figs. 1–3 with the tabulated data in Tables 2 and 3.

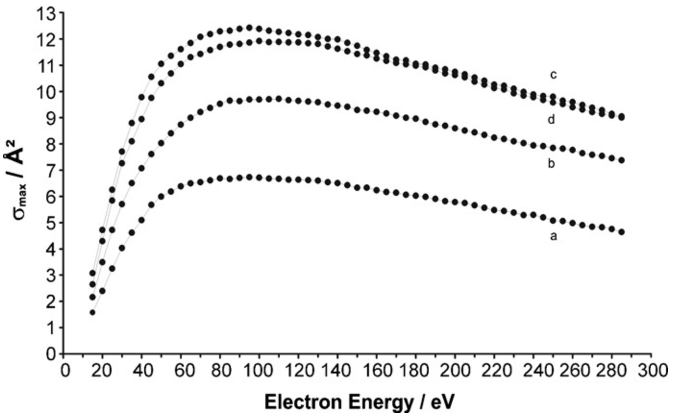

Fig. 1. Ionization cross-section versus electron energy for the aldehydes: a = ethanal; b = propanal; c = butanal; d = 2-methylpropanal.

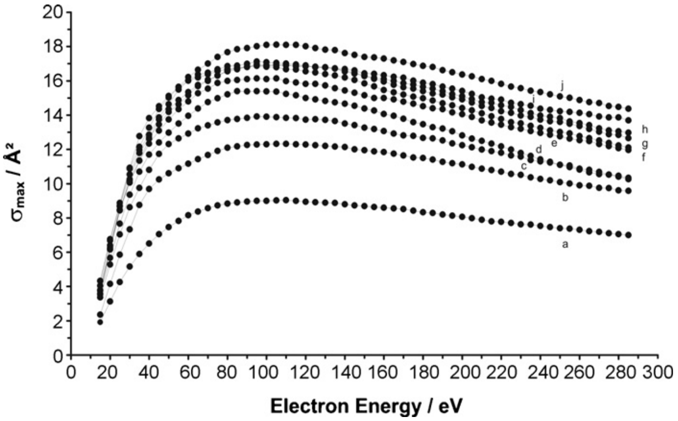

Fig. 2. Ionization cross-section versus electron energy for the ketones: a = propanone; b = butanone; c = pentan-2-one; d = pentan-3-one; e = 3-methylbutan-2-one; f = hexan-3-one; g = hexan-2-one; h = 3,3-dimethylbutan-2-one; i = 3-methylpentan-2-one; j = 4-methylpentan-2-one.

We have previously reported on relationships between the maximum total electron impact ionization cross-section and molecular electrostatic parameters. Polarisability volumes are used in the calculation of a range of physical parameters, including: modelling

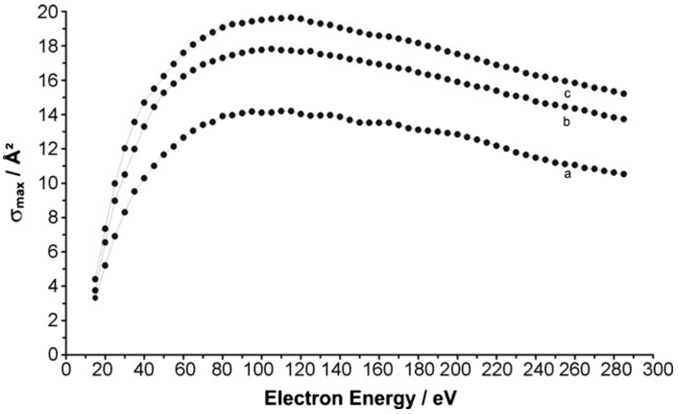

Fig. 3. Ionization cross-section versus electron energy for the symmetric ethers: a = ethoxyethane; b = propoxypropane; c = 2-isopropoxypropane.

Table 2
Total ionization cross-section as a function of electron energy for the aldehydes and ethers

EE (eV)	Ionization cross-section (Å^2)						
	Aldehydes				Ethers		
	a	b	c	d	a	b	c
15	1.6	2.2	3.1	2.7	3.3	3.8	4.4
20	2.4	3.5	4.7	4.3	5.2	6.5	7.3
25	3.3	4.7	6.2	5.8	6.9	9.0	10.0
30	4.0	5.7	7.7	7.3	8.3	10.5	12.0
35	4.6	6.5	8.8	8.1	9.5	12.0	13.6
40	5.1	7.1	9.8	8.9	10.3	13.3	14.7
45	5.7	7.6	10.6	9.8	11.0	14.4	15.5
50	6.0	8.0	11.1	10.3	11.7	15.3	16.2
55	6.2	8.4	11.4	10.7	12.1	15.8	16.9
60	6.4	8.7	11.6	11.0	12.7	16.2	17.6
65	6.5	9.0	11.8	11.3	13.0	16.6	18.1
70	6.5	9.2	12.1	11.4	13.4	16.9	18.5
75	6.6	9.4	12.2	11.6	13.6	17.1	18.8
80	6.7	9.5	12.3	11.7	13.9	17.3	19.1
85	6.7	9.6	12.3	11.8	14.0	17.5	19.3
90	6.7	9.6	12.4	11.8	14.1	17.6	19.3
95	6.7	9.7	12.4	11.9	14.2	17.7	19.4
100	6.7	9.7	12.4	11.9	14.1	17.8	19.5
105	6.7	9.7	12.3	11.9	14.1	17.8	19.6
110	6.7	9.7	12.3	11.9	14.2	17.8	19.6
115	6.6	9.7	12.2	11.9	14.2	17.7	19.6
120	6.6	9.6	12.2	11.9	14.0	17.7	19.6
125	6.6	9.6	12.1	11.8	13.9	17.7	19.4
130	6.6	9.6	12.1	11.8	13.9	17.5	19.3
135	6.5	9.5	12.0	11.7	14.0	17.5	19.2
140	6.5	9.5	12.0	11.6	13.9	17.4	19.1
145	6.4	9.4	11.8	11.5	13.7	17.2	18.9
150	6.3	9.3	11.7	11.4	13.5	17.1	18.8
155	6.3	9.3	11.6	11.4	13.5	17.0	18.7
160	6.2	9.2	11.5	11.3	13.5	16.9	18.6
165	6.2	9.2	11.3	11.2	13.5	16.8	18.5
170	6.1	9.1	11.2	11.1	13.4	16.7	18.4
175	6.1	9.0	11.2	11.0	13.2	16.6	18.3
180	6.0	9.0	11.0	11.0	13.1	16.4	18.2
185	6.0	8.8	11.0	10.9	13.1	16.3	18.0
190	5.9	8.7	10.9	10.8	13.0	16.2	17.9
195	5.8	8.7	10.8	10.7	12.9	16.0	17.7
200	5.8	8.6	10.7	10.6	12.8	15.9	17.5
205	5.7	8.5	10.7	10.5	12.7	15.8	17.4
210	5.7	8.4	10.5	10.4	12.5	15.6	17.2
215	5.6	8.3	10.4	10.3	12.4	15.5	17.1
220	5.5	8.2	10.3	10.1	12.2	15.4	16.9
225	5.4	8.2	10.2	10.1	12.0	15.2	16.8
230	5.4	8.1	10.1	9.9	11.8	15.1	16.6
235	5.3	8.0	10.0	9.8	11.6	15.0	16.4
240	5.3	7.9	9.9	9.8	11.5	14.8	16.3
245	5.2	7.9	9.8	9.7	11.4	14.6	16.2
250	5.1	7.8	9.8	9.6	11.2	14.6	16.0
255	5.1	7.8	9.6	9.5	11.1	14.5	15.9
260	5.0	7.8	9.6	9.4	11.1	14.3	15.8
265	4.9	7.6	9.5	9.3	10.9	14.2	15.7
270	4.8	7.6	9.4	9.2	10.8	14.1	15.6
275	4.8	7.5	9.3	9.1	10.7	14.0	15.5
280	4.8	7.5	9.1	9.1	10.6	13.8	15.3
285	4.6	7.4	9.0	9.0	10.5	13.7	15.2

For the aldehydes: a = ethanal; b = propanal; c = butanal; d = 2-methylpropanal. For the ethers: a = ethoxyethane; b = propoxypropane; c = 2-isopropoxypropane.

Table 3
Total ionization cross-section as a function of electron energy for the ketones

EE (eV)	Ionization cross-section (Å^2)									
	a	b	c	d	e	f	g	h	i	j
15	1.9	2.4	3.4	3.6	4.0	4.3	4.3	3.8	3.8	3.5
20	3.1	4.2	5.3	5.7	6.4	6.8	6.7	6.2	6.2	6.2
25	4.3	5.9	7.0	7.7	8.5	8.9	8.7	8.5	8.4	8.7
30	5.2	7.3	8.6	9.4	10.2	10.9	10.5	10.1	10.3	10.9
35	5.9	8.8	9.8	10.7	11.3	12.2	12.0	11.4	11.8	12.8
40	6.5	9.7	10.8	11.7	12.3	13.3	12.9	12.6	12.7	13.8
45	7.1	10.2	11.7	12.4	13.1	14.4	13.9	13.8	13.5	14.5
50	7.5	10.6	12.3	13.0	13.7	15.0	14.6	14.3	14.2	15.1
55	7.8	10.9	12.6	13.5	14.3	15.6	15.5	14.9	14.6	15.7
60	8.2	11.2	12.9	14.0	14.8	16.0	16.0	15.3	15.2	16.2
65	8.4	11.4	13.2	14.4	15.3	16.2	16.4	15.8	15.7	16.7
70	8.6	11.7	13.4	14.8	15.5	16.4	16.5	16.1	16.0	17.0
75	8.7	11.9	13.6	15.0	15.9	16.6	16.7	16.3	16.3	17.4
80	8.8	12.1	13.7	15.2	16.0	16.7	16.9	16.5	16.6	17.7
85	8.9	12.2	13.8	15.4	16.1	16.7	16.9	16.7	16.8	17.8
90	9.0	12.3	13.8	15.4	16.1	16.8	17.0	16.8	16.8	17.9
95	9.0	12.3	13.9	15.4	16.1	16.9	17.1	16.9	17.0	18.0
100	9.0	12.3	13.9	15.4	16.1	16.8	17.1	16.9	16.9	18.1
105	9.0	12.3	13.9	15.4	16.1	16.8	17.1	16.9	16.9	18.1
110	9.0	12.3	13.8	15.2	16.0	16.7	17.0	16.9	16.9	18.1
115	9.0	12.3	13.8	15.2	15.9	16.7	17.0	16.9	16.9	18.1
120	8.9	12.3	13.7	15.0	15.8	16.6	16.9	16.9	16.8	18.0
125	8.9	12.2	13.8	14.9	15.8	16.5	16.8	16.8	16.8	17.9
130	8.9	12.2	13.7	14.8	15.7	16.4	16.8	16.8	16.8	17.8
135	8.9	12.2	13.7	14.8	15.6	16.3	16.7	16.7	16.7	17.8
140	8.8	12.1	13.5	14.7	15.4	16.2	16.6	16.5	16.7	17.6
145	8.7	12.0	13.4	14.5	15.3	16.0	16.5	16.4	16.6	17.5
150	8.7	12.0	13.3	14.4	15.2	15.8	16.3	16.3	16.4	17.4
155	8.6	11.9	13.2	14.3	15.0	15.7	16.1	16.2	16.4	17.4
160	8.6	11.8	13.1	14.1	15.0	15.5	15.9	16.1	16.3	17.3
165	8.6	11.8	12.9	14.0	14.9	15.3	15.8	16.0	16.2	17.2
170	8.5	11.7	12.8	13.8	14.8	15.2	15.6	15.9	16.2	17.1
175	8.4	11.5	12.8	13.6	14.7	15.1	15.5	15.8	16.0	17.0
180	8.3	11.5	12.7	13.5	14.5	15.0	15.4	15.7	15.9	16.9
185	8.3	11.4	12.6	13.3	14.4	14.8	15.3	15.5	15.8	16.8
190	8.2	11.3	12.5	13.2	14.3	14.7	15.2	15.4	15.7	16.6
195	8.1	11.2	12.4	13.1	14.2	14.6	15.0	15.2	15.5	16.5
200	8.1	11.1	12.2	12.8	14.0	14.4	14.9	15.1	15.4	16.4
205	8.0	11.0	12.1	12.6	13.9	14.3	14.7	14.9	15.2	16.3
210	7.9	10.9	12.0	12.5	13.7	14.1	14.5	14.8	15.0	16.1
215	7.8	10.8	11.9	12.3	13.6	13.9	14.4	14.7	15.0	16.0
220	7.8	10.7	11.8	12.2	13.4	13.8	14.2	14.6	14.9	15.8
225	7.7	10.6	11.6	12.0	13.3	13.6	14.1	14.5	14.7	15.7
230	7.6	10.5	11.6	11.8	13.2	13.5	14.0	14.3	14.6	15.6
235	7.6	10.4	11.4	11.6	13.1	13.4	13.9	14.1	14.5	15.4
240	7.5	10.3	11.3	11.4	13.0	13.3	13.7	14.0	14.4	15.3
245	7.5	10.2	11.2	11.3	12.8	13.1	13.6	13.9	14.3	15.2
250	7.4	10.1	11.1	11.1	12.8	13.0	13.6	13.8	14.2	15.1
255	7.4	10.0	11.1	11.0	12.6	12.9	13.5	13.6	14.2	15.0
260	7.3	9.9	10.9	10.8	12.5	12.8	13.4	13.5	14.1	14.9
265	7.2	9.9	10.8	10.7	12.5	12.7	13.2	13.4	14.1	14.8
270	7.2	9.8	10.7	10.6	12.3	12.5	13.0	13.2	13.9	14.7
275	7.1	9.7	10.5	10.5	12.2	12.4	12.9	13.1	13.9	14.5
280	7.1	9.6	10.5	10.4	12.1	12.2	12.8	13.1	13.9	14.5
285	7.0	9.6	10.3	10.3	12.0	12.1	12.7	13.0	13.7	14.4

a, propanone; b, butanone; c, pentan-2-one; d, pentan-3-one; e, 3-methylbutan-2-one; f, hexan-3-one; g, hexan-2-one; h, 3,3-dimethylbutan-2-one; i, 3-methylpentan-2-one; j, 4-methylpentan-2-one.

of refraction by polar and non-polar molecules; the calculation of dielectric constants and diamagnetic susceptibility; ion mobility in gases; long-range electron–molecule and ion–molecule interaction energies; Langevin capture cross-sections and rate constants for polar and non-polar molecules; van der Waals constants; oscillator strengths. It has been shown from first principles [10,11] and confirmed experimentally [20] that a linear relationship exists between the maximum cross-section $\sigma_{\max}$ and the molecular polarisability volume α. A plot of $\sigma_{\max}$ in Å^2 versus α in Å^3 for 72 atoms and molecules from He to $C_{10}H_{22}$ for which the polarisability volume has been determined, including small molecules such as H_2, N_2, O_2, H_2O, NH_3, hydrocarbons, perfluorocarbons, chlorocarbons, nitriles, mixed halocarbons, alcohols, methanoates and ethanoates [21–28] gave a proportionality constant of 1.40. Inclusion of the data for the aldehydes, ethers and ketones, Table 1, gives the plot shown in Fig. 4 with proportionality constant of 1.48 (Eq. (3)).

$$\sigma_{\max}(\text{expt}) = 1.48\alpha \tag{3}$$

A plot of the literature values for polarisability (9 of the 17 molecules reported here) versus the values calculated from Eq. (3) using experimentally measured values from Tables 1 and 2 are shown in Fig. 5. The literature values are calculated from measure-

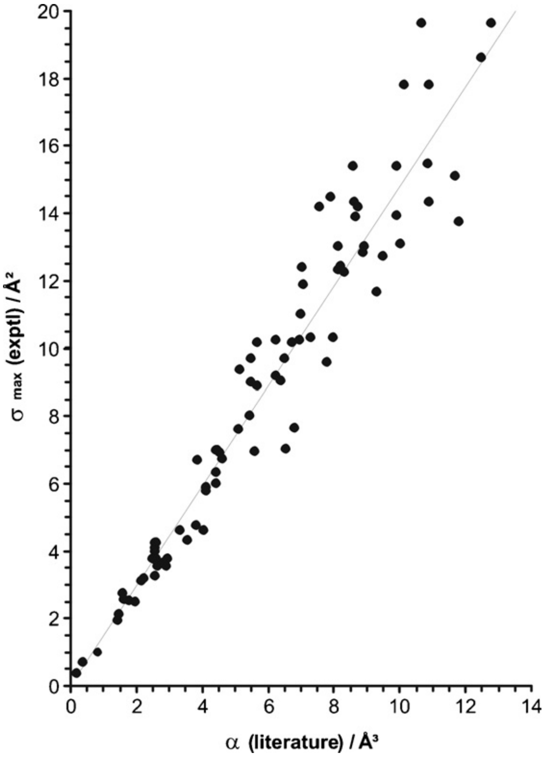

Fig. 4. Plot of the maximum ionization cross-section versus literature polarisability volume for a wide range of molecules including the aldehydes, ketones and ethers for which data is available (as listed in Table 1). The best line fit to the data is given by Eq. (3).

ments of dipole moment, dielectric constant and molar refraction. It is evident from the plot represented by Eq. (4) that this relationship offers an acceptable route to the estimation of unknown polarisability volumes in the absence of *ab initio* molecular orbital calculations.

$$\alpha(\text{Eq. (3)}) = \frac{\sigma_{\max}(\text{expt})}{1.48} = 1.06\alpha(\text{lit}) - 0.38 \qquad (4)$$

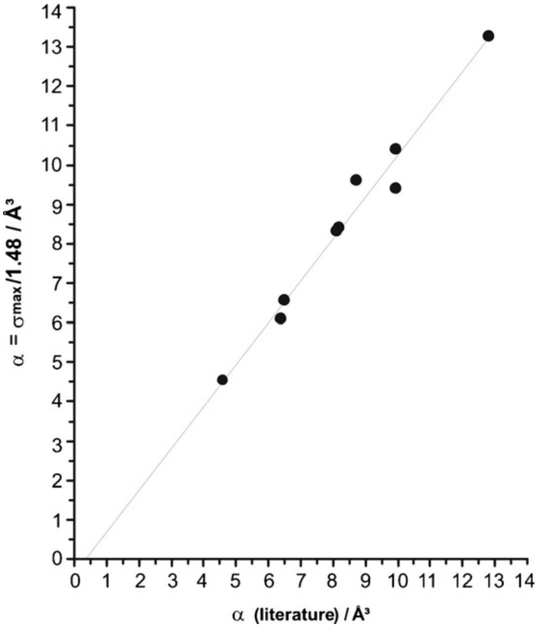

Fig. 5. Plot of the polarisability volume calculated from Eq. (3) versus literature values. The best line fit to the data is given by Eq. (4).

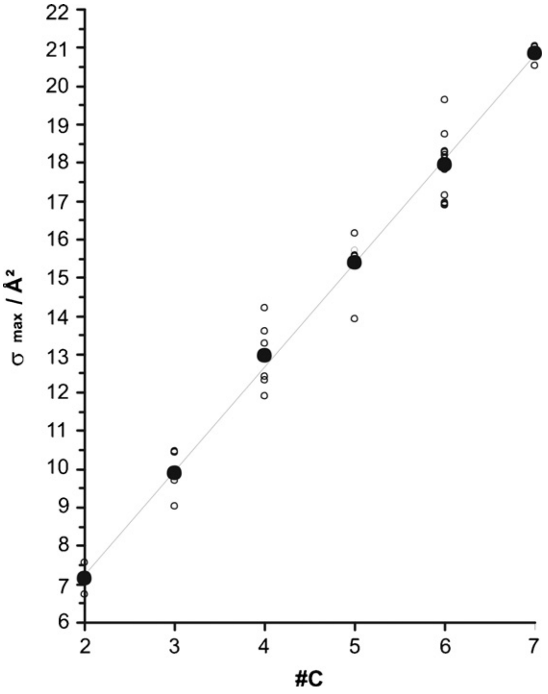

Fig. 6. Plot of maximum ionization cross-section versus the number of carbon atoms in the skeletal structure of the molecule. The larger solid points are averaged values of the maximum ionization cross-section for all of the aldehydes, ketones and ethers measured and the smaller open circles are values for the individual molecules (including isomers). The best line fit to the average data is given by Eq. (5).

Since ionization cross-section increases with molar mass, a plot of the maximum ionization cross-section with the number of carbons in the skeletal structure of the molecule might also be expected to reveal a useful correlation. It is evident from the data that for a given number of carbon atoms in the molecule there is a spread in the maximum ionization cross-section reflecting differences between structural and functional isomeric forms. For example, the maximum ionization cross-section for 2-methylpropanal with four carbon atoms was found to be 11.9 $Å^2$ compared to 12.4 $Å^2$ for butanal, 12.3 $Å^2$ for butanone and 14.2 $Å^2$ for ethoxyethane. The higher value for the ether is most likely to be the consequence of the oxygen atom incorporated into the skeletal chain. However, a plot of the average value of the maximum cross-section versus the number of carbon atoms, #C, for the aldehydes, ethers and ketones reported here and the formates and acetates reported earlier (total of 36 molecules) [6] exhibits a surprisingly good correlation as shown in Fig. 6 and Eq. (5). The filled points are the average values of $\sigma_{\max}$(expt) for all molecules with the same number of carbon atoms and the small open circles are the individual values. This is the first time that we have measured significant differences between isomeric forms and although they are less than 10% they do reflect the differences in the three-dimensional profiles of the molecules as viewed by an inbound ionizing electron.

$$\sigma_{\max}(\text{expt}) = 2.72\#\text{C} + 1.81 \qquad (5)$$

For the implementation of the BEB model, *ab initio* gas phase electronic structure calculations were performed on all 19 closed shell compounds. MP2//6–311G++(2d,p) optimizations and energy calculations were carried out with PCGAMESS 7.0 [29], which is based on GAMESS [30]. Orbital kinetic energies were computed in order to satisfy the virial ratio. A plot of experimentally measured maximum ionization cross-sections, $\sigma_{\max}$, against the values calculated using the BEB formalism is shown in Fig. 7. The relationship between the experimental and the calculated BEB values given by Eq. (6) shows that the correspondence is within 10% as found for

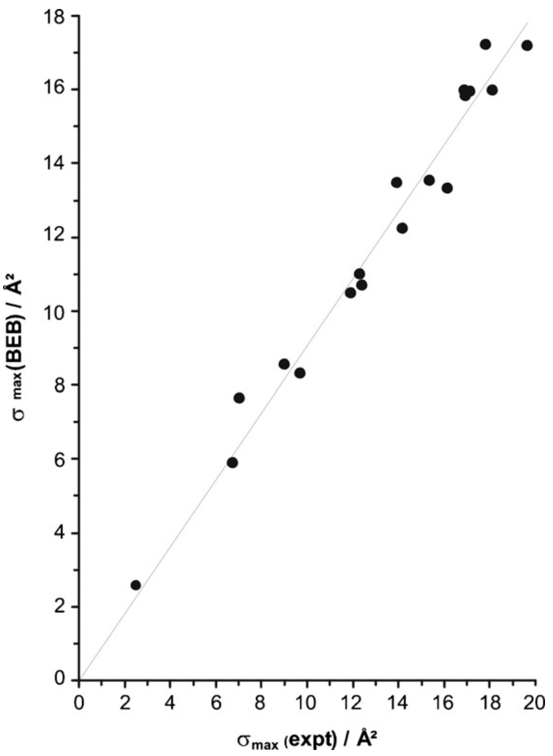

Fig. 7. Plot of the experimental versus calculated (BEB) maximum ionization cross-sections. The best line fit to the data is given by Eq. (6).

the methyl and ethyl methanoates and ethanoates in which the BEB values were typically 9–10% lower than those measured.

$$\sigma_{\max}(\mathrm{BEB}) = 0.91\,\sigma_{\max}(\mathrm{expt}) \tag{6}$$

4. Conclusion

Total absolute ionization cross-sections from 15 to 285 eV have been measured for the C_2 to C_4 aldehydes, the C_{2v} symmetric C_4 and C_6 ethers and C_3 to C_6 ketones. A correlation between the maximum ionization cross-section and the number of skeletal carbons may be used to predict cross-sections. In addition, a correlation between the maximum ionization cross-section for a wide range of molecules and the polarisability volume can be used to estimate values for polarisability volume when ionization cross-sections are available. Cross-sections measured in this report and those calculated using the BEB theory agree to within better than 10%.

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