

6 Cross sections for scattering- and excitation-processes in electron-molecule collisions

6.1 Total scattering cross sections

6.1.1 Introduction

6.1.1.1 Subject

This contribution presents a collection of total cross sections for electron scattering on molecules from the lowest energies examined experimentally up to 1000 eV. Some data at higher energies can be found, for example in [96Zec1, 01Kar1, 01Kar2]. Although the electron-atom scattering is not discussed explicitly, some references on electron-noble gases scattering are given while discussing experimental methods.

The bibliography mainly covers papers printed later than 1970. A description of experimental methods (on atoms) was given in [71Bed1], the list of early experiments in [33Bro1, 33Ram1], tabulated data for cross sections in [89Shi1], recommended cross sections in [92Hay1]. We quote also several other review articles and books on electron scattering [84Shi1, 84Chr1, 89McD1, 90Kau1, 94Ino1, 96Zec1, 00Kim1, 01Kar1, 01Kar2].

6.1.1.2 Measured quantities

6.1.1.2.1 Total cross section

Most of the total cross section (TCS) measurements on molecules have been performed by the transmission method. In this type of experiments the attenuation of an electron beam passing through a gas cell is monitored. The total cross section σ_{tot} is obtained from the deBeer-Lambert formula

$$I = I_0 \exp\left(-\frac{p}{kT} l \sigma_{\text{tot}}\right) \quad (1)$$

where I_0 and I stand for the electron current at the entrance and exit of the gas cell respectively, T and p for the gas temperature and pressure respectively, l -for the length of the scattering region and k for Boltzmann's constant.

The total cross section can be described as a sum of the cross sections for scattering into all channels opened at a given energy. In the case of molecules these channels are elastic scattering, rotational and vibrational excitation, electronic excitation, dissociative and non-dissociative attachment, dissociation into neutrals, dissociative and non-dissociative ionization. This definition has been used to check the quality of total cross sections by comparison with the sum of partial integral values [96Zec1, 01Kar1, 01Kar2]. Nevertheless the amount of data available as partial integral cross sections is rather sparse, and does not help in the assessment of total cross section recommended values.

6.1.1.2.2 Integral and momentum transfer cross sections

A few other experimental methods allow to evaluate the total cross sections whenever it is difficult to be measured by the transmission method. For example, below the threshold for inelastic processes, the total cross section coincides with the integral cross section for elastic scattering σ_{el} which can be obtained by integrating experimental differential cross sections $d\sigma_{\text{el}}/d\omega$ over the full solid angle

$$\sigma_{\text{el}} = 2\pi \int_0^\pi \frac{d\sigma_{\text{el}}}{d\omega} \cdot \sin\theta \cdot d\theta \quad (2)$$

where θ is the scattering angle.

Note that although the rotational excitation channel is opened also at the lowest energies experimentally achievable, the rotational excitation is usually not discriminated in the experiment. In this way the measured integral elastic cross section equals to the total one below the vibrational excitation thresholds, see section 6.2 in this volume. In some gases, like HCl, the rotational cross sections have been measured [89Rad1] and can be summed to check the total cross section.

In the limit of isotropic scattering (e.g. low energy scattering for non polar molecules) the total cross section can be evaluated by comparison with the momentum transfer cross section σ_{m} obtained from the analysis of diffusion coefficients (see section 6.4).

$$\sigma_{\text{m}} = 2\pi \int_0^\pi \frac{d\sigma_{\text{el}}}{d\omega} \cdot (1 - \cos\theta) \cdot \sin\theta \cdot d\theta \quad (3)$$

Practically, the total and momentum transfer cross sections coincide at low energies (say below 1 eV) for non polar molecules, like N₂. For molecules showing a Ramsauer-Townsend minimum, σ_{tot} and σ_{m} coincide only for energies below the minimum. The momentum transfer cross section at higher energies is lower than the total cross section.

6.1.1.2.3 Other measurements

Sporadically, other methods have been used to measure total cross sections. In the recoil method, the electron beam crosses at right angle the molecular beam and the current I_s of recoiled atoms is measured. The total cross section is determined from the formula

$$\sigma_{\text{tot}} = \frac{I_s}{I_m} \frac{hu}{I_e} \quad (4)$$

where u is the velocity of atoms in the beam, h is the height of the electron beam, I_m is the molecular beam intensity and I_e the electron beam intensity. Targets measured by this method are alkali atoms dimers [73Mil1, 82Mil1], alkali halides [74Sla1, 84Jad1, 89Vus1] and oxygen [67Sun1].

At very low energies (at meV range) the Rydberg atoms quenching method has been used to evaluate total cross section. Electrons in high Rydberg orbits can be considered as almost free so they scatter on perturbing gas molecules. Rydberg electrons with principal quantum numbers above 100 have mean kinetic energies below 1 meV [92Lin1]. Quenching rate constants in the presence of a perturbing gas are measured. The interpretation of these data is not straightforward. Quenching of the Rydberg atoms can be caused by such processes as electron attachment, like in CCl₄ [92Lin1]; by formation of intermediate molecular complexes, like in C₆H₆ [93Pop1]; by rotational excitation of the molecule, like in CH₃I [93Lin1].

In the limit of zero-energy $E = 0$, the Fermi method [34Fer1] can be used to evaluate the scattering length A_0 :

$$\sigma_{\text{tot}}(E = 0) = 4\pi A_0^2 \quad (5)$$

The method consists in measurements of the shift in the optical emission from molecular gases (like C_6H_6 , CH_3I) [90Rup1] in presence of a perturber. Targets for which the scattering length has been determined in this way are noble gases [90Rup1], CO_2 [91Asa1], CH_4 , C_2H_6 , C_3H_8 [91Mey1].

6.1.1.3 Experimental methods

6.1.1.3.1 Absolute measurements

In absolute measurements, all quantities in eq. (1) are monitored directly. The typical systematic error of most of the absolute measurements performed in the last decades (apart from the angular resolution error, see below), is less than 5 %. The most difficult is the pressure evaluation, which requires, for example, corrections for the temperature difference between the scattering cell and the pressure gauge (the thermal transpiration error). A few experiments used indirect methods of pressure evaluation, like ionization [78Szm1] or optical emission [86Gar1]. Indirect methods are likely to introduce additional errors.

In normalized measurements, some of the quantities (often the electron path length inside the gas cell) are unknown. Sometimes this uncertainty is related to gas outflow from the scattering through entrance and exit orifices [85Wag1]; for this reason long scattering cells are privileged. In other apparatuses the uncertainty is introduced by the use of electron-guiding magnetic fields [77Kau1, 80McM1, 84Sue1]. Here the real length of the electron path is determined by spiralling in the magnetic field. This is a difficult quantity to evaluate.

The normalized measurements can be useful to assess the shape of the cross section vs. energy curve, but are of no use for the evaluation of the recommended (absolute) values.

6.1.1.3.2 Angular resolution error

An inherent error of the transmission technique is due to the lack of discrimination for electrons scattered into small angles, within the angular acceptance of the detector. The absolute error $\Delta\sigma_\omega$, leading to underestimation of the measured cross section, depends on the angular acceptance $\Delta\omega(x)$ of the detector, as seen from the position x of the scattering event and on the small-angle differential cross section $d\sigma/d\omega$ for a specified scattering channel [80Win1, 83Laz1]

$$\Delta\sigma_\omega = \frac{1}{I} \int_0^I dx I'(x) \int_0^{\Delta\omega(x)} \frac{d\sigma}{d\omega} d\omega, \quad (6)$$

with $I'(x) = I(x)/I_0$, see eq. (1), and the first integral to be evaluated over the interaction region length (I). The angular resolution error, similarly as the total cross section, is a sum over all possible scattering processes. However, many experiments use retarding-field analyzers, preventing a part of the inelastically scattered electrons to reach the detector. The energy resolution of such detectors, in any case, hardly allows to discriminate the lowest inelastic channels, like the rotational and vibrational excitation.

The angular resolution error, for a given apparatus, rises if the differential cross section is forward peaked. For any given apparatus it depends also on the total cross section partitioning between elastic and inelastic channels. For the apparatuses used in the last decades, the angular resolution error becomes comparable with the remaining systematic errors essentially in two limits: at energies lower than a few eV for polar molecules (like H_2O and NH_3) [92Yua1, 94Ham2, 00Kim1] and at energies above several hundreds eV for all targets [92Zec1, 96Gar2].

Some authors correct the measured total cross sections for the angular resolution error [79Jos1, 82Nog1, 83Jos1, 00Kim1], using theoretical or extrapolated into zero-angle experimental differential cross sections. The reliability of such corrections is often limited.

6.1.1.3.3 Survey of the experimental methods

As stated in subsect. 6.1.1.2.1, reliable electron - molecule total cross section measurements have been performed using the attenuation method. The attenuation of an electron beam is measured when it passes through a region containing the sample gas. Other measurement principles have been occasionally proposed, but the few data produced are considered of low reliability (see subsect. 6.1.1.2.3). Fig. 6.1.1 is a block diagram of a transmission measurement showing all the possible functional blocks.

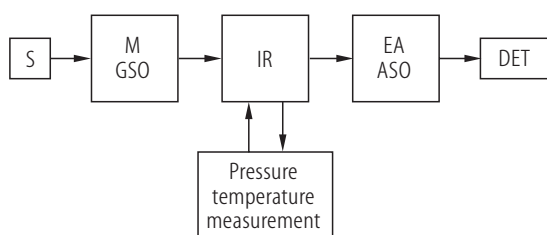


Fig. 6.1.1. Block diagram showing all the functional blocks of a transmission measurement.

Here S stands for the electron source. Electrons are then monochromatized (M) and geometrically selected (GSO) to form a beam. This beam is passed through an interaction region (IR) where the target gas is confined. The confinement is performed in a gas cell or by the use of a molecular beam. Different techniques are used to measure the gas density with the needed accuracy. Transmitted electrons are energy selected by an energy analyzer (EA) and geometrically selected by a suitable angular selection optics (ASO) to be admitted in the detector (DET). The beam forming and the monochromatization functions are often mixed in a single device; the same applies for the geometrical selection and the energy analysis functions. In real experimental set-ups some of these functional blocks can be absent. As an example, the monochromator function is sometimes missing: at energies higher than several tens of eV, this can be justified by the fact that $\Delta E/E$ is smaller than 1/100 for standard thermionic sources.

Attenuation measurements are performed with a variety of different set-ups. Among these, we can distinguish two broad classes: the time of flight techniques (TOF) and the beam techniques. The former rely on fast timing to obtain a velocity (energy) spectrum of transmitted electrons. TOF apparatuses cannot deconvolve energy losses introduced by the scattering event from the original electron energy distribution of the source; therefore they have been used mostly in the very low energy range, where inelastic channels are closed. TOF spectrometers are (typically) more difficult to operate than beam spectrometers: below 1 eV, difficulties in obtaining stable beams increase, rendering the TOF technique more interesting [80Ken1, 81Fer1, 86Buc2, 96Al1].

Beam techniques can be implemented as linear apparatuses or as curved beams. The pioneering works of Ramsauer [21Ram1] and Ramsauer and Kollath [29Ram1], Brüche [27Bru1] and others in the twenties have been performed with a 180° magnetic spectrometer. This type of apparatus suffers from a poor energy discrimination of the inelastically scattered electrons [81Dal1]. Linear apparatuses [80Bla1] can more easily implement an energy analyzer (see Fig. 6.1.1) to improve this discrimination.

Errors affecting the measured cross section can arise mainly from:

1. Determination of the interaction region length; this is more difficult when axial magnetic fields are used.
2. Target density measurement.
3. Electron emission instabilities.

4. Poor energy and/or angle discrimination of the scattered electrons - at the high energy limit of each apparatus.
5. Apparatus instabilities - at the low energy limit of each apparatus.

Table 6.1.1 gives a short form description of the apparatuses used in the total cross section measurements referenced throughout this paper. Table 6.1.1 quotes those parameters which are more important for the assessment of the quality of the measured cross sections. This table does not give a detailed description of each apparatus: this is hindered by the fact that each apparatus has undergone continuous improvements during its life. The relevant parameters often change from one paper to the next. In particular, the errors quoted by the authors often change in the measurement of different gases. The energy range also changes frequently.

The order in which the apparatuses appear in the table is in accordance with the lower limit of the energy span. The symbols used in the table are listed in the table caption. The most relevant references are given in the last column and are listed in the reference list below the table.

Table 6.1.1. Overview of transmission-method experiments for total cross section measurements.

Laboratory	Method Monochr. Analyzer	Energy range [eV]	Energy resolution ΔE [eV]	Stat. error [%]	Syst. error [%]	L_{scat} L_{cell} [cm]	Ω_{geom} [10^{-4} sr]	Source	Ref.
LURE-ACO, Orsay (France)	LTE No RF	0.01 - 6	0.0055 - 0.015	NQ	NQ	3 3	NQ	Ph-S	A1, A2
SRS-SERC, Daresbury (UK)	LTE No SE	0.02 - 20	0.0035		ND Tot: 8	3 3	NQ	Ph-S	B1, B2
University of Bielefeld (Germany)	TOF	0.08 - 20	0.003 - 2.9, DoE	2 - 3	< 1	27.1 24.7	2.4 to 15	ThC	C
Australian National University, Canberra (Australia)	TOF	0.12 - 20	>0.003, DoE	3 - 3.75	2.2	25.5 NQ	7.0	WF	D
Forschungsinstitut der AEG	RT MAG MAG	1.16 - 2.2	0.09 at 0.5 eV		NQ	3.14 3.14	240	PhC	E
University of Maryland (USA)	LTM (axial) TR RF	0.2 - 12	0.05 - 0.08, DoE	< 10	10 - 43 DoE	NQ NQ	NQ	ThC	F
Technical University of Gdańsk (Poland)	LTE CE RF	0.25 - 250	0.07	< 1	4 - 10	3.05 3.05	10	WF	G
University of Trento (Italy)	LTE RPD RPD	0.3 - 100	0.5		ND Tot: 1.7 - 7 DoE	(a)	NQ	ThC	H
Indiana University Bloomington (USA)	TOF	0.5 - 100	0.06 - 2.8 DoE		ND Tot: 3-15	38 38	0.22 to 1.4	SE	I
Phys. Research Lab., Navrangpura Ahmedabad-India	LTE CE RF	0.7 - 10	NQ	1.5	5.3	2.37 NQ	NQ	Ph	J

Table 6.1.1 (continued)

Laboratory	Method Monochr. Analyzer	Energy range [eV]	Energy resolution ΔE [eV]	Stat. error [%]	Syst. error [%]	L_{scat} L_{cell} [cm]	Ω_{geom} [10^{-4} sr]	Source	Ref.
Technische Hochschule Danzig	RT MAG MAG	1 - 50	0.2 at 1.2 eV		NQ	1.8 1.8	$9 \cdot 10^2$	PhC	K
Tokyo-Yamaguchi, University (Japan)	RP-TOF +axial B field	1 - 400	1.8	ND Tot: 3 - 15		7.17 (b) 6.38	NQ	SE	L1, L2
Wayne State University, Detroit (USA)	LTM (axial) No RF	1 - 700	0.15 at 5 eV	1	5	109 109	NQ	ThC WF for O ₂	M
Lockheed Research Laboratory, Palo Alto (USA)	RT MAG MAG	2 - 21	0.07 - 0.7, DoE	ND Tot: 3 - 10		NQ NQ	NQ	ThC WF	N
Jet Propulsion Lab., Pasadena, California (USA)	LTE-linear No RF	4 - 300	0.35	0.2 - 2	2	14.43 14.43	2.2	WF	O
Niigata University (Japan)	LTE No RF	7 - 500	1.25 at 100 eV	0.2 - 6	13 - 18	2.52 2.52	NQ	WF	P
University of Bielefeld (Germany)	LTE CE RF	5 - 400	> 0.5	> 5	3	51.8 51.5	NQ	ThC SE	Q
FOM-Inst. Atom. Mol. Phys., Amsterdam-Holland	LTE-linear No RF	16 - 700	0.4	Stat. 1 Tot: < 4		4.2 4.2	0.785	ThC	R
University of Trento (Italy)	RT MAG MAG	75 - 4000	NQ	< 1.5	2.4 - 3	14.02 14.02	3.4	ThC	S1, S2
Universidad Complutense Madrid (Spain)	LTE No SE	380 - 5200	1	Stat. 2 Tot: 3		7 - 12.7 7 - 12.7	0.35	WF	T1, T2
University of Science and Techn., Hefey (China)	LTE-linear No RF	400 - 4250	0.85	2.5 - 3	1 - 3	20.2 20.2	0.63	WF	U

Symbols

- 1st column: laboratories.
- 2nd column: *First line*, method, apparatuses used to measure TCS: **RT** Ramsauer-type; **TOF** time of flight; **RP-TOF** time of flight + retarding potential; linear transmission methods with (i) electrostatic transport **LTE** or with (ii) with magnetic transport **LTM**.
Second line, monochromator: **SE** spherical electrostatic, **CE** cylindrical electrostatic, **TR** trochoidal, **RPD** retarding potential difference, **MAG** magnetic 180°, **No** no monochromator.
Third line, analyser: **SE** spherical electrostatic; **RF** retarding field, **MAG** magnetic 180°, **No** no analyser.
- 3rd column: energy range of the measured TCS.
- 4th column: energy resolution of the apparatus.
- 5th and 6th columns: statistical and systematic errors. Where not distinguished, the total error is given.
- 7th column: length of the scattering path and of the scattering cell.
- 8th column: angular discrimination of the apparatus after the interaction region.
- 9th column: source: **ThC** thermoionic cathode, **WF** tungsten filament, **SE** secondary, electrons, **Ph** – photoionization, **Ph-S** photoionization with synchrotron radiation, **PhC** photocathode.
- 10th column: selected references regarding the gases measured with the corresponding apparatus.

ND: not distinguished; **NQ**: not quoted; **DoE**: depends on energy

Notes

- (a) A cell (and a scattering) length of (1.8 ± 0.02) cm and (5.0 ± 0.02) cm in the 0 - 10 eV and 10 - 100 eV energy range was respectively used.
- (b) Obtained by normalization of positron-scattering TCS in N₂ with those of [82Hof1].

References and targets

- A1** 84Fie1 (CF₄, N₂, O₂); 94Lun1 (CH₄, C₂H₄, C₂H₆)
- A2** LTE with an axial magnetic field: 93Zie1 (O₂); 93Ran1 (CF₃Cl, CF₂Cl₂, CFCl₃, CCl₄); 96Ran1 (CO)
- B1** with crossed beam: 91Fie1; 88Fie1 (O₂); 91Fie2 (CO₂); 94Lun1 (CH₄, C₂H₄, C₂H₆)
- B2** LTE with an axial magnetic field: 98Gul1 (C₆H₆, C₆D₆, C₆H₅D); 98Gul2 (O₃, ClO₂); 98Gul3 (Cl₂); 98Lun1 (CH₄, C₂H₆, C₃H₈, C₃H₆); 99Lun1 (C₆H₅F, C₆H₅Cl, C₆H₅Br, C₆H₅I)
- C** 80Fer1 (H₂, O₂); 81Fer1 (CO₂); 85Fer1 (Ar); 85Fer2 (CH₄); 89Fer1 (CO₂); 91Fer1 (N₂)
- D** 86Buc1 (CO); 86Buc2 (He, Ar); 86Loh1 (CH₄); 87Buc1 (CO₂); 95Sun1 (N₂); 94Gul1 (Ne); 96All1 (NO)
- E** 21Ram1 (He, Ne, Ar), 29Ram1 (He-Xe), 30Ram1 (H₂, N₂, O₂, CO, CO₂, CH₄); 30 Ram2 (H₂, N₂O)
- F** 88Ben1 (CH₃I, CH₃Br, CH₃F, CH₃Cl); 89Wan1 (SiH₄, SiH₂Cl₂, SiHCl₃, SiH₄, SiF₄, SiCl₄, SiBr₄, SiI₄); 91Wan1 (CCl₄, CHCl₃, CH₂Cl₂, CHCl₃, CH₄); 93Wan1 (SO₂); 94Und1 (CF₃Cl, CF₃Br, CF₃I, CF₂Cl₂, CF₂Br₂); 98San1 (CHF₃, C₂F₆, C₃F₈, c-C₄F₈)
- G** 78Szm1 (CO₂); 84Szm1 (N₂O, OCS); 86Zec1 (O₂); 86Szm1 (H₂S); 86Szm2 (SO₂); 87Szm1 (H₂O); 87Szm2 (CS₂); 87Szm3 (CO₂); 89Szm1 (NH₃, OCS, N₂O); 91Szm2 (D₂O); 91Szm1 (NO); 92Szm1 (NO₂); 92Szm2 (CF₄, CCl₄); 93Szm1 (CH₃I); 94Krz1 (CH₃Br); 95Krz1 (CH₃F, CH₃Cl); 95Szm1 (C₂H₆, CH₃OH, CH₃NH₂); 95Szm2 (CH₃SH); 96Moz1 (GeH₄); 96Moz2 (C₆H₆); 96Szm1 (He-Xe, H₂, N₂, O₂, CO, NO); 96Szm2 (SO₂); 96Szm3 (N₂O, OCS, SO₂); 97Szm1 (SiH₄, GeCl₄); 98Kar1 (SiF₄); 98Szm1 (GeF₄); 99Moz1 (SiCl₄)
- H** 80Dal1 (H₂); 86Zec1 (O₂)
- I** 78Ken1 (He); 79Ken1 (SF₆); 80Ken1 (N₂); 85Jon1 (H₂); 85Jon2 (CH₄); 86Jon1 (CF₄, CF₃Cl, CF₂Cl₂, CFCl₃, CCl₄)
- J** 87Kum1 (He); 89Sub1 (H₂); 90Sub1 (O₂)
- K** 27Bru1 (HCl), 27Bru2 (N₂, H₂), 27Bru3 (O₂, CO, NO, CO₂, N₂O, CH₄); 29Bru1 (C₂H₂, C₂H₄), 29Bru2 (NH₃, H₂O), 30Bru1 (CH₄, C₂H₆, C₃H₈, n-C₄H₁₀), 30Bru2 (n-C₄H₁₀, iso-C₄H₁₀)

- L1** different L_{cell} and L_{scatt} 84Sue1 (N₂, CO, CO₂)
- L2** 86Sue1 (CH₄, C₂H₄, C₂H₆); 86Sue2 (H₂O); 87Sue1 (NH₃); 88Sue1 (C₆H₆); 89Sue1 (C₂H₂); 94Ham1 (HCl); 94Ham2 (H₂O, NH₃); 94Sue1 (SiH₄, CF₄); 95Ham1 (CCl₄); 97Kim1 (CO₂); 98Sue1 (CHF₃); 99Sue1 (OCS); 99Tan1 (C₃F₈, C₃H₈); 00Kim1 (H₂O, HCl, CO, CO₂, OCS, CH₄, CH₂F₂, CF₄, CCl₄, SiH₄, C₂H₂, C₂H₄, C₂H₆, C₃H₈, C₃F₈, CH₃OH, HCOOH, CH₃COCH₃, C₆H₆, n-C₅H₁₂, n-C₆H₁₄, c-C₆H₁₂)
- M** 77Kaul (He, Ar); 82Hof1 (CO₂, N₂); 83Kwal (CO₂); 84Kwal (N₂O); 86Dab1 (OCS, SO₂); 88Dab1 (O₂, CH₄, SF₆)
- N** 65Gol1 (He); 66Gol1 (N₂); 66Gol2 (H₂, D₂); 70Sal1 (O₂, Ne)
- O** 85Nic1 (He, Ne, Ar, Xe); 90Sag1, 91Sag1 (H₂O); 92Kan1 (Kr, O₂, CO); 92Nic1 (H₂, N₂); 92Kan2 (CH₄)
- P** 88Nis1 (Ar, N₂, H₂O, D₂O); 90Nis1 (CH₄); 91Nis1 (C₂H₄, C₂H₆, C₃H₆, cyclo-C₃H₆, C₃H₈)
- Q** 83Deul (H₂); 85Flo1 (CH₄, C₂H₆, C₂H₄, C₃H₈, C₃H₆, C₄H₁₀, C₄H₈)
- R** 80Blal (N₂, He); 80Win1 (H₂)
- S1** Ω_{geom} $1.6 \cdot 10^{-4}$ sr in the 250-3000 eV energy range, $3.4 \cdot 10^{-4}$ sr in the 100-360 eV energy range: 81Dal1 (He); 80Dal2 (O₂, N₂, NO); 87Zec2 (Ne, Ar)
- S2** Ω_{geom} $3.4 \cdot 10^{-4}$ sr in the 75 - 4000 eV energy range: 87Zec1 (H₂O); 87Szm3 (CO₂); 91Zec1 (CH₄); 91Szm2 (D₂O); 92Zec1 (NH₃, SiH₄, H₂S); 92Zec2 (CF₄, CClF₃, CCl₂F₂, CCl₃F, CCl₄); 92Zec3 (SF₆); 93Kar1 (CO); 95Zec1 (NO₂, OCS, SO₂); 95Kar1 (GeH₄); 96Moz2 (C₆H₆); 98Kar1 (SiF₄); 99Kar1 (CH₃Cl, CH₂Cl₂, CHCl₃); 99Moz1 (SiCl₄); 00Kar1 (WF₆)
- T1** different energy resolution and L_{cell} 88Gar1 (N₂)
- T2** 90Gar1 (CO); 96Gar1 (CO₂); 96Gar2 (NH₃); 98Gar1 (CH₄)
- U** 94Xin1 (N₂); 95Xin1 (C₂H₂, CO); 97Xin1 (N₂O)

6.1.1.4 Semiempirical methods

In some cases (very low or high-energies) semiempirical formulae have been used to extrapolate measured total cross sections. As far as these methods have been originally developed for atoms, numerous authors use them also for molecules. In the zero-energy limit, the modified effective-range theory [62OMa1, 89Buc1] gives for σ_{el} the following formula:

$$\sigma_{\text{el}} = 4\pi \left[A_0^2 + \frac{2\pi}{3a_0} \alpha A_0 k + \frac{8\pi}{3a_0} \alpha A_0^2 k^2 \ln(ka_0) + Bk^2 + \dots \right] \quad (7)$$

where α is the electric polarizability, a_0 is the Bohr radius, A_0 the scattering length, E is the electron energy and k its wavenumber. The modified effective-range theory has been used to extrapolate towards zero-energy the elastic cross sections in targets like CF₄ [92Man1] and C₂H₆ [98Mer1]; below inelastic thresholds it is also used to extrapolate total cross sections [80Fer1].

In the high energy limit, the Born-Bethe approximation [71Ino1] is the most frequently used. For the elastic cross sections this approximation gives:

$$\sigma_{\text{el}} = A_1 \frac{R}{E} + A_2 \frac{R^2}{E^2} + \dots \quad (8)$$

where R is the Rydberg energy and the coefficients A_i are related to the atomic number Z and atomic form factors [74Ino1]. For the inelastic cross section it yields:

$$\sigma_{\text{in}} = 4\pi a_0^2 R \left[M_{\text{tot}}^2 \frac{\ln(E)}{E} + M_{\text{tot}}^2 \frac{\ln(4C_{\text{tot}}/R)}{E} + \gamma_{\text{tot}} \frac{R}{E^2} + \dots \right] \quad (9)$$

where the coefficients M_{tot}^2 , C_{tot} , and γ_{tot} can be obtained theoretically from the distributions of electronic moments. The Born-Bethe formulae (eqs. 8 and 9) have been indicated as the very high energy (above 10 keV) limit for the total cross section in targets like N₂ [88Gar1], CH₄ [98Gar1], NH₃ [96Gar2].

Note that other approximating formulae have been given for total cross section in the few hundreds eV - few keV range. As an example we quote the one based on Born's scattering from a screened Coulomb potential [91Zec1]

$$\sigma_{\text{tot}} = \frac{\sigma_z b}{b + \sigma_z E} \quad (10)$$

where σ_z and b are found by a fitting procedure.

In the case of polyatomic molecules, like CF_3Cl [92Zec2] or WF_6 [00Kar1] a more complex formula, similar to the one giving the integral elastic cross section for scattering on a double Yukawa potential (see [92Zec2], [00Zec1]) was used to fit the observed total cross section energy dependence.

$$\sigma = \frac{1}{A(B+E)} + \frac{1}{C(D+E)} + \frac{2}{E} \sqrt{\frac{BD}{AC}} \frac{1}{|B-D|} \left| \ln \frac{E/D+1}{E/B+1} \right| \quad (11)$$

where A, B, C, D are fitting parameters.

In some cases, in particular at low energies, the TCS almost coincides with the integral cross section for inelastic processes, like vibrational and rotational excitation. In other molecules, like CCl_4 [92Lin1] CFCl_3 , C_6F_6 [88Mar1], CH_3I [88Ala1] the zero-energy total cross section is governed by electron attachment processes. Some approximate formulae allow to evaluate the TCS in these cases. For the rotational and vibrational excitation cross sections, the Born approximation [66Tak1, 74Iti1] can be used:

$$\sigma_{\text{rot}}(J \rightarrow J \pm 1) = \frac{8\pi}{3k^2} D^2 \frac{J_{\pm}}{2J+1} \ln \frac{k+k'}{|k-k'|} \quad (12)$$

with k being the incident electron wavenumber and k' being the scattered electron wave number, J – initial rotational number; D is the permanent dipole moment of the molecule. For example, the TCS below 0.1 eV for polar molecules like NO and CO [96Ran1] is determined by the rotational excitation.

Similarly, the vibrational excitation cross section equals

$$\sigma_{\text{vib}}(v \rightarrow v') = \frac{8\pi}{3k^2} g' \left| \langle v' | D | v \rangle \right|^2 \ln \frac{k+k'}{|k-k'|} \quad (13)$$

with $\langle v' | D | v \rangle$ being the transient dipole moment matrix element for the $v \rightarrow v'$ vibrational transition and g' being the degeneration factor for this transition. Vibrational excitation determines the total cross section at energies below 1 eV in targets like CF_4 [98Lun1] or SiF_4 [98Kar1].

For the electron attachment cross sections, the experiments in the few meV energy range [87Dun1, 92Lin1] showed the applicability of Wannier's [54Vog1] threshold law: $\sigma_{\text{att}} \propto E^{1/2}$ in the zero-energy limit for targets, like CCl_4 or SF_6 [92Lin1]. At energies in the few tens of meV other types of approximating formulae have been proposed [88Ala1].

Finally, for total cross sections at intermediate and high energies we quote numerous additivity rule formulations [96Jos1, 95Jia1, 96Liu1, 99Zec1, 99Kar1] which have been published in the last years. These allow to calculate molecular cross sections starting from those of the atomic constituents. At present, the reliability of such additivity rules has not been validated, mainly due to the noise present in total cross section measurements. In the future it is possible that these rules will become useful for the evaluation of total cross section for "exotic" targets where little experimental data exist.

6.1.1.5 Data selection and analysis criteria

In this section we list the criteria used to select the experimental cross section data. After this selection, the accepted data have been handled to obtain the recommended values. The handling procedure has been codified in order to obtain criteria as uniform and as objective as possible for the various gases and various authors.

The selection has been made according to the following criteria. Total cross section data sets have been rejected when:

1. The number of measured points was very small.
2. The energy span of the measurement was much less than a decade.
3. The measurements were performed with a relative method: i.e. when the cross section values were normalized or when the values of one key parameter were obtained through a normalization procedure.
4. The measurements were in large disagreement with the majority of other existing measurements in the same energy range.

In several instances isolated data points or groups of points were rejected when metadata obtained from more recent articles of the same research group or from more recent articles from competing groups give evidence of systematic errors limited to those points.

We note that in all the cases where we have found measurements from one group only, we have relaxed the above conditions giving those values as the recommended cross sections. Obviously, in such cases the error bar on the recommended values is at least as large as the error bars declared by the authors. We warn that sometimes these error bars have been underestimated.

The selected data have been handled to obtain the recommended values. We note here the different role of statistic and systematic errors. Systematic errors can be described as introducing an unknown multiplicative factor, so that the published values can be thought as the product of the "real" cross section times this factor. Statistic errors can be described as introducing an additional random noise on the "real" cross sections and thus in the published values. As a consequence of this distinction, we have first smoothed each published data set in order to reduce the random noise. The smoothing has been done by filtering the data or by fitting them with appropriate functions. Different filtering and fitting functions have been chosen for different gases and for different energy ranges according to the density of data points and to the behaviour of the cross section as a function of the energy. This smoothing operation results normally in a reduction of the statistical noise by a factor 5 to 10.

The smoothed data sets from different laboratories have been averaged giving a weight to each of them. Normally all data, for a given gas and a given energy range, had the same weight. A differentiated weighting has been used whenever the absolute errors published by the authors were significantly different. A differentiated weighting has been used in some instances when available metadata have evidenced the possibility of systematic errors larger than those declared by the authors.

We note here that different authors have measured cross sections at different energy values, so that only rarely it is possible to have data from different groups at the same given energy. The use of a smoothing procedure circumvents this difficulty, allowing us to make averages at any chosen energy and to give recommended values for different gases with the same "comb" on the energy axis.

The region of resonances (see for instance the N_2 molecule) has been handled in the following way. The recommended values have been obtained as averages over several measurements performed by different methods. Additionally, the resonant region has been presented with an extra table with values from a high resolution, low noise measurements, like [80Ken1] for N_2 . An extra figure (Fig. 6.1.3, p. 6-13) with a resonant structure from "backward" scattering [93Zie1, 96Ran2] has been added for NO and O_2 , for comparison reasons. Note that the data presented in Fig. 6.1.3 are not exactly total cross sections.

Recommended values obtained through this procedure are presented in numerical form in Tables 6.1.2 to 6.1.13. Figures 6.1.2 and 6.1.4 to 6.1.9 present the recommended values as bold continuous lines. In these figures also the original (uncorrected) experimental data are presented as data points or thin lines. The figures are intended to give a visual representation of the cross section dependence on the energy. The scatter of the points (where more than one measurement exist) allows an immediate evaluation of the probable error bar in each energy range.

We note that the grouping of targets in the figures does not follow the grouping in the tables. This has been done to optimize the use of printed space. We also note that Tables 6.1.11, 6.1.12 and 6.1.13 do not contain recommended values but rather the experimental data from a single group. These are the only data available for the targets and therefore can be considered as recommended data.

6.1.2 Diatomic molecules

Table 6.1.2. Recommended total cross sections for diatomic molecules.

Energy [eV]	Cross section [10^{-16} cm^2]				
	H ₂	N ₂	O ₂	CO	NO
0.1	9.23	4.88	3.83 (c1)		
0.12	9.47	5.13	4.02	(d1)	
0.15	9.76	5.56	4.22		(e1)
0.17	9.93	5.85	4.33		
0.2	10.1	6.25	4.47		
0.25	10.5	6.84	4.65		
0.3	10.7	7.32	4.79	9.13	
0.35	11.0	7.72	4.91	9.69	
0.4	11.2	8.06	5.07	10.2	
0.45	11.4	8.33	5.20	10.6	
0.5	11.6	8.61	5.31 (c2)	10.9	
0.6	11.9	8.96	5.49	11.7	
0.7	12.3	9.25	5.64	12.2	
0.8	12.8	9.48	5.77	12.7	
0.9	13.2	9.66	5.87	13.3	
1.0	13.5 (a1)	9.85	5.97	14.1	
1.2	14.2	10.2	6.18	16.7	
1.5	15.0	11.2	6.36	29.1	
1.7	15.5	13.3	6.45	38.9	
2.0	16.0	25.7	6.56 (c3)	43.3 (d2)	
2.5	16.5	28.5 (b1)	6.68	33.3	9.70
3.0	16.6	21.0	6.84	23.8	9.47
3.5	16.6	14.6	7.01	18.9	9.32
4.0	16.3	13.2	7.18	16.4	9.25
4.5	15.9	12.3	7.36	15.2	9.22
5.0	15.4	11.8	7.55	14.5	9.23
6.0	14.4	11.4	7.93	13.7	9.32
7.0	13.3	11.4	8.39	13.5	9.48
8.0	12.4	11.5	9.16	13.6	9.68
9.0	11.6	11.7	9.91	13.5	9.92
10	10.9	12.0	10.4	13.2	10.2
12	9.61	12.4	10.8	13.3	11.0
15	8.19	13.2	10.7	13.9	11.5
17	7.46	13.5	10.7	14.3	11.6
20	6.60	13.7	10.8	14.5	11.4
25	5.61	13.5	11.0	14.1	11.1
30	4.97	13.0	11.0	13.6	10.7
35	4.54	12.4	10.9	13.2	10.3
40	4.19	12.0	10.7	12.7	9.97
45	3.91	11.6	10.5	12.3	9.73
50	3.68	11.3	10.3	11.9	9.53
60	3.36	10.7	9.87	11.2	9.18
70	3.06	10.2	9.52	10.7	8.89
80	2.86	9.72	9.23	10.2	8.64
90	2.68	9.30	8.98	9.69	8.42

Table 6.1.2 (continued)

Energy [eV]	Cross section [10^{-16} cm^2]				
	H ₂	N ₂	O ₂	CO	NO
100	2.54	8.94	8.68	9.27	8.22
120	2.25	8.33	7.97	8.53	7.86
150	1.98	7.48	7.21	7.64	7.44
170	1.84	7.02	6.78	7.15	7.13
200	1.66	6.43	6.24	6.53	6.64
250	1.43	5.66	5.51	5.71	5.93
300	1.24	5.04	4.94	5.09	5.25
350	1.11	4.54	4.55	4.57	4.75
400	1.00	4.15	4.17	4.16	4.34
450	0.914	3.82	3.85	3.82	4.00
500	0.841	3.55	3.58	3.54	3.70
600	0.700	3.14	3.11	3.13	3.23
700	0.614	2.79	2.76	2.79	2.87
800	0.516	2.55	2.49	2.52	2.58
900	0.464	2.32	2.26	2.31	2.34
1000	0.422 (a2)	2.13	2.08 (c4)	2.13	2.15

Notes

The following sets of data (the energy ranges are given in brackets) have been used to obtain the recommended TCS.

H₂: [80Fer1] (0.02-1.0); [96Szm1] (0.4-250); [80Dal1] (0.6-100); [85Jon1] (1-50), corrected by 0 % at 4 eV up to + 3 % at 50 eV; [92Nic1] (4-300); [82Hof1] (4.9-500); [80Win1] (25-750); [96Kar1] (70-1000). See Fig. 6.1.2.

N₂: [95Sun1] (0.1-10); [96Szm1] (1.0-250); [91Fer1] (0.1-1); [80Ken1] (0.5-50) corrected by 0 % at 5 eV up to + 7 % at 50 eV; [82Hof1] (3.8-700); [92Nic1] (4-300); [88Nis1] (10-500); [80Bla1] (100-750); [93Kar1] (121-1000); [94Xin1] (500-1000); [88Gar1] (600-1000). See Fig. 6.1.2.

O₂: [90Sub1] (0.15-1.1); [96Szm1] (0.4-250); [70Sal1] (2.3-7); [86Zec1] (0.15-100), Trento data; [86Zec1] (2-15), Gdańsk data; [92Kan1] (5-300); [88Dab1] (51-500); [80Dal2] (100-1000); [96Kar1] (100-1000). See Fig. 6.1.2 and Fig. 6.1.3.

CO: [86Buc1] (0.5-4.9); [96Szm1] (0.4-250); [83Kwa1] (4.8-500); [92Kan1] (5-300); [93Kar1] (80-1000); [95Xin1] (400-1000); [90Gar1] (380-1000). See Fig. 6.1.2.

NO: [91Szm1] (2.5-160); [96Szm1] (2.5-250); [74Zec1] (2.5-9.5); [80Dal2] (144-1000). See Fig. 6.1.2 and Fig. 6.1.3.

(a1) All different sets of data at low energies are in good agreement apart from data in [80Fer1] which are somewhat lower than the recommended set above 1 eV.

(a2) Note that scattering in H₂ at high energies is extremely forward centred; existing data [96Kar1] could be underestimated due to angular resolution error.

(b1) A vibrational structure due to the presence of $^2\Pi_g$ resonant state is visible in TCS in the 2 - 4 eV energy region. See Table 6.1.3a for detailed values of TCS in this range.

(c1) The 0.1 eV point has been extrapolated from data in [90Sub1] and [86Zec1]. The early TCS measurements in O₂ [30Ram1] indicated a rise of TCS below 0.1 eV up to about $6 \cdot 10^{-16} \text{ cm}^2$ at 0.04 eV [see 96Zec1].

(c2) A resonant structure is present in O₂ TCS between 0.2 - 1 eV [74Lan1, 80Fer1, 86Zec1]. A series of narrow peaks was observed also in other experiments [62Sch1, 70Bon1, 71Lin1, 88Fie1, 94Ran1, 95All1]. Only recent TCS measurements [99Buc1] have been performed with an energy resolution sufficient to distinguish the structure. See also Fig. 6.1.3.

- (c3) Different TCS measurements [70Sal1, 86Zec1, 90Sub1, 96Szm1] in O_2 at 1.5 - 6 eV are in serious disagreement. Present recommended values are average of results quoted in the table caption above. They agree well with TCS from Tokyo lab [85Kat1]. The recent elastic cross sections between 1 - 5 eV [95Sul1, see also [97Gre1] are slightly higher than our recommended TCS, with differences remaining well within the declared [95Sul1] error bar. In this energy range the scattering into inelastic channels (vibrational and $a^1\Delta_g$, $b^1\Sigma_g^+$ electronic excitation) is in the 10^{-18} cm^2 range and contributes less than 1 % to TCS [71Lin1, 92Mid1, 93Shy1].
- (c4) Present high energy TCS in O_2 are slightly lower than in N_2 and CO, being average values of only Trento TCS [80Dal2, 96Kar1]. Comparative measurements, say at 2500 eV, [93Kar1, 96Kar1] show that O_2 TCS is higher ($0.92 \cdot 10^{-16} \text{ cm}^2$) than the N_2 ($0.89 \cdot 10^{-16} \text{ cm}^2$) value.
- (d1) The backward-scattering measurements from Daresbury lab [96Ran1] indicate a rise of TCS below 0.12 eV, attributed to the rotational excitation, see formula (eq.12) in the introduction.
- (d2) A $^2\Pi$ resonant state is present between 1 and 4 eV. A maximum TCS is reached at 2 eV.
- (e1) TCS at very low energies in NO is dominated by the presence of resonant states. See Table 6.1.3b for detailed values of TCS in the 0.16 - 2.0 eV energy region.

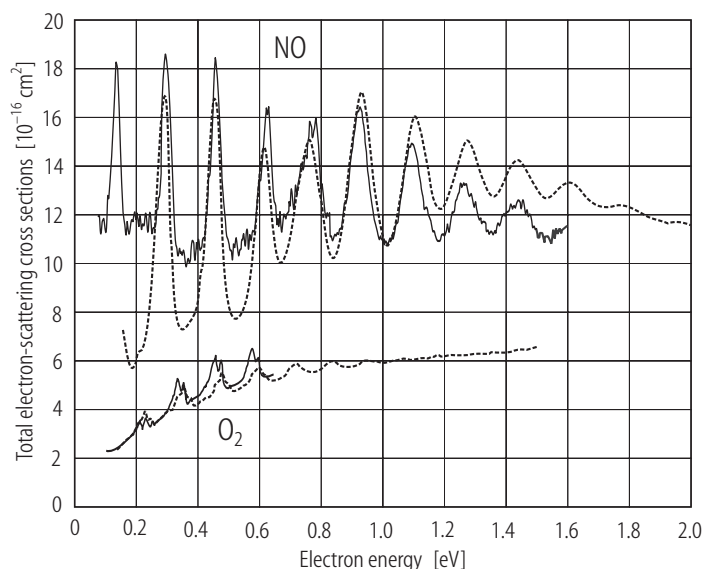


Fig. 6.1.3. Low-energy resonance region in O_2 and NO (solid lines: Orsay and Daresbury experiments using synchrotron-radiation electron sources; broken lines: total cross sections from Canberra lab).

Synchrotron radiation experiments:
 O_2 , total cross section obtained with use of a strong guiding magnetic field [93Zie1];
 NO, signal of electrons elastically scattered into 60° - 120° angle [96Ran2].

Total cross sections:
 O_2 [99Buc1], NO [96All1].

Notes. A resonant structure in NO total cross section was observed in numerous measurements [74Zec1, 91Szm1] but only in Canberra lab it was measured with a high (3 meV) energy resolution [96All1]. Also in O_2 , only the measurement from Canberra lab yielded a well-distinct structure [99Buc1]. Therefore, in this figure we compare two available "scattered electrons" measurements in NO and O_2 from a synchrotron-radiation electron-source spectrometer with the TCS data from Canberra laboratory. Note the above mentioned difference in the detection method in the experiments with the synchrotron-radiation electron source. Note also that the Orsay data show in O_2 a double structure of the peaks due to the spin-orbit coupling in the $^2\Pi_g O_2^-$ resonant state. Such a structure was observed, for example, also in time-of-flight measurements of [74Lan1].

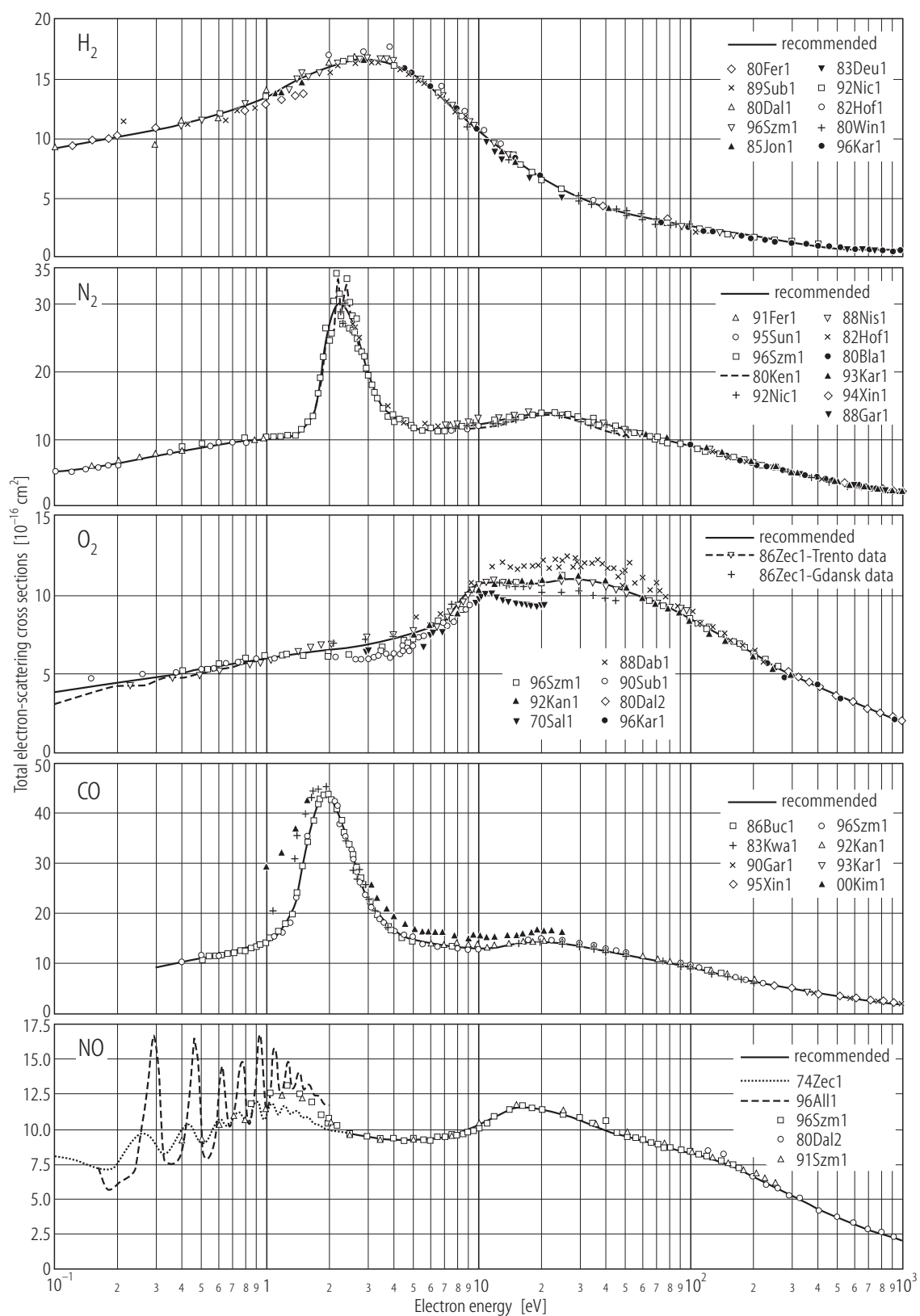


Fig. 6.1.2. Overview of experimental and recommended total cross sections for H_2 , N_2 , O_2 , CO , NO .

Table 6.1.3a. Resonant structure in N₂ total cross section (from [80Ken1]).

Energy [eV]	σ [10 ⁻¹⁶ cm ²]	Energy [eV]	σ [10 ⁻¹⁶ cm ²]	Energy [eV]	σ [10 ⁻¹⁶ cm ²]	Energy [eV]	σ [10 ⁻¹⁶ cm ²]
1.002	9.91	1.584	11.79	2.290	28.32	3.267	16.75
1.012	9.88	1.604	11.86	2.308	27.14	3.298	16.69
1.023	9.86	1.625	12.04	2.326	26.19	3.328	16.60
1.033	9.96	1.647	12.30	2.345	26.36	3.360	16.51
1.044	10.05	1.668	12.66	2.364	27.64	3.391	16.02
1.055	10.04	1.691	13.00	2.383	28.82	3.423	15.90
1.066	10.01	1.713	13.51	2.403	30.79	3.456	15.37
1.078	10.21	1.736	13.79	2.422	32.06	3.489	15.16
1.089	10.10	1.760	14.44	2.463	31.80	3.523	15.05
1.101	10.17	1.784	15.28	2.483	30.85	3.557	15.05
1.113	10.07	1.809	16.36	2.504	29.19	3.591	14.55
1.125	10.06	1.834	17.46	2.525	27.25	3.626	14.51
1.137	9.95	1.853	18.61	2.546	25.83	3.662	14.16
1.150	10.03	1.866	19.12	2.567	25.18	3.698	14.14
1.162	10.22	1.879	20.23	2.589	25.19	3.734	13.86
1.175	10.31	1.892	21.19	2.611	25.63	3.772	13.71
1.188	10.15	1.906	22.26	2.633	27.03	3.809	13.63
1.202	10.14	1.922	23.23	2.656	27.90	3.848	13.34
1.215	10.34	1.936	24.26	2.679	27.78	3.886	13.50
1.229	10.27	1.951	25.40	2.702	26.74	3.926	13.31
1.243	10.33	1.965	25.95	2.725	25.90	3.966	13.09
1.258	10.32	1.980	25.88	2.749	24.33	4.007	13.21
1.272	10.43	1.994	25.84	2.773	22.95	4.048	12.92
1.287	10.42	2.009	25.61	2.798	22.19	4.090	12.89
1.302	10.31	2.024	25.37	2.822	22.32	4.132	12.88
1.317	10.44	2.039	24.52	2.848	22.49	4.176	12.48
1.333	10.36	2.055	23.81	2.873	22.84	4.220	12.44
1.349	10.61	2.070	23.69	2.899	23.28	4.264	12.54
1.365	10.66	2.086	23.83	2.925	22.39	4.310	12.34
1.381	10.55	2.102	24.13	2.951	21.64	4.356	12.31
1.398	10.75	2.118	25.26	2.978	20.51	4.402	12.25
1.415	10.76	2.134	27.18	3.005	19.73	4.450	12.19
1.432	10.80	2.151	29.13	3.033	19.29	4.498	12.15
1.450	10.96	2.167	30.77	3.061	19.30	4.547	11.95
1.468	10.97	2.184	32.78	3.089	19.17	4.597	12.00
1.487	10.98	2.201	33.22	3.118	19.24	4.648	11.99
1.505	11.24	2.219	33.58	3.147	18.69	4.700	11.89
1.524	11.29	2.236	32.62	3.176	18.22	4.752	11.90
1.544	11.40	2.254	31.11	3.206	17.46	4.806	11.79
1.563	11.58	2.272	29.75	3.236	16.95	4.860	11.74

Notes

This structure is due to the presence of $^2\Pi_g$ resonant state [62Sch2] which manifests itself in total, elastic and vibrational excitation cross sections, see e.g. [85All1]. Different recent TCS measurements [95Sun1, 96Szm1] agree on the position and height of the peaks. The resonant structure in N₂, in particular as measured in Ref. [80Ken1] is the most frequently used as standard in the energy scale calibration for low-energy electron scattering.

Table 6.1.3b. Resonant structure in NO total cross section (digitized from Fig. 1 in Ref. [96All1]).

Energy [eV]	σ [10^{-16} cm ²]	Energy [eV]	σ [10^{-16} cm ²]	Energy [eV]	σ [10^{-16} cm ²]	Energy [eV]	σ [10^{-16} cm ²]
0.160	7.28	0.445	14.52	0.785	14.73	1.160	13.21
0.165	6.74	0.452	16.03	0.792	13.97	1.177	12.46
0.170	6.20	0.454	16.28	0.799	13.40	1.197	12.13
0.174	5.67	0.458	16.79	0.803	12.79	1.217	12.53
0.191	5.63	0.460	16.25	0.814	11.68	1.224	12.89
0.207	6.42	0.465	15.93	0.818	11.17	1.237	13.47
0.224	6.42	0.470	15.60	0.821	10.78	1.240	13.72
0.234	6.71	0.475	15.42	0.831	10.35	1.253	14.26
0.241	7.25	0.480	14.09	0.838	10.31	1.260	14.65
0.247	7.79	0.483	12.51	0.855	10.49	1.273	14.91
0.250	8.65	0.488	10.86	0.861	11.18	1.290	14.91
0.253	9.52	0.492	9.64	0.868	11.54	1.301	14.55
0.259	10.34	0.499	8.89	0.874	11.82	1.311	14.08
0.268	11.64	0.503	8.02	0.884	12.29	1.325	13.54
0.274	13.15	0.520	7.77	0.890	13.44	1.335	13.15
0.277	13.72	0.547	7.88	0.900	14.02	1.352	12.79
0.284	14.51	0.553	8.24	0.903	14.52	1.379	12.87
0.286	15.55	0.569	9.32	0.910	15.06	1.396	13.26
0.288	15.81	0.582	10.37	0.916	16.14	1.412	13.77
0.290	15.99	0.592	11.62	0.942	17.00	1.432	14.09
0.292	16.20	0.598	12.31	0.949	16.57	1.445	14.24
0.294	16.52	0.601	12.95	0.953	16.14	1.469	13.84
0.296	16.88	0.607	13.60	0.960	15.60	1.490	13.31
0.298	16.42	0.614	14.21	0.964	14.92	1.513	12.91
0.300	16.20	0.620	14.75	0.971	14.27	1.527	12.73
0.302	15.95	0.634	14.29	0.982	12.59	1.557	12.84
0.304	15.77	0.638	13.64	0.992	11.69	1.574	13.06
0.306	15.52	0.641	12.88	1.000	11.19	1.587	13.24
0.308	15.09	0.649	12.02	1.030	10.94	1.601	13.35
0.310	14.94	0.653	11.23	1.039	11.62	1.652	12.92
0.320	9.59	0.660	10.66	1.053	12.05	1.675	12.60
0.327	8.48	0.663	10.16	1.062	13.09	1.713	12.35
0.331	7.72	0.683	10.09	1.068	13.92	1.753	12.43
0.348	7.26	0.693	10.59	1.078	14.43	1.793	12.43
0.385	7.76	0.696	10.84	1.085	14.93	1.830	12.14
0.402	8.45	0.706	11.49	1.088	15.32	1.868	11.90
0.411	9.46	0.716	11.92	1.101	15.79	1.912	11.75
0.414	10.21	0.726	12.68	1.114	16.01	1.935	11.68
0.420	10.89	0.739	13.54	1.125	15.51	1.949	11.79
0.430	11.76	0.745	14.26	1.128	15.36	1.996	11.65
0.433	12.65	0.752	14.73	1.135	14.97		
0.442	13.70	0.772	14.98	1.149	13.78		

Notes

This resonant structure in NO was detected with different methods [71Spe1, 75Tro1, 96Ran2]. Below 0.7 eV only one "shape" resonance state is present; at 0.7 - 2.0 eV it overlaps with two more states [77Tei1, 86Ten1]. The TCS measurements in ref. [96All1] were performed with a much better (± 3 meV at 0.3 eV) energy resolution than other TCS experiments in this range [74Zec1, 91Szm1, 96Szm1]. Differently than the N₂ data given in Table 6.1.3a, the resonant structure in NO is not an established standard.

6.1.3 Triatomic molecules

Table 6.1.4. Recommended total cross sections for triatomic molecules.

Energy [eV]	Cross section [10^{-16} cm^2]					
	CO ₂	N ₂ O	NO ₂	OCS	SO ₂	CS ₂
0.1	49.7					
0.12	44.3					
0.15	38.1	10.3				
0.17	34.9	9.69				
0.20	31.1	8.96		51.6 (d1)	40.3 (e1)	
0.25	26.4	8.08		48.0	38.9	
0.30	23.0	7.48		44.0	37.8	
0.35	20.5	7.06		39.9	36.8	
0.40	18.6	6.77		36.0	36.0	22.4 (f1)
0.45	17.0	6.58		32.7	35.2	21.1
0.5	15.7	6.48		29.8	34.5	20.0
0.6	13.6	6.57	16.9	25.8	33.3	18.4
0.7	11.9	6.70	16.4	25.7	32.3	17.6
0.8	10.5	6.98	16.0	29.0	31.2	17.6
0.9	9.25	7.37	15.6	34.3	30.3	18.1
1.0	8.29	8.08	15.3 (c1)	42.5	29.8	19.1
1.2	7.22	10.2	14.7	51.3 (d2)	29.4	22.0
1.5	6.32	14.2	14.1	31.8	29.9	27.7
1.7	6.02	18.1	13.7	24.4	30.6	30.8
2.0	5.94	25.6	13.3	20.3	31.8	33.4 (f2)
2.5	6.81	26.9 (b1)	12.9	19.4	33.0 (e2)	37.5
3.0	8.77	18.6	12.7	22.5	33.4	42.2
3.5	13.3	13.6	12.6	26.3	33.7	46.9
4.0	14.9 (a1)	11.0	12.6	27.5	33.8	50.0
4.5	11.3	9.73	12.7	27.5	33.8	51.1
5.0	9.06	9.24	12.8	27.5	33.6	51.8 (f2)
6.0	8.44	9.37	13.2	28.2	32.2	52.3
7.0	9.21	10.4	13.7	29.4	31.5	52.4
8.0	10.3	11.9	14.3	30.6	31.1	52.4
9.0	11.3	13.4	14.7	31.7	30.8	52.4
10	12.2	14.5	14.9	32.3	30.7	52.3
12	14.2	15.9	14.8	32.8	30.7	51.8
15	15.8	16.4	14.5	32.2	29.5	50.4
17	16.4	16.6	14.7	31.2	28.4	48.7
20	17.0	17.4	14.7	30.0	26.4	45.7
25	17.8	17.7	14.4	28.5	25.0	39.3
30	18.0 (a2)	17.6	14.1	27.4 (d3)	24.0 (e3)	34.7
35	17.6	17.2	13.9	26.5	23.2	32.0
40	17.0	16.7	13.7	25.7	22.7	30.8
45	16.4	16.3	13.6	24.8	22.3	29.9
50	15.8	15.8 (b2)	13.4	23.9	22.0	28.1
60	14.8	15.0	13.2	22.3	21.1	25.2
70	14.1	14.4	12.9	21.1	20.1	23.8
80	13.5	13.8	12.6	20.2	19.1	22.5 (f3)
90	13.1	13.2	12.2	19.2	18.1	

Table 6.1.4 (continued)

Energy [eV]	Cross section [10^{-16} cm^2]					
	CO ₂	N ₂ O	NO ₂	OCS	SO ₂	CS ₂
100	12.6	12.6	11.8	18.4	17.2	
120	11.8	11.6	10.9	16.9	15.7	
150	10.6	10.4	9.87	15.1	13.9	
170	10.0	9.78	9.28	14.2	13.1	
200	9.24	8.87	8.55	13.0	12.2	
250	8.20	7.80	7.65	11.5	11.0	
300	7.39	7.12	6.97	10.3	9.99	
350	6.73	6.46	6.40	9.39	9.16	
400	6.08	5.92	5.92	8.63	8.46	
450	5.62	5.47	5.50	7.98	7.87	
500	5.23	5.08	5.14	7.43	7.35	
600	4.63	4.44	4.55	6.58	6.51	
700	4.16	3.94	4.07	6.08	5.84	
800	3.78	3.56	3.69	5.50	5.30	
900	3.47	3.26	3.37	5.02	4.85	
1000	3.20	3.01	3.11	4.63	4.48	

Notes

The following sets of data (the energy ranges are given in brackets) have been used to obtain the recommended TCS.

- CO₂** [87Buc1] (0.1-5); [81Fer1] (0.07-3); [97Kim1] (1.0-2.9, 4.8-90); [83Kwa1] (3-500); [87Szm3] (0.5-80) Gdańsk data; [87Szm3] (72-1000) Trento data; [96Gar1] (400-1000). See Fig. 6.1.4.
- N₂O** [30Ram2] (0.15-1.25), [84Szm1] (0.6-16.5), [96Szm3] (17-250), [84Kwa1] (1.2-500), [97Xin1] (600-1000). See Fig. 6.1.4.
- NO₂** [92Szm1] (0.6-220), [95Zec1] (100-1000). See Fig. 6.1.4.
- OCS** [84Szm1] (0.2-40), [89Szm1] (40-100), [86Dab1] (1.6-40), [99Sue1] (1.6-600) [95Zec1] (121-1000). See Fig. 6.1.4.
- SO₂** [96Szm3] (0.5-200); [93Wan1] (0.2-12); [95Zec1] (144-1000). See Fig. 6.1.4.
- CS₂** [87Szm2] (0.4-80).

- (a1) TCS between 2.5 - 5 eV is characterized by a $^2\Pi_u$ shape resonance. A maximum value of $15.8 \cdot 10^{-16} \text{ cm}^2$ is reached at 3.8 eV.
- (a2) We note some discrepancy at intermediate energies where TCS from the Gdańsk lab [87Szm3] are lower than those from Detroit lab [83Kwa1] and TCS corrected for the angular resolution error from Tokyo lab [97Kim1]; the recommended TCS are averaged over all the three laboratories.
- (b1) TCS between 1 - 4 eV is characterized by two resonances [84And1]. A maximum value of $28.4 \cdot 10^{-16} \text{ cm}^2$ is reached at 2.3 eV.
- (b2) Earlier TCS from Gdańsk lab [84Szm1, 89Szm1] at 20 - 100 eV have not been included in the averaged values being lower than the successive data from the same group [96Szm3] and those from the Detroit lab [84Kwa1].
- (c1) Electron transmission spectra [73San1] and vibrational excitation studies [91Ben1] indicate the presence of resonant states between 0.1 - 1.8 eV; no structures were seen in TCS [92Szm1].
- (d1) The sum of elastic and vibrational excitation cross section [87Soh1] exceeds TCS from Gdańsk lab [84Szm1] and amounts to 57.2 at 0.4 eV and $39.4 \cdot 10^{-16} \text{ cm}^2$ at 0.6 eV. Note that Gdańsk data at very low energies could be effected by a high uncertainty in the electron current measurement, in the 10^{-13} A range.

-
- (d2) TCS between 0.7 - 2 eV is characterized by a $^2\Pi$ resonance, seen also in the vibrational excitation [87Soh1] and dissociative attachment [75Zie1] channels. A maximum TCS of $52.8 \cdot 10^{-16} \text{cm}^2$ is reached at 1.15 eV.
- (d3) Differently than in SO_2 and N_2O , the successive measurements in OCS at intermediate energies from Gdańsk lab [96Szm1] coincide with earlier data [84Szm1]. However, they disagree with the data in [86Dab1] and recent TCS from the Tokyo apparatus [99Sue1]; the recommended TCS are averaged over all three laboratories.
- (e1) Low energy data in SO_2 show large discrepancies [86Szm2, 86Dab1, 93Wan1, 96Szm2].
- (e2) Two resonant states are present in electron scattering on SO_2 at 2 - 5 eV [73San1, 83And1, 94Gul1].
- (e3) More recent TCS from Gdańsk lab [96Szm2, 96Szm3] differ rather seriously at intermediate energies from the previous ones [86Szm1] but coincide with TCS from the Detroit lab [86Dab1].
- (f1) The only existing TCS data [87Szm2] agree in shape with elastic cross sections [87Soh1] at 0.3 - 5 eV.
- (f2) At low energies TCS shows two weak shoulder structures, at about 2 and 5 eV, probably due to resonant states, as seen in the dissociative attachment channel [87Dre1].
- (f3) At 80 eV the TCS from [87Szm2] and therefore also our recommended values, can be underestimated, being lower than the theory [97Raj1].

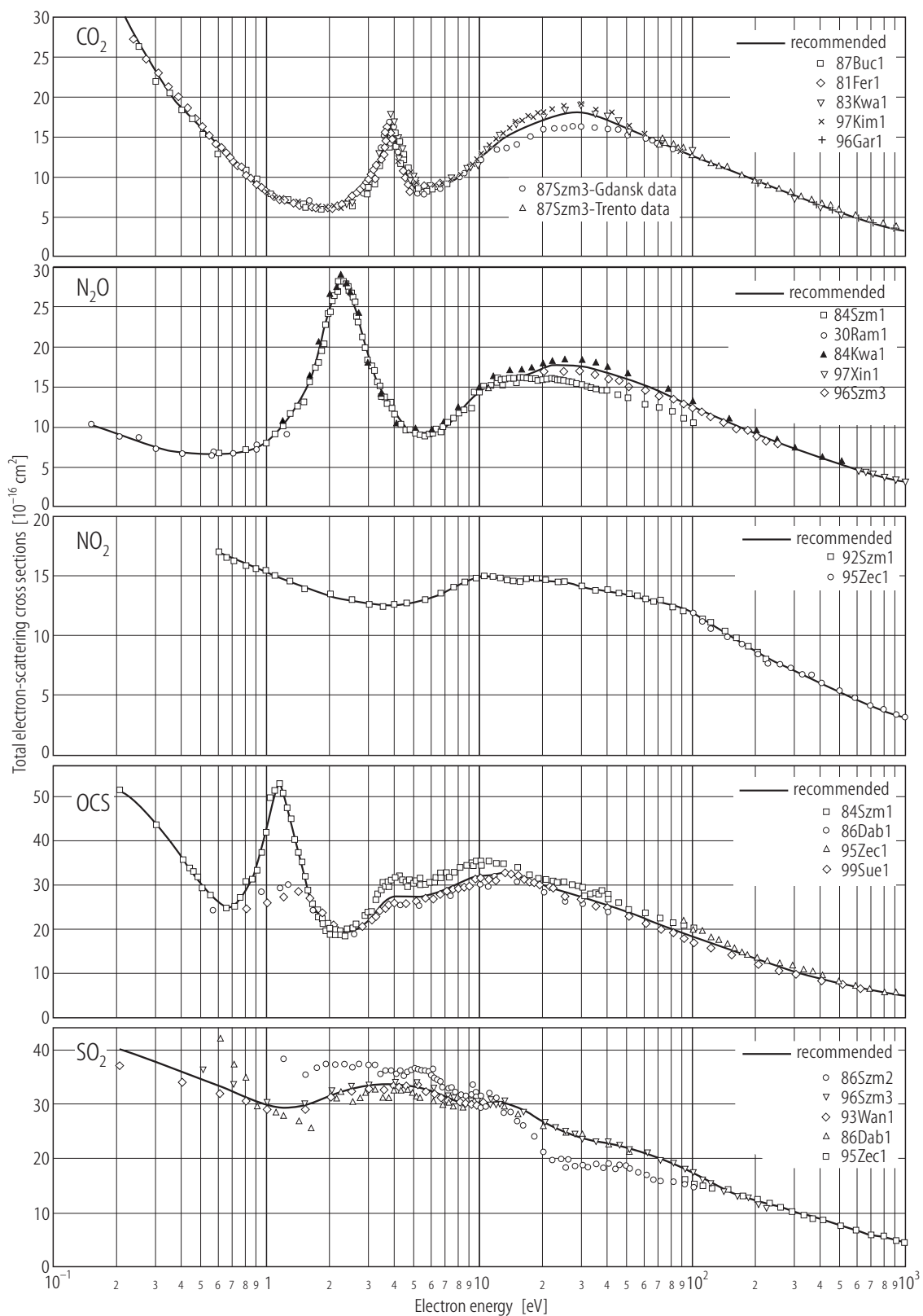


Fig. 6.1.4. Overview of experimental and recommended total cross sections for CO_2 , N_2O , NO_2 , OCS , SO_2 .

6.1.4 Hydrides

Table 6.1.5. Recommended total cross sections for some hydrides.

Energy [eV]	Cross section [10^{-16} cm^2]			
	NH ₃	H ₂ O (b1)	H ₂ S	HCl (d1)
0.5		71.4		
0.6		61.4		
0.7		53.8		
0.8		47.9		35.5
0.9		43.2		33.9
1.0	14.5 (a1)	39.4 (b2)	32.0	32.2
1.2	13.3	33.8	28.4	28.9
1.5	12.0	28.4	25.1	25.3
1.7	11.4	26.1	25.9	23.7
2.0	10.8	23.7	29.1 (c1)	22.4
2.5	10.5	21.6	31.8	22.1
3.0	10.7	20.5	31.7	23.1 (d2)
3.5	11.4	20.0	31.3	23.5
4.0	12.6	19.5	31.2	23.6
4.5	14.0	19.5	31.6	23.6
5.0	15.6	19.7	32.5	23.6
6.0	18.0	20.2	35.5	23.6
7.0	20.3	20.7	38.7	24.2
8.0	21.9	21.1	39.9 (c1)	25.6
9.0	22.8	21.2	39.8	27.4
10	22.9	20.9	39.0	28.0
12	21.8	19.1	36.4	28.0
15	20.1	17.3	32.1	26.6
17	19.1	16.5	30.9	24.9
20	17.8	15.6	30.0	22.2
25	16.1	14.0	28.0	20.5
30	14.8	12.7	25.0	19.0
35	13.8	11.7	22.1	17.2
40	13.0	10.9	20.4	15.9
45	12.3	10.3	19.1	14.9
50	11.8	9.78	18.2	14.0
60	10.9	8.98	17.3	12.7
70	10.3	8.37	16.1	11.7
80	9.68	7.89	15.0	10.9
90	9.10	7.56	14.0	10.2
100	8.57	7.17	13.1	9.67
120	7.64	6.50	11.7	8.79
150	6.67	5.74	10.3	7.81
170	6.17	5.34	9.57	7.29
200	5.55	4.83	8.71	6.66
250	4.76	4.17	7.61	5.85
300	4.21	3.68	6.79	5.23
350	3.75	3.26	6.14	4.74
400	3.38	2.95	5.61	4.34
450	3.13	2.71	5.17	
500	2.88	2.50	4.80	

Table 6.1.5 (continued)

Energy [eV]	Cross section [10^{-16} cm^2]			
	NH ₃	H ₂ O (b1)	H ₂ S	HCl (d1)
600	2.50	2.19	4.20	
700	2.21	1.93	3.74	
800	1.99	1.73	3.37	
900	1.81	1.56	3.06	
1000	1.66	1.43	2.81	

Notes

The following sets of data (the energy ranges are given in brackets) have been used to obtain the recommended TCS.

H₂O [87Szm1] (0.5-80), [90Sag1] (25-300), [88Nis1] (40-500), [87Zec2] (80-1000). See Fig. 6.1.5.

NH₃ [89Szm1] (1-100), [92Zec1] (75-1000), [96Gar2] (300-1000). See Fig. 6.1.5.

H₂S [86Szm1] (1-100), [92Zec1] (75-1000). See Fig. 6.1.5.

HCl [94Ham1] (0.8-400). See Fig. 6.1.5.

- (a1) At low energies two sets of TCS in NH₃ from Tokyo lab – those uncorrected for forward scattering [87Sue1] and the corrected ones [94Ham2] differ substantially. The data in [87Sue1] agree well in shape with the data in [87Szm3] and differ by 0 % at 4 eV, 28 % at 8 eV and 0 % at 400 eV. The TCS in [94Ham2] does not show a maximum and rises towards the zero energy reaching 29.0 at 5 eV, 45.7 at 2 eV and $76.2 \cdot 10^{-16} \text{ cm}^2$ at 1 eV.
- (b1) D₂O total cross sections as measured by [91Szm2] and [88Nis1] practically coincide with the H₂O data from the same laboratories, [87Szm1] and [88Nis1], respectively.
- (b2) Low energy TCS in H₂O is subject to a big uncertainty. Two sets of data from Tokyo lab, the uncorrected for forward scattering [86Sue2] and the corrected one [94Ham2, 00Kim1], differ substantially, see Fig. 6.1.5. The TCS in [94Ham2] does not show a maximum and rises towards the zero energy reaching 30.2 at 5 eV, 54.2 at 2 eV and $110 \cdot 10^{-16} \text{ cm}^2$ at 1 eV. These data are in agreement with the theory [92Yua1] who suggested that maxima observed in H₂O [29Bru2, 87Szm1, 91Sag1] and NH₃ could be experimental artifacts due to angular resolution errors.
- (c1) Structures in TCS in H₂S at about 2.5 and 8 eV are due to resonant scattering. An enhancement of the cross section was seen at 2-3 eV in the vibrational channel [78Roh1, 93Gul1]. Several maxima between 2 eV and 10 eV were observed in the dissociative attachment channel [72Azr1, 73Tro1, 85Bel1, 93Rao1].
- (d1) Recommended TCS in HCl are based exclusively on the Tokyo lab results [94Ham1]. We note, that these experimental data are lower than the early TCS measurements [27Bru1] in the 4 - 35 eV range and lower than the sum of elastic + rotational excitation cross [89Rad1, 95Got1], by 20 - 30 % in the 0.8 - 20 eV energy range.
- (d2) The hump in TCS at about 3 eV reflects the presence of a $^2\Sigma^+$ resonant state [89Rad1], seen also in the vibrational [75Roh1, 89Kno1, 89Kno2] and rotational [89Rad1] excitation channels.

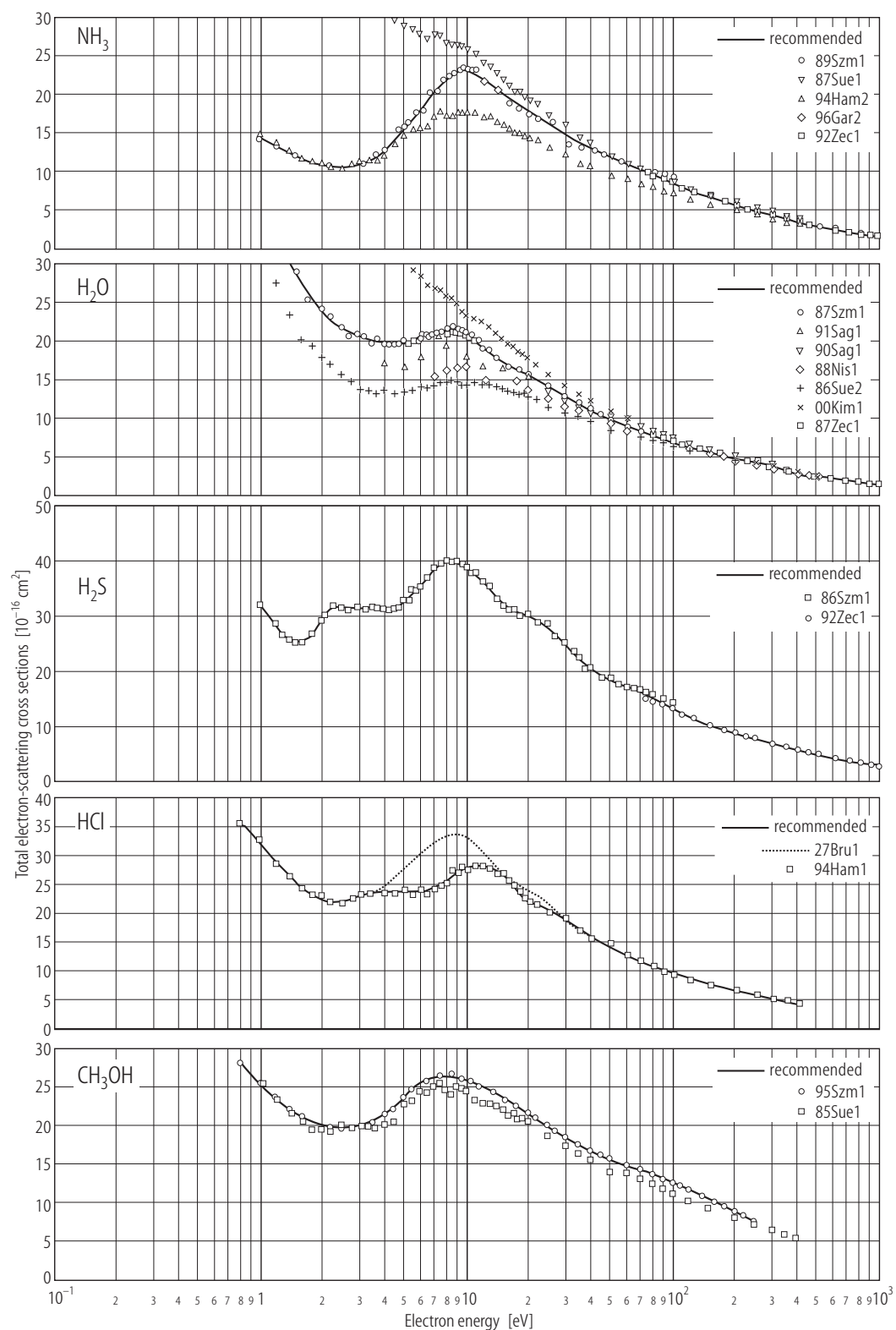


Fig. 6.1.5. Overview of experimental and recommended total cross sections for NH_3 , H_2O , H_2S , HCl , CH_3OH .

6.1.5 Hydrocarbons

Table 6.1.6. Recommended total cross sections for hydrocarbons.

Energy [eV]	Cross section [10^{-16} cm^2]					
	CH ₄	C ₂ H ₂	C ₂ H ₄	C ₂ H ₆	C ₃ H ₈	C ₆ H ₆
0.1	4.20	9.41 (b1)			(e1)	
0.12	3.45	9.20				
0.15	2.72	9.50				
0.17	2.46	9.90				
0.2	2.13	10.6				
0.25	1.77	11.7				
0.3	1.55	12.7				
0.35	1.42	13.4				
0.4	1.39	14.0				
0.45	1.40	14.5				
0.5	1.41	15.0				
0.6	1.51	15.7		3.18 (d1)		32.7
0.7	1.64	16.2		4.19		32.5
0.8	1.81	16.7		5.10	15.3	32.3
0.9	2.01	17.3		5.92	15.6	32.3
1	2.23	17.8	14.6	6.86	15.9	32.5
1.2	2.76	19.2	17.2	8.03	16.4	33.1 (f1)
1.5	3.73	22.4	22.0	9.50	17.2	33.2
1.7	4.42	25.4	23.7	10.3	17.7	32.8
2	5.64	30.4	24.2	11.6	18.5	34.0
2.5	7.43	35.4 (b2)	20.8	13.8	20.0	35.7
3	9.60	34.9	19.0	16.0	22.0	37.5
3.5	12.0	31.9	18.7	18.2	24.6	40.7
4	14.5	29.2	19.7	20.0	28.1	44.6
4.5	16.9	27.2	21.4	22.2	31.4	48.1 (f2)
5	19.3	25.1	22.7	24.6	33.9	50.5
6	23.4	24.1	25.3	29.4	38.3	52.2
7	25.6	24.8	27.2	32.5	42.3	55.6
8	26.2 (a1)	24.7	28.0	33.4	44.9	57.7
9	26.1	23.7	28.3	33.0	45.4	57.9
10	25.7	23.0	28.3 (c1)	31.9 (d2)	43.3 (e2)	56.8
12	24.3	22.2	27.9	29.6	40.6	54.1
15	22.3	20.6	26.5	28.9	38.9	50.3
17	21.2	19.6	25.6	28.4	38.4	48.2
20	19.6	18.4	24.4	27.4	37.5	45.9
25	17.6	16.8	22.5	25.5	35.8	43.3
30	16.2	15.9	21.1	23.9	34.0	41.7
35	15.1	15.2	20.0	22.7	32.4	40.5
40	14.2	14.7	19.1	21.8	31.1	39.5
45	13.5	14.2	18.4	20.9	29.9	38.6
50	12.8	13.7	17.7	20.2	28.9	37.7 (f3)
60	11.8	13.0	16.6	18.9	27.0	35.9
70	11.0	12.4	15.7	17.8	25.4	34.1
80	10.3	11.8	14.9	16.9	24.1	31.8
90	9.75	11.3	14.2	16.1	22.9	30.2

Table 6.1.6 (continued)

Energy [eV]	Cross section [10^{-16} cm^2]					
	CH ₄	C ₂ H ₂	C ₂ H ₄	C ₂ H ₆	C ₃ H ₈	C ₆ H ₆
100	9.24	10.9	13.6	15.3	21.8	29.0
120	8.38	10.1	12.5	14.1	19.9	26.9
150	7.37	9.15	11.2	12.5	17.7	24.3
170	6.83	8.62	10.5	11.7	16.4	22.9
200	6.16	7.93	9.62	10.6	14.9	21.0
250	5.30	7.00	8.43	9.25	12.9	18.5
300	4.66	6.28	7.51	8.24	11.4	16.4
350	4.10	5.73	6.78	7.41	10.2	14.8
400	3.71	5.30	6.18	6.73	9.19	13.5
450	3.38	4.94	5.67	6.15	8.38	12.4
500	3.11	4.60	5.25	5.65	7.71	11.4
600	2.74	4.01				9.94
700	2.42	3.56				8.79
800	2.17	3.19				7.88
900	1.97	2.90				7.13
1000	1.81	2.65				6.52

Notes

The following sets of data (the energy ranges are given in brackets) have been used to obtain the recommended TCS.

- CH₄** [85Fer2] (0.09-12); [86Loh1] (0.1-20); [88Dab1] (1.4-500); [85Jon2] (1.3-50), corrected linearly from 0 % at 4 eV to +7 % at 50 eV; [91Zec1] (1.2-100) Gdańsk data; [91Zec1] (77-1000) Trento data; [90Nis1] (5-500); [92Kan2] (5-300); [98Gar1] (400-1000). See Fig. 6.1.6.
- C₂H₂** [87Dre1] (0.1-4.8) normalized to [89Sue1] at 2.5 eV, [89Sue1] (1-400), energy scale corrected linearly by +10 % at 1 eV down to 0 % at 20 eV, TCS corrected by 0 % at 5 eV up to +14 % at 400 eV; [95Xin1] (400-1000). See Fig. 6.1.7.
- C₂H₄** [86Sue1] (1-400); [91Nis1] (4-500), [85Flo1] (5-400). See Fig. 6.1.7.
- C₂H₆** [95Szm1] (0.6-250); [86Sue1] (1-400); [91Nis1] (4-500), [85Flo1] (5-400). See Fig. 6.1.7.
- C₃H₈** [99Tan1] (0.8-500); [91Nis1] (4-500). See Fig. 6.1.7.
- C₆H₆** [96Moz2] (0.6-250) Gdańsk data; [96Moz2] (90-3500) Trento data. See Fig. 6.1.7.

- (a1) The agreement between all used sets of data is very good. At the TCS maximum, five sets of TCS [85Jon2, 90Nis1, 91Zec1, 92Kan2, 00Kim1] agree within 4 %.
- (b1) [87Dre2] reported a "total" transmission spectrum between 0.07 - 4.8 eV in arbitrary units. These data normalized to TCS in [89Sue1] at 2.5 eV agree very well in shape with [89Sue1] in the whole energy range of overlap.
- (b2) Early data [29Bru1], not included in the averaged values, are above 2 eV slightly (about 10 %) higher than those in [89Sue1]. TCS maximum in [29Bru1] amounts to about $40 \cdot 10^{-16} \text{ cm}^2$.
- (c1) The agreement between existing data is rather bad above 5 eV. At 10 eV, measurements performed with a guiding magnetic field [86Sue1, 85Flo1] are 15 % lower than the data obtained in [91Nis1].
- (d1) Present recommended values below 2 eV are based on TCS in [95Szm1] and [86Sue1], in good mutual agreement. A quick fall of TCS below 2 eV with a Ramsauer-Townsend minimum at about 0.15 eV [98Lun1] is indicated also by relative TCS measurements from Daresbury and Orsay labs [94Lun1, 98Lun1]. However, TCS measurements [95Szm1, 86Sue1] below 2 eV are not compatible with the elastic cross sections in [98Mer1].

-
- (d2) The agreement between different data [86Sue1, 91Nis1, 95Szm1] is very good up to 6 eV. At higher energies the agreement is poor: at 10 eV the data in [85Flo1] are 25 % lower than those in [91Nis1].
 - (e1) "Backward scattering" from Orsay lab indicates a Ramsauer-Townsend minimum at about 0.1 eV [98Lun1].
 - (e2) The TCS from Tokyo lab corrected [99Tan1] for the angular resolution error are slightly (7 % at 10 eV) higher than TCS in [91Nis1]. TCS in [85Flo1], much lower than the two other sets of data [99Tan1, 91Nis1], have not been included in the averaged values.
 - (f1) A $^2E_{2u}$ resonant state is present in the 1.2 - 1.6 eV energy region [75Won1]. In TCS measurements with a moderate energy-resolution [88Sue1, 96Moz2, 00Kim1] only an enhancement of TCS was observed (reproduced in the present table). A resonant structure, seen in TCS measurements [98Gul1] performed with a high energy resolution (3.5 meV) is reported in Table 6.1.12.
 - (f2) The shoulder in TCS at about 4.8 eV is attributed to a short-lived $^2B_{2g}$ resonant state, seen also in the vibrational excitation channel [75Azr1, 89All1] and in electron-transmission spectra [73San1].
 - (f3) The recommended data for C_6H_6 are based on two sets (Gdańsk and Trento labs) of TCS from [96Moz2], in good agreement in the energy overlap region. The more recent set of TCS from Tokyo lab [00Kim1] agrees within the error bar with results in [96Moz2] up to 10 eV but is 15 % lower at 50 eV. These data [00Kim1] are higher than previous results from the Tokyo lab [88Sue1] by 20 % at 10 eV and 6 % at 50 eV.

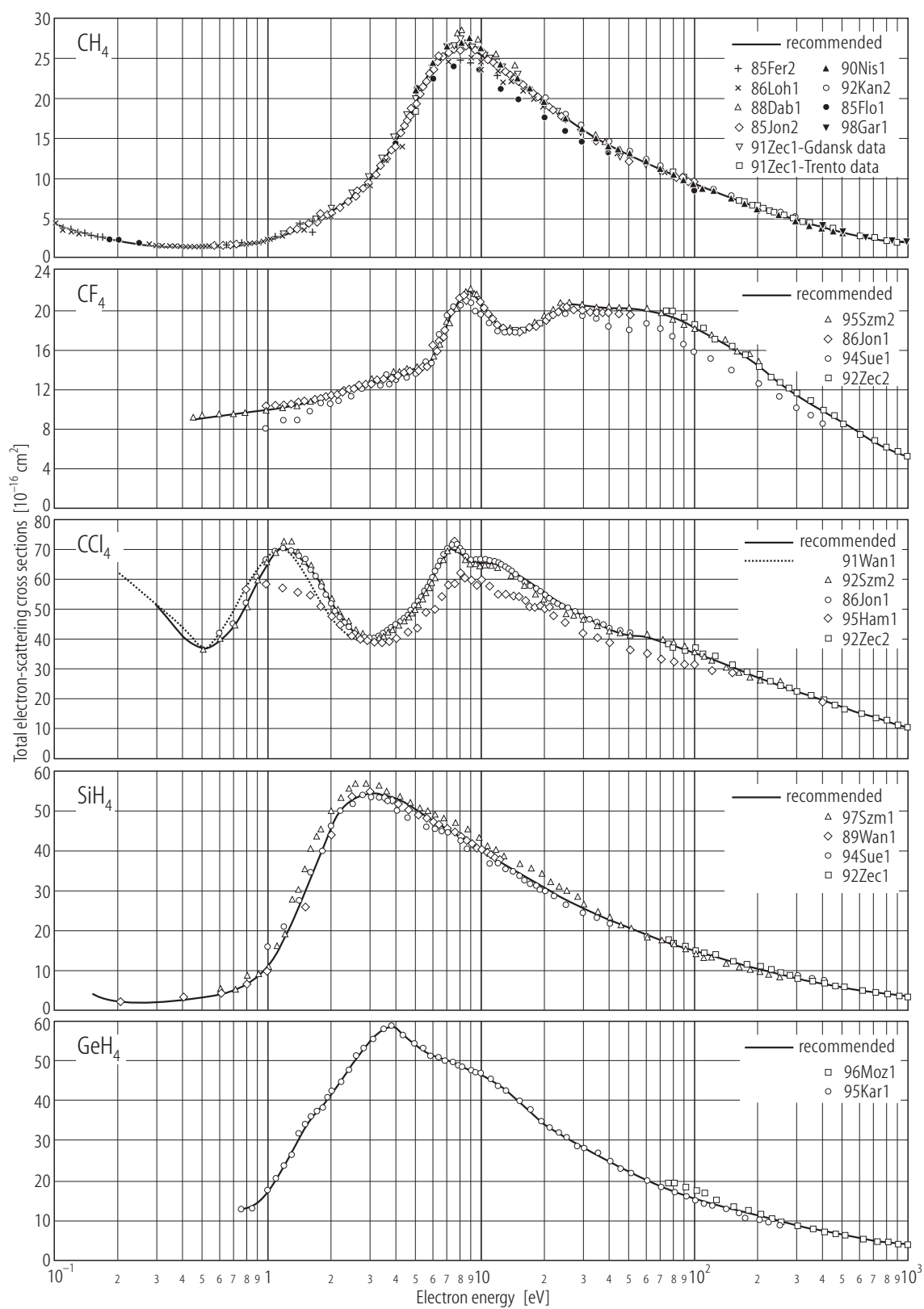


Fig. 6.1.6. Overview of experimental and recommended total cross sections for CH₄, CF₄, CCl₄, SiH₄, GeH₄.

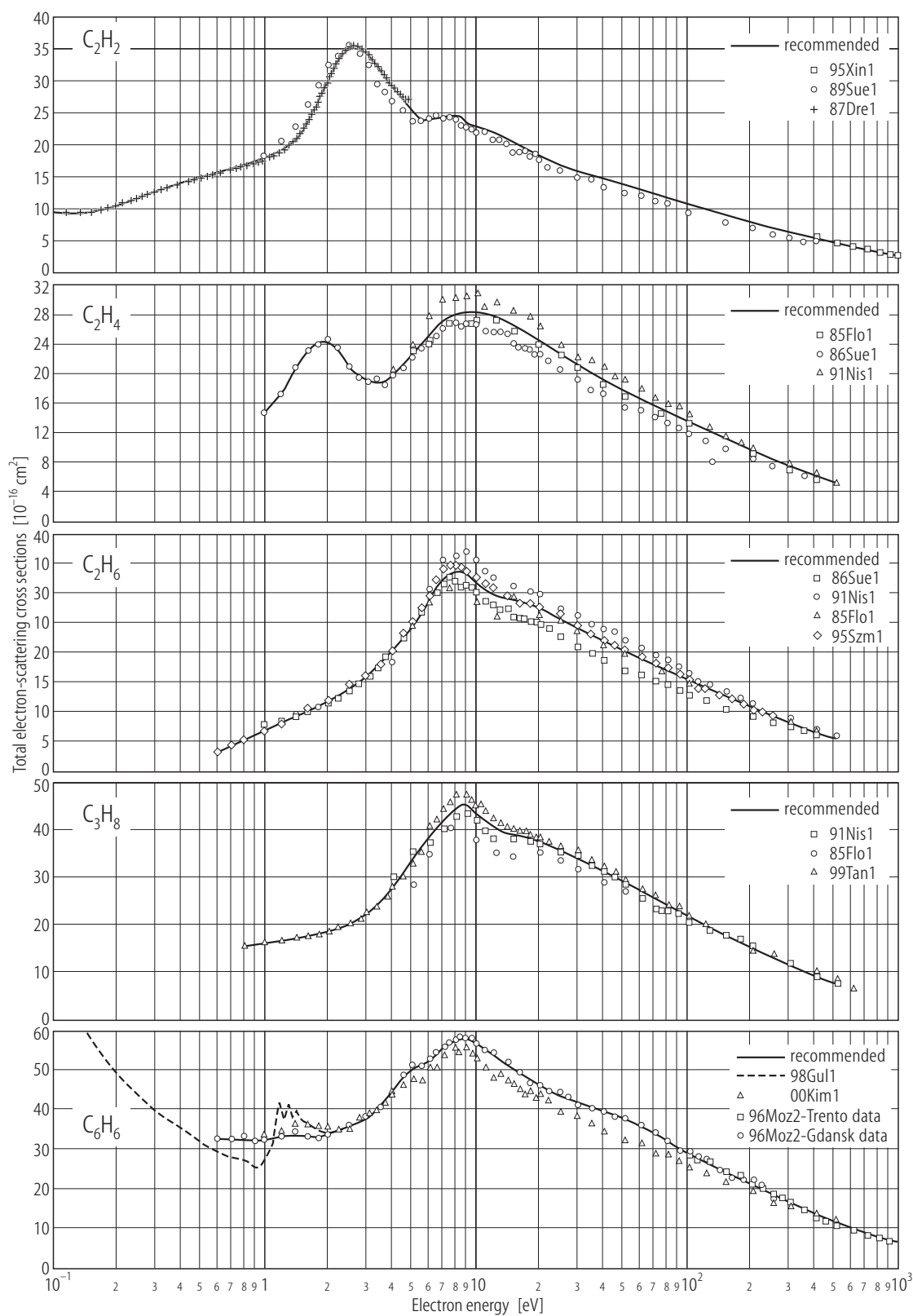


Fig. 6.1.7. Overview of experimental and recommended total cross sections for C_2H_2 , C_2H_4 , C_2H_6 , C_3H_8 , C_6H_6 .

6.1.6 Halomethanes

Table 6.1.7. Recommended total cross sections for some halomethanes.

Energy [eV]	Cross section [10^{-16} cm^2]					
	CHF ₃ (a1)	CF ₄	CF ₃ Cl	CF ₂ Cl ₂	CFCl ₃	CCl ₄
0.10	(a2)	(b1)	(c1)	(d1)	96.7 (e1)	(f1)
0.12					88.4	
0.15					78.9	
0.17					74.4	
0.20				73.3	69.4	
0.25			41.9	60.7	64.0	
0.30			31.7	53.0	60.5	51.7
0.35			25.7	47.2	57.4	45.7
0.40			22.1	42.4	55.2	41.2
0.45		8.97	19.8	38.6	53.2	38.3
0.5		9.15	18.4	35.6	51.3	36.5
0.6		9.35	17.3	32.2	47.3	39.5
0.7		9.47	17.2	32.9	43.6	44.0
0.8	32.1	9.59	17.3	36.6	40.2	51.4
0.9	30.9	9.73	17.6	40.0	36.8	58.9
1.0	30.2	9.87	18.2	41.4 (d2)	34.8	65.0 (f2)
1.2	29.5	10.2	20.3	38.3	39.6	71.0 (f3)
1.5	29.1	10.6	25.5	30.3	51.2	66.5
1.7	28.6	10.9	29.2	29.4	53.9 (e2)	60.6
2.0	27.4	11.3	31.8 (c2)	32.4	52.5	52.0
2.5	25.8	12.0	27.2	38.5 (d2)	46.1	42.5
3.0	24.8	12.6	23.6	38.0	42.4	39.6
3.5	24.2	13.1	23.2	38.2	44.1	41.4
4.0	24.0	13.5	24.9	39.9 (d2)	44.9 (e2)	44.1
4.5	24.1	13.8	27.8	40.6	44.7	47.7
5.0	24.5	14.0	31.3	41.7	45.2	51.9
6.0	26.1 (a3)	15.2	33.7 (c2)	43.6	49.8	61.3
7.0	26.7	18.6	33.1	44.3	56.4	69.8 (f3)
8.0	26.7	21.2	33.8	46.6	59.9	69.1
9.0	26.3	21.9 (b2)	34.6	49.0	60.4	65.7
10	25.4	21.0	35.0	50.8	60.5	65.2
12	23.2	18.6	36.1	50.6	59.7	64.2
15	22.8	18.0	33.9	46.0	54.5	59.9
17	22.7	18.3	32.2	43.8	51.8	56.9
20	23.3	19.3	30.8	41.4	48.9	53.5
25	23.3	20.6	30.0	39.2	45.6	49.4
30	22.8	20.4 (b3)	28.6	37.3	43.4	46.6
35	22.2	20.3	28.0	36.1	41.7	44.6
40	21.6	20.3	27.4	35.1	40.3	43.2
45	21.0	20.3	26.9	34.2	39.1	42.2
50	20.5	20.2	26.3	33.4	38.1	41.5
60	19.6	20.0	25.4	32.0	36.3	40.8
70	18.4	19.7	24.5	30.7	34.8	39.4
80	17.4	19.4	23.7	29.5	33.6	37.8
90	16.4	18.8	23.0	28.4	32.4	36.5

Table 6.1.7 (continued)

Energy [eV]	Cross section [10^{-16} cm^2]					
	CHF ₃ (a1)	CF ₄	CF ₃ Cl	CF ₂ Cl ₂	CFCl ₃	CCl ₄
100	15.6	18.3	22.3	27.4	31.4	35.4
120	14.3	17.3	21.0	25.7	29.6	33.3
150	12.7	16.3	19.3	23.4	27.3	30.5
170	11.9	15.6	18.4	22.1	26.0	29.0
200	10.8	14.4	17.1	20.5	24.2	27.1
250	9.48	12.8	15.1	18.4	21.5	24.6
300	8.49	11.6	13.6	16.7	19.6	22.4
350	7.72	10.7	12.5	15.3	18.0	20.6
400	7.12	9.87	11.5	14.1	16.7	19.1
450	6.64	9.18	10.7	13.2	15.6	17.9
500	6.26	8.59	10.1	12.3	14.6	16.7
600	5.70	7.60	8.98	10.9	13.0	14.9
700		6.83	8.13	9.80	11.7	13.4
800		6.19	7.43	8.91	10.7	12.2
900		5.67	6.86	8.16	9.83	11.3
1000		5.22	6.36	7.53	9.09	10.4

Notes

The following sets of data (the energy ranges are given in brackets) have been used to obtain the recommended TCS.

CHF₃ [98Sue1] (0.8-600).

CF₄ [92Szm2] (0.45-200); [86Jon1] (1-50) corrected linearly from 0 % at 4 eV to 5 % at 50 eV, according to the angular resolution error; [92Zec2] (75-1000). See Fig. 6.1.6 (p. 6-27).

CF₃Cl [94Und1] (0.2-1.8); [86Jon1] (0.6-50) corrected linearly from 0 % at 4 eV to +7 % at 50 eV, according to the angular resolution error given in [86Jon1]; [92Zec2] (75-1000). See Fig. 6.1.8.

CF₂Cl₂ [94Und1] (0.2-2); [86Jon1] (0.6-50) corrected linearly from 0 % at 4 eV to +7 % at 50 eV, according to the angular resolution error given in [86Jon1]; [92Zec2] (75-1000). See Fig. 6.1.8.

CFCl₃ [93Ran1] (0.1-0.9) backward scattering, normalized to [86Jon1] at 0.9 eV; [86Jon1] (0.6-50) corrected linearly from 0 % at 4 eV to +7 % at 50 eV, according to the angular resolution error given in [86Jon1]; [92Zec2] (75-1000). See Fig. 6.1.8.

CCl₄ [86Jon1] (0.6-50), corrected linearly from 0 % at 4 eV to +7 % at 50 eV, according to the angular resolution error given in [86Jon1]; [92Szm2] (0.5-200); [91Wan1] (0.2-9); [92Zec2] (75-1000). See Fig. 6.1.6 (p. 6-27).

(a1) The recommended TCS are based on the recent data from the Tokyo lab [98Sue1]. Note that the recent TCS from this lab in CH₄ and CF₄, cited together with CHF₃ [98Sue1] are in a very good agreement with recommended values.

(a2) Low energy measurements indicate a rise TCS in the limit of zero energy: from about $20 \cdot 10^{-16} \text{ cm}^2$ at 1 eV to $45 \cdot 10^{-16} \text{ cm}^2$ at about 0.1 eV [98San1].

(a3) Measurements from Maryland lab [98San1] at 0.1 - 20 eV are generally lower in the energy overlap region than the TCS in [98Sue1] and at the 6.5 eV maximum amount to about $17.5 \cdot 10^{-16} \text{ cm}^2$.

(b1) The "backward-scattering" measurements from the Orsay lab [84Fie1, 98Lun1] indicate a fall of TCS below 0.2 eV and a Ramsauer minimum at about 0.15 eV. Normalizing the data from [84Fie1] at 0.4 eV to the TCS in [92Szm2] one gets a good agreement of this fall with the Born approximation for the vibrational excitation (see eq. 13).

- (b2) The peak in TCS at 8.87 eV [86Jon1] is due to resonant scattering, seen as a dip structure in elastic cross section [92Boe1, 92Man1], as an enhancement in the vibrational [92Boe1, 92Man2] and in the dissociative attachment cross sections [92Iga1].
- (b3) The recent measurements from Tokyo lab [94Sue1] are very close to the recommended data, being at 30 eV only 5 % lower.
- (c1) The measurements from the Maryland lab [94Und1], lower by 25 % on the average than those in [86Jon1], indicate a rise of TCS in the low energy limit. These data [94Und1] normalized at 1 eV by a factor of 1.25 to the TCS from [86Jon1] yield a value of about $42 \cdot 10^{-16} \text{ cm}^2$ at 0.25 eV.
- (c2) The TCS maxima at 2.0 and 5.94 eV [86Jon1] are due to the presence of resonances, which have been observed at about the same energies in the vibrational excitation [92Man3] and electron attachment [89Ost1, 95Und1] channels.
- (d1) TCS from the Maryland lab [94Und1] show a rise below 0.5 eV, see Fig. 6.1.8. These data normalized at 1 eV by a factor of 1.33 to the TCS in [86Jon1] reach about $73 \cdot 10^{-16} \text{ cm}^2$ at 0.2 eV. We note also that a peak at 0.2 eV was observed in the dissociative attachment cross section [95Und1].
- (d2) Two peaks and a shoulder at 1.02, 2.64 and 4.0 eV were reported in [86Jon1]. Resonances were observed at about the same energies in the vibrational excitation [92Man4] and dissociative attachment cross sections [79Pej1, 89Ost1, 95Und1].
- (e1) The "backward scattering" measurements [93Ran1] indicate a rise of TCS below 1 eV. This rise is due to electron attachment [80McC1, 87Dun1]. In Fig. 6.1.8 relative data from [93Ran1] have been normalized to TCS from [86Jon1] at 0.8 eV.
- (e2) Maxima in TCS were observed at 1.76 and 4.0 eV in [86Jon1]. Peaks in electron attachment cross sections were observed at slightly lower energies, 1.6 and 3.3 eV [89Ost1].
- (f1) The measurements from the Maryland lab [91Wan1] indicate a rise of TCS in the limit of zero-energy, up to approximately $120 \cdot 10^{-16} \text{ cm}^2$ at 0.1 eV (data digitized from Fig. 3. in [91Wan1]). This rise is due to electron attachment [85Chu1, 92Lin1, 95Mat1].
- (f2) Different sets of TCS in CCl_4 [86Jon1, 91Wan1, 92Szm2, 95Ham1] are in good agreement. TCS in [95Ham1] are somewhat lower at the low-energy maximum at 1 eV, probably due to a poorer energy resolution.
- (f3) The TCS maxima at 1.22 and 7.51 eV [86Jon1] are due to resonant scattering. These maxima were also seen in dissociative attachment [91Wan1, 90Chu1, 89Ost1].

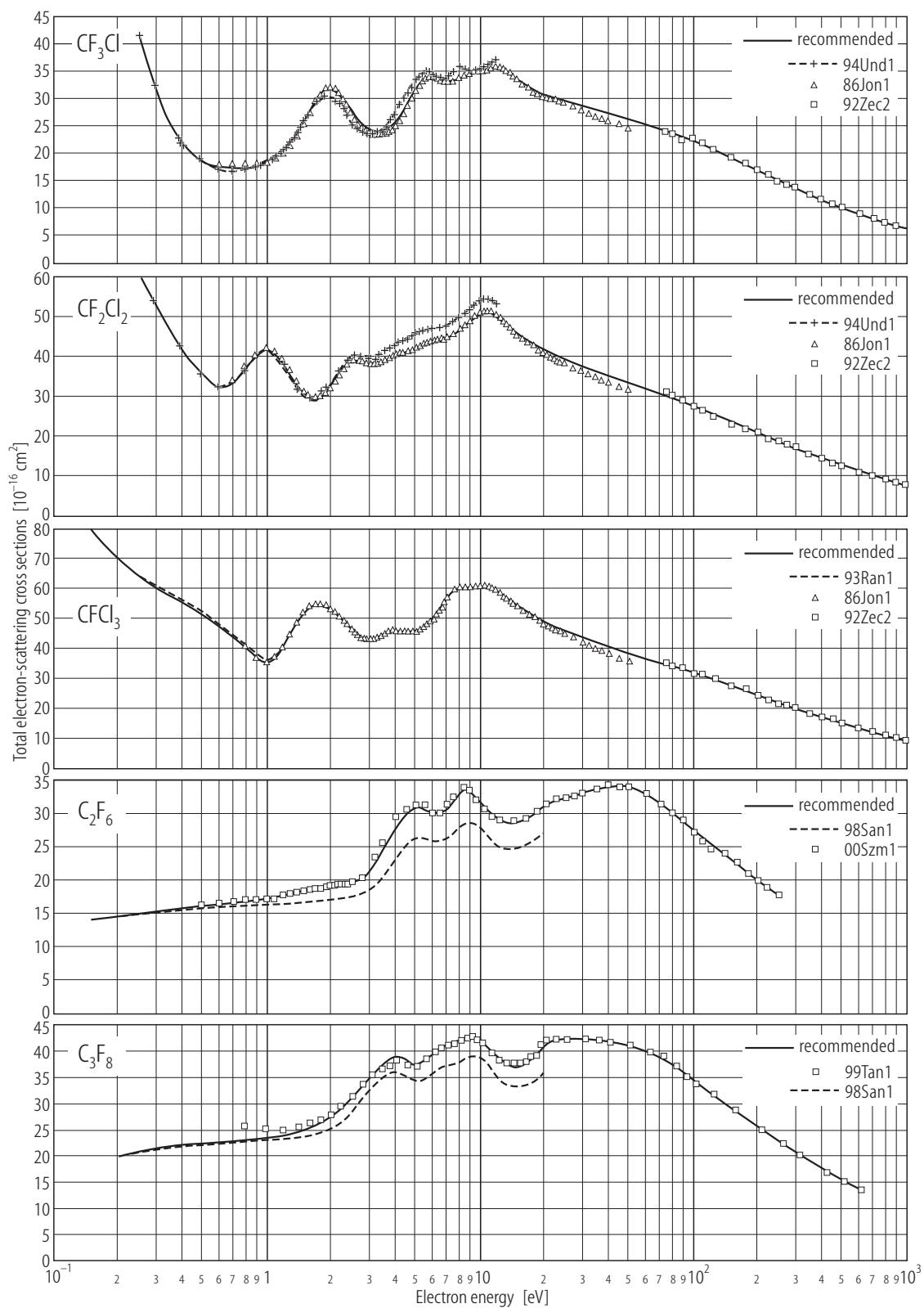


Fig. 6.1.8. Overview of experimental and recommended total cross sections for CF₃Cl, CF₂Cl₂, CFCF₃, C₂F₆, C₃F₈.

6.1.7 Methyl compounds

Table 6.1.8. Recommended total cross sections for some methyl compounds.

Energy [eV]	Cross section [10^{-16} cm ²]				
	CH ₃ OH	CH ₃ F	CH ₃ Cl	CH ₃ Br	CH ₃ I
0.25			58.4 (c1)		
0.30			54.4		
0.35		38.8 (b1)	51.0		
0.40		37.5	48.1	62.4 (d1)	
0.45		36.3	45.6	60.3	95.6 (e1)
0.5		35.1	43.5	58.4	90.6
0.6		32.8	40.2	55.4	82.9
0.7		30.8	37.7	52.9	76.9
0.8	28.2	29.0	35.9	51.0	72.0
0.9	26.8	27.4	34.6	49.4	67.8
1.0	25.6	25.9	33.6	48.1	64.2
1.2	23.6	23.6	32.4	46.1	58.4
1.5	21.6	21.1	31.7	45.2	52.6
1.7	20.7	19.9	31.6	44.5	50.7
2.0	19.9	19.2	31.9	42.9 (d2)	49.9
2.5	19.5	19.2	32.6	39.8	49.8
3.0	19.7	19.8	33.5	39.0	49.8
3.5	20.5	20.6	34.2	38.8	50.4
4.0	21.4 (a1)	21.4	34.7	38.9	52.0
4.5	22.5	22.3	34.6	39.1	53.7
5	23.6	23.2	34.6	39.4	55.0
6	25.4	24.1	35.0	40.0	57.2
7	26.3 (a2)	24.4	35.5	40.3	58.0
8	26.6	24.1	35.5	40.1	56.0
9	26.5	23.5	34.3	39.4	54.4
10	26.1	22.8	33.1	38.2	53.4
12	24.8	21.8	31.7	36.1	52.1
15	23.4	20.2	30.3	33.6	50.7
17	22.7	19.4	29.4	32.6	49.2
20	21.6	18.6	28.0	31.4	46.2
25	20.0	17.5	25.9	29.6	42.5
30	18.5	16.8	24.4	28.4	39.8
35	17.4	16.2	23.5	27.3	37.6
40	16.6	15.7	22.6	26.3	35.9
45	16.2	15.3	21.9	25.3	34.4
50	15.7	14.9	21.2	24.4	33.0
60	14.9	14.1	20.1	22.7	30.8
70	14.2	13.5	19.1	21.3	29.0
80	13.5	12.9	18.2	20.1	27.4
90	12.9	12.4	17.4	19.0	26.0
100	12.4	11.9	16.6 (c2)	18.0	24.8
120	11.5	11.0	15.4	16.4	22.6
150	10.3	9.79	13.8	14.4	19.7
170	9.70	9.07	12.9	13.4	18.1
200	8.83	8.10	11.8	11.9	15.8

Table 6.1.8 (continued)

Energy [eV]	Cross section [10^{-16} cm ²]				
	CH ₃ OH	CH ₃ F	CH ₃ Cl	CH ₃ Br	CH ₃ I
250	7.55	6.70	10.4	9.91	
300			9.22		
350			8.30		
400			7.55		
450			6.93		
500			6.40		
600			5.55		
700			4.90		
800			4.39		
900			3.98		
1000			3.63		

Notes

The following sets of data (the energy ranges are given in brackets) have been used to obtain the recommended TCS.

CH₃OH [95Szm1] (0.8-250). See Fig. 6.1.5 (p. 6-23)

CH₃F [95Krz1] (0.35-250).

CH₃Cl [95Krz1] (0.25-250); [99Kar1] (75-1000).

CH₃Br [94Krz1] (0.4-250).

CH₃I [93Szm1] (0.45-220).

- (a1) TCS in [85Sue1] agree well with those in [95Szm1] up to 4 eV, are lower by 10 - 15 % at 7 - 150 eV and merge again in the 250 eV limit.
- (a2) The more recent TCS from the Tokyo lab [00Kim1] are higher than the previous data [85Sue1] and amount to $31 \cdot 10^{-16}$ cm² at 7 eV. The recent data [00Kim1] report also a narrow maximum at 2 eV.
- (b1) TCS in [95Krz1] agree well in shape with TCS in [88Ben1] at 0.35 - 7 eV but are up to 20 % higher.
- (c1) TCS from Maryland lab [88Ben1, 91Wan1] agree well in shape with those from Gdańsk lab [95Krz1] in the whole energy overlap region up to 12 eV but are 30 % lower on the average.
- (c2) TCS from Gdańsk lab [95Krz1] and Trento lab [99Kar1] merge poorly in the 75 - 250 eV region with differences up to 15 %. A fit with formula (eq. 11) on both sets of data together was used to get recommended values.
- (d1) TCS in [94Krz1] agree well in shape with TCS measurements from the Maryland lab [88Ben1] in the whole energy region of overlap (0.4 - 7 eV). Absolute values in these two sets of data differ by less than 10 %.
- (d2) A shoulder structure at about 2 eV [94Krz1] was seen as a weak maximum in TCS measurements presented in [88Ben1]. A weak resonant state was predicted theoretically at this energy [92Mod1].
- (e1) TCS measurements from the Maryland lab [88Ben1] are higher than in [93Szm1] by 10 - 15 % in the whole energy region of overlap (0.45 - 7 eV) but agree well in shape.

6.1.8 Fluorides

Table 6.1.9. Recommended total cross sections for some fluorides.

Energy [eV]	Cross section [10^{-16} cm^2]				
	C_2F_6	C_3F_8	C_6F_6	SF_6	WF_6
0.10				156 (d1)	
0.12				131	
0.15	14.1 (a1)			106	
0.17	14.2			94.6	
0.20	14.5	19.7 (b1)	(c1)	81.4	
0.25	14.9	20.7		66.4	
0.30	15.2	21.2		56.5	
0.35	15.5	21.6		49.5	
0.40	15.7	21.9		44.3	
0.45	15.9	22.1		40.3	
0.5	16.1	22.2		37.1	
0.6	16.3	22.5	31.6	32.7	
0.7	16.5	22.7	32.8	29.7	
0.8	16.7	22.9	33.2	27.0	
0.9	16.9	23.1	33.2	24.9	
1.0	17.1	23.3	33.1 (c2)	23.5	
1.2	17.4	23.7	32.6	22.4	21.7
1.5	17.9	25.0	31.8	21.9	22.1
1.7	18.2	25.8	31.4	22.1	22.3
2.0	18.7	27.2 (b2)	30.8	22.6	23.3
2.5	19.5	30.8	29.9	23.3 (d2)	29.4
3.0	21.1	34.8	29.1	23.1	30.8 (e1)
3.5	24.7	37.7	29.0	22.8	27.9
4.0	27.9	38.8	29.8	22.4	26.1
4.5	29.9 (a2)	38.0	31.0	22.5	24.5
5.0	30.7	37.4	32.5	23.5	23.4
6.0	29.9	39.6	36.0	27.9	22.7
7.0	30.7	41.1	39.9	31.3 (d2)	23.1
8.0	33.0 (a2)	41.7	44.1	28.9	23.5
9.0	33.1	42.9	48.4 (c3)	27.0	24.4
10	31.6 (a3)	42.2	47.7	27.1	26.7 (e1)
12	29.2	38.8	53.4	33.3 (d2)	28.1
15	28.6	36.9	56.2 (c3)	26.3	30.6
17	29.5	37.9	56.3	26.2	34.7
20	31.1	41.1	57.7	27.3	36.5
25	32.4	42.4	59.7	29.1	36.6
30	33.1	42.4	60.5	29.3	37.1
35	33.6	42.2	60.4	29.3	37.9
40	34.0	42.0	59.5	29.3	37.8
45	34.2	41.6	58.2	29.4	37.5
50	34.1	41.2	56.7	29.3	37.0
60	33.0	40.2	53.7	28.8	36.1
70	31.5	38.9	51.2	28.0	35.2
80	30.0	37.5	49.0	27.3	34.4
90	28.6	35.8	47.0	26.4	33.5

Table 6.1.9 (continued)

Energy [eV]	Cross section [10^{-16} cm^2]				
	C_2F_6	C_3F_8	C_6F_6	SF_6	WF_6
100	27.3	34.1	45.2	25.6	32.6
120	25.2	31.9	42.1	24.3	30.9
150	22.9	29.2	38.3	22.5	28.9 (e2)
170	21.7	27.6	36.1	21.5	27.8
200	20.1	25.6	33.3	20.1	26.3
250	17.7	22.8	29.5	18.1	24.2
300		20.6		16.4	22.4
350		18.8		15.2	20.9
400		17.3		14.2	19.6
450		16.1		13.3	18.3
500		15.1		12.6	16.8
600		13.5		11.5	14.8
700				10.4	13.3
800				9.47	12.2
900				8.69	11.3
1000				8.04	10.6

Notes

The following sets of data (the energy ranges are given in brackets) have been used to obtain the recommended TCS.

- C₂F₆** [00Szm1] (0.5-250); [98San1] (0.15-20) corrected linearly from 0 % at 0.15 up to +15 % at 3.4 eV and then by 15 % at 3.4 - 20 eV. See Fig. 6.1.8 (p. 6-32).
- C₃F₈** [99Tan1] (1.4-600); [98San1] (0.2-20), corrected linearly from 0 % at 0.2 eV to +10 % at 20 eV. See Fig. 6.1.8 (p. 6-32).
- C₆F₆** [97Kas1] (0.6-250).
- SF₆** [82Fer1] (0.1-1); [97Kas1] (0.6-250); [88Dab1] (2.8-500); [79Ken1] (0.5-95), corrected linearly from 0 % at 1 eV up to +10 % at 100 eV (angular resolution error); [92Zec3] (75-1000). See Fig. 6.1.9.
- WF₆** [00Szm1] (1.2-250), [00Kar1] (150-3500). See Fig. 6.1.9.

- (a1) The "backward scattering" measurement from Orsay lab indicates a quick fall of the cross section below 0.15 eV, with a Ramsauer-Townsend minimum at 0.08 eV [98Lun1].
- (a2) The C₂F₆ TCS [00Szm1, 97Sue1, 98San1] shows two maxima: of about $31 \cdot 10^{-16} \text{ cm}^2$ at 5 eV and $34 \cdot 10^{-16} \text{ cm}^2$ at 8 eV [00Szm1]. The vibrational excitation [94Tak1] shows resonances at 4.3 and 8.5 eV. The data in [98San1] are probably underestimated, see note (b1).
- (a3) The TCS from the Tokyo lab [97Sue1] show the same shape as our recommended values, but are somewhat (15 % at 10 eV) lower.
- (b1) The data in [98San1] obtained with a trochoidal spectrometer are possibly underestimated due to the uncertainty in determining the effective length of the scattering cell. We have corrected data in [98San1] by a factor linearly rising from 0 % at 0.2 eV to 10 % at 20 eV. Below 1.5 eV our recommended values follow the data of [98San1] which extend down to 0.2 eV. Low energy data in [99Tan1] amount to: 25.4 at 0.8 eV, 25.0 at 1 eV, 24.7 at 1.2 eV, $25.2 \cdot 10^{-16} \text{ cm}^2$ at 1.4 eV.
- (b2) The large discrepancy between the two sets of data suggest a large error bar on the recommended values. The data in [98San1] agree in shape with those in [99Tan1] but are systematically lower; we have corrected them by a factor linearly rising with energy from 0 % at 0.2 eV to 10 % at 20 eV.

- (c1) The "backward scattering" measurement from Orsay lab indicates a slowly diminishing cross section down to 0.2 eV then a quick fall, with a Ramsauer-Townsend minimum at 0.08 eV [98Lun1].
- (c2) An enhancement of electron attachment was observed around 1 eV [94Shi1].
- (c3) Two weak structures can be discerned in the TCS at 9.5 and 14 eV [97Kas1]. Peaks in dissociative attachment have been seen at 4.5 and 8 - 12 eV [89Fen1].
- (d1) The rise of TCS below 1 eV is caused both by vibrational excitation [79Roh1, 92Ran1] and electron attachment [85Chu1, 92Lin1, 92Shi1].
- (d2) TCS in SF₆ below 20 eV shows three maxima: a weak one of 23.3 at 2.5 eV and two distinct of 31.3 and $33.5 \cdot 10^{-16} \text{ cm}^2$ at 7.1 and 11.9 eV, respectively. Electron transmission spectra [79Ken1] evidenced resonant states at 2.52, 7.05, 11.87 eV; their symmetries were discussed in [78Deh1].
- (e1) TCS in WF₆ [00Szm1] shows a maximum of $31.4 \cdot 10^{-16} \text{ cm}^2$ at 3.0 eV and a shoulder structure at 8 - 10 eV on the slope of the low-energy edge of the very broad hump. An enhancement of the electron attachment has been seen at 2.8 eV and 10 eV [73Thy1].
- (e2) The two existing sets of TCS [00Szm1, 00Kar1] are in rather serious disagreement in the overlap region. For this reason an unique fit with formula (eq. 11), extending from 100 to 450 eV was used.

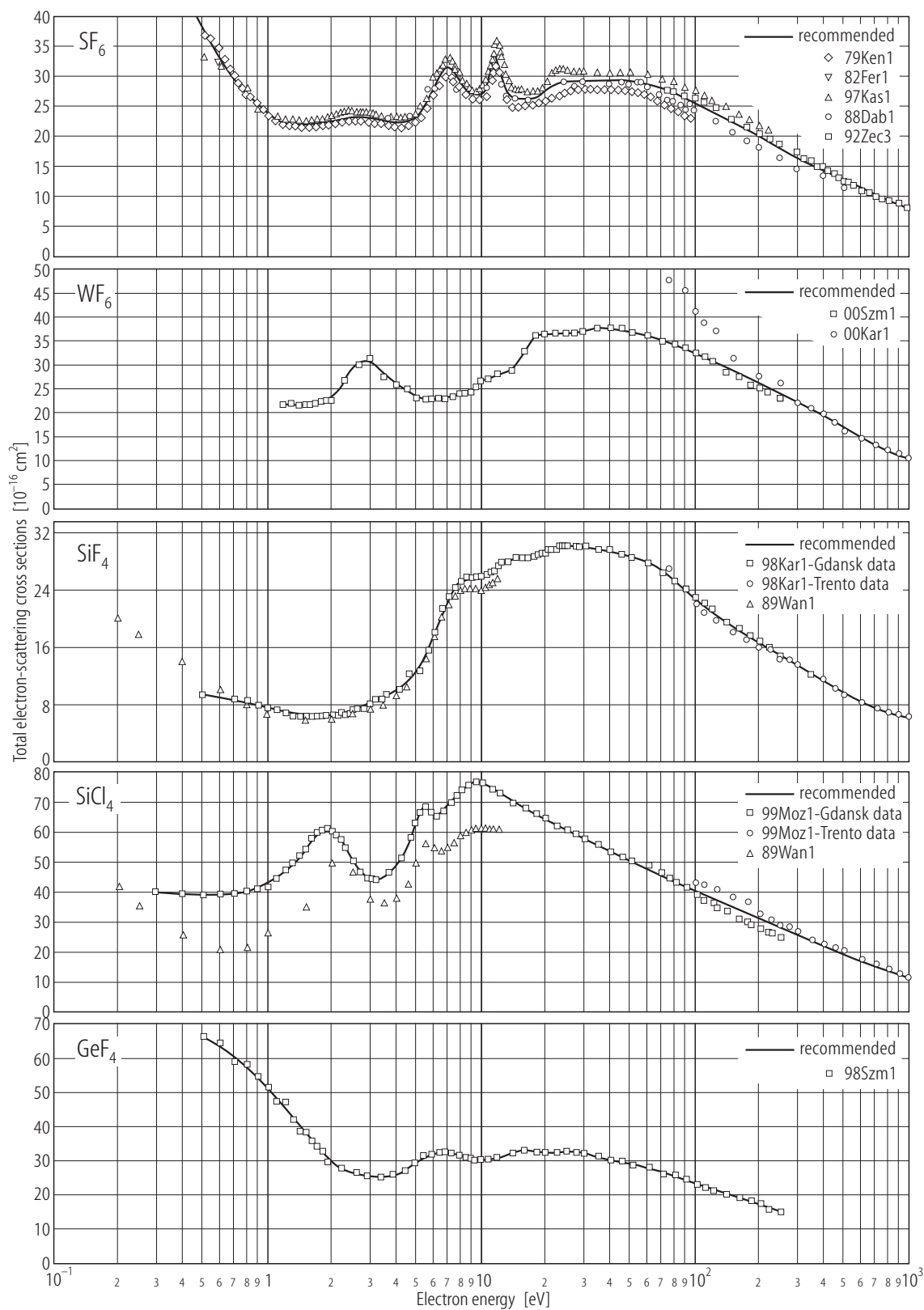


Fig. 6.1.9. Overview of experimental and recommended total cross sections for SF_6 , WF_6 , SiF_4 , SiCl_4 , GeF_4 .

6.1.9 Silicon and germanium compounds

Table 6.1.10. Recommended total cross sections for silicon and germanium compounds.

Energy [eV]	Cross section [10^{-16} cm^2]					
	SiH ₄	SiF ₄	SiCl ₄	GeH ₄	GeF ₄	GeCl ₄
0.15	3.86					
0.17	2.84					
0.20	2.00					
0.25	1.53					
0.30	1.55		39.7			
0.35	1.77		39.6			
0.40	2.08		39.3			
0.45	2.45		39.1			
0.5	2.87	9.26	38.9		66.4	
0.6	4.00	8.97	38.9		63.3	36.9
0.7	5.05	8.65	39.2		60.3	42.3
0.8	6.13	8.30	40.0	12.7	57.3	45.5
0.9	7.81	7.93	41.2	14.2	54.2	47.8
1.0	11.0	7.55 (b1)	42.7	16.7	51.1	49.8
1.2	17.9	6.81	46.8	23.6	45.3	53.2
1.5	29.3	6.23	54.8	33.7	37.7	56.3
1.7	36.4	6.22	59.9	37.4	33.7	57.0 (f1)
2.0	46.1	6.44	60.2 (c1)	41.9	29.4	57.0
2.5	53.1 (a1)	7.11	50.1	49.2	26.6	50.9
3.0	54.6 (a2)	7.99	44.3	55.0	25.4	47.5
3.5	54.1	9.04	45.0	58.0	25.2	48.3
4.0	52.9	10.1	49.2	57.9 (d1)	26.2	50.1
4.5	51.4	11.1	55.5	55.4	27.8	53.0
5.0	49.9	12.8	64.3 (c2)	53.5	30.0	57.9 (f2)
6.0	47.3	17.7	65.4	51.1	32.4 (e1)	70.6
7.0	45.2	22.7	68.5	49.6	32.4	74.2
8.0	43.5	25.2 (b2)	73.6	48.4	31.6	75.3
9.0	42.0	25.7	76.4	47.3	30.7	77.8
10	40.7	25.9	76.5	46.1	30.1	79.6
12	38.0	27.3	73.2	43.7	30.9	78.3
15	34.4	28.5	68.6	39.9	32.9	73.9
17	32.6	28.7	66.9	37.3	32.8	71.1
20	30.5	29.3	64.3	34.0	32.4	67.3
25	27.8	30.2	60.7	30.5	32.7	63.0
30	25.7	30.1	57.8	28.1	32.2	60.3
35	24.1	29.8	55.5	26.1	31.3	58.0
40	22.7	29.4	53.6	24.5	30.5	55.9
45	21.6	29.1	51.8	23.0	29.7	53.8
50	20.6	28.8	50.0	21.7	29.0	52.2
60	18.8	27.8	47.4	19.6	27.7	49.3
70	17.4	26.6	45.2	18.0	26.5	46.7
80	16.4	25.4	43.4	16.8	25.5	44.2
90	15.4	23.9	41.8	15.9	24.5	41.9
100	14.6	22.7	40.4 (c3)	15.2	23.5	39.9
120	13.6	20.7	37.9	14.1	21.9	36.5

Table 6.1.10 (continued)

Energy [eV]	Cross section [10^{-16} cm^2]					
	SiH ₄	SiF ₄	SiCl ₄	GeH ₄	GeF ₄	GeCl ₄
150	12.1	18.7	34.9	12.7	19.9	32.8
170	11.3	17.7	33.3	11.9	18.7	30.8
200	10.2	16.5	31.1	10.8	17.2	28.4
250	8.86	14.7	28.1	9.46	15.3	25.1
300	7.82	13.2	25.6	8.47		
350	7.01	12.0	23.6	7.66		
400	6.35	11.0	21.9	7.01		
450	5.91	10.2	20.4	6.48		
500	5.44	9.58	19.1	6.03		
600	4.70	8.51	16.9	5.32		
700	4.14	7.68	15.2	4.76		
800	3.70	7.01	13.8	4.32		
900	3.34	6.46	12.8	3.96		
1000	3.05	5.99	12.0	3.66		

Notes

The following sets of data (the energy is given in brackets) have been used to obtain the recommended TCS.

SiH₄ [89Wan1] (0.15-12); [97Szm1] (0.6-100); [94Sue1] (1-400); [92Zec1] (75-1000); Fig. 6.1.6 (p. 6-27).

SiF₄ [98Kar1] (0.5-250) Gdańsk data, (80-1000) Trento data. See Fig. 6.1.9 (p. 6-38).

SiCl₄ [99Moz1] (0.3-250) Gdańsk data, (100-1000) Trento data. See Fig. 6.1.9 (p. 6-38).

GeH₄ [96Moz1] (0.75-200); [95Kar1] (150-1000). See Fig. 6.1.6 (p. 6-27).

GeF₄ [98Szm1] (0.5-200). See Fig. 6.1.9 (p. 6-38).

GeCl₄ [97Szm1] (0.6-250).

- (a1) An enhancement of the dissociative attachment [69Pot1] and the vibrational excitation [90Tan1] cross sections at 2.5 eV suggest the existence of a resonance state at about this energy.
- (a2) The TCS from the Tokyo lab [94Sue1] are generally higher, at 3 eV by 15 %, than the preliminary measurements [85Mor1] from the same laboratory.
- (b1) A rise of TCS below 2 eV was also observed in the data from the Maryland lab [89Wan1], see Table 6.1.11.
- (b2) A shoulder structure in TCS at 8 eV has been also observed in [89Wan1], see Fig. 6.1.9 (p. 6-38).
- (c1) The TCS reaches a sharp maximum of about $62 \cdot 10^{-16} \text{ cm}^2$ at 1.9 eV [99Moz1]. A resonant state at 2.07 eV has been seen in electron transmission spectra [98Mod1]; an enhancement of the dissociative attachment cross section has been observed around 2 eV [74Wan1, 90Moy1].
- (c2) The TCS reaches a weak maximum of $68 \cdot 10^{-16} \text{ cm}^2$ at 5.5 eV and a broader one ($77 \cdot 10^{-16} \text{ cm}^2$) at about 9.5 eV. A resonant state has been seen in electron transmission spectra at 5.4 eV [98Mod1]; an enhancement of the dissociative attachment has been seen between 8 - 12 eV [74Wan, 90Moy1].
- (c3) The TCS from Gdańsk and Trento labs [99Moz1] merge poorly in the 100 - 200 eV region. For this reason the recommended data were obtained by fitting formula (eq. 11) to all data points from 30 to 3000 eV.
- (d1) The maximum of TCS ($59 \cdot 10^{-16} \text{ cm}^2$) has been reported [96Moz1] at 3.8 eV, while the elastic cross section reaches a maximum at about 5 eV and the vibrational one a maximum at 2 - 2.5 eV [93Dil1].
- (e1) A maximum of $33 \cdot 10^{-16} \text{ cm}^2$ has been observed at 6.5 eV [98Szm1]. We are not aware of resonances in GeF₄.
- (f1) TCS reaches a maximum of $57.8 \cdot 10^{-16} \text{ cm}^2$ at 2.0 eV [97Szm1]. Electron transmission spectra [96Gui1, 98Mod1] indicate the presence of a resonant state at 1.7 eV.
- (f2) Electron transmission and electron attachment spectra [98Mod1] indicate the presence of a resonant state at 5.6 eV; a shoulder is visible in TCS [97Szm1] at about this energy.

6.1.10 Halogen substituted silanes

Table 6.1.11. Experimental total cross section for halogen substituted silanes (a1).

Energy [eV]	Cross section 10^{-16} cm^2						
	SiH ₄ (a2)	SiH ₂ Cl ₂	SiHCl ₃	SiCl ₄ (a2)	SiF ₄ (a2)	SiBr ₄	SiI ₄
0.2	1.9	36.6	26.5	41.2	19.9 (c1)	87.9	95.6
0.4	2.7	33.9	23.7	24.9	13.7	50.1	82.6
0.6	4.0	45.9	32.0	20.1 (b1)	9.9	34.7	61.2
0.8	6.2	55.2	39.0	21.1	7.7	36.9	39.7
1.0	9.5	60.8	45.4	25.7	6.5	48.6 (b1)	35.0
1.5	25.7	64.1 (b1)	58.0 (b1)	34.4	5.6 (b1)	45.5	42.7
2.0	44.0	60.8	58.5	49.1 (b1)	5.7	25.9	59.0
2.5	53.4	57.6	51.8	45.9	6.4	22.9	73.8
3.0	54.7 (b1)	57.2 (b1)	48.1	36.9	7.2	26.8	95.4
3.5	53.1	53.5	46.6	35.9	7.7	33.2	108.0 (b1)
4.0	51.6	50.7	46.8	37.9	8.9	42.3	104.4
4.5	50.1	49.7	48.1	41.9	10.1	53.7	102.0
5.0	48.9	50.5	51.6	49.3	12.4	58.4 (b1)	100.4
5.5	48.0	51.5 (b1)	56.0 (b1)	55.7 (b1)	14.3	57.1	100.9
6.0	47.1	51.5	56.5	54.3	17.4	54.9	100.3
6.5	45.7	51.1	55.0	53.3	19.8	55.6	101.9
7.0	45.2	51.1	54.8	54.5	21.6 (b1)	58.3	103.3
7.5	44.1	51.2	55.4	56.2	22.9	59.8	102.0
8.0	43.3	51.1	56.1	58.2	23.7	61.0	100.3
8.5	42.4	51.0	56.7	59.4	24.0	61.8	100.0
9.0	41.5	51.2 (b1)	57.1	60.1	24.0	60.5	99.9
9.5	40.5	51.4	57.4 (b1)	60.8	23.9	60.3	99.3
10.0	40.2	51.6	57.5	60.7	23.8	61.4	99.0
10.5	39.6	51.1	57.7	60.5	24.2	61.7	99.9
11.0	39.0	51.0	58.1	60.9	24.6	61.3	100.3
11.5	38.3	51.0	57.8	60.6	24.9	60.1	100.0
12.0	38.0	51.6	57.9	60.7	25.6	59.9	100.3

Notes

- (a1) All data are from Table 1 in [89Wan1]; for recommended data in SiH₄, SiF₄, SiCl₄ see Table 6.1.10. Electron transmission spectra in all seven gases were given in the same reference [89Wan1].
- (a2) The data in [89Wan1] for SiH₄, SiF₄ and SiCl₄ given in this table are slightly different from recommended values given in table 10. In particular in SiF₄ and SiCl₄ at the minima of the TCS (1.5 and 0.6 eV respectively) the measurements from the trochoidal spectrometer [89Wan1] are lower than the recommended data; the difference amounts to 15 % in SiF₄ and 50 % in SiCl₄. This is probably due to non-complete discrimination of forward scattered electrons in the Maryland apparatus [89Wan1]. The data for SiH₄, SiF₄ and SiCl₄ are given again in Table 6.1.11 in order to give a hint about the quality of TCS for other halosilanes in [89Wan1].
- (b1) These maxima and shoulders in TCS can be caused by resonances; see a detailed discussion in [89Wan1].
- (c1) The rise of TCS in SiF₄ below 1.0 eV can be well reproduced [98Kar1] by the Born approximation for the vibrational excitation, see eq. 13 in the introduction.

6.1.11 Very low energy (0.01 - 10 eV) TCS for some targets

Table 6.1.12. Experimental total cross sections for Cl₂, ClO₂, O₃ and C₆H₆.

Energy [eV]	σ [10^{-16} cm ²]			Energy [eV]	σ [10^{-16} cm ²]
	Cl ₂	ClO ₂	O ₃		
0.010			117	0.040	153
0.012			108	0.045	145
0.015			99.0	0.05	135
0.017			93.9	0.06	109
0.020	40.3	308 (b1)	87.6	0.07	91.9
0.022	39.9	277	84.0	0.08	86.0
0.025	38.8	227	79.4	0.09	90.3
0.030	35.6	131	73.1	0.10	89.7 (d1)
0.035	31.2	55.0	68.1	0.12	74.0
0.040	26.3	42.2	63.9	0.15	61.9
0.045	21.6	85.3	60.3	0.17	56.5
0.05	17.2	117	57.3	0.20	50.7
0.06	10.6	132 (b2)	52.3	0.25	44.7
0.07	7.5 (a1)	121	48.2	0.30	40.9
0.08	8.2	116	45.0	0.35	38.3
0.09	10.3	109	42.2	0.40	36.4
0.10	9.74	101	39.8	0.45	34.8
0.12	8.96	88.2	35.9	0.50	33.5
0.15	9.08	76.3	31.6	0.60	31.2
0.17	7.25	70.5	29.4	0.70	29.1
0.20	5.19	62.8	26.7	0.80	27.2
0.22	4.56	58.1	25.2	0.90	25.6
0.25	3.99	52.2	23.4	1.00	26.8
0.30	3.63	44.9	21.0	1.05	29.0
0.35	3.64	40.0	19.2	1.10	32.5
0.40	3.84	36.4	17.8	1.15	40.5 (d2)
0.45	4.11	33.4	16.7	1.17	42.0
0.5	4.43	30.8	15.8	1.19	40.2
0.6	5.12	25.8	14.5	1.21	37.7
0.7	5.81	22.3	13.7	1.23	37.3
0.8	6.50	20.1	13.1	1.25	38.5
0.9	7.18	18.5	12.8	1.27	40.8
1.0	7.87	17.5	12.6	1.29	41.8
1.2	9.14	16.0	12.2	1.31	40.8
1.5	10.9	14.8	12.0	1.34	38.3
1.7	12.2	14.2	12.1	1.37	39.4
2.0	13.8	13.6 (b2)	12.3	1.40	39.9
2.2	14.7	13.4	12.6	1.42	39.3
2.5	16.0 (a2)	12.9	13.0	1.45	38.0
3.0	17.8	12.0	13.8	1.47	37.1
3.5	19.7	11.0	14.8	1.50	37.8
4.0	21.8	9.94	15.4	1.52	38.1
4.5	24.3	8.97	14.6	1.55	37.8
5	27.1	8.11	14.1 (c1)	1.60	37.4
6	34.1	7.50	14.2	1.65	36.9

Table 6.1.12 (continued)

Energy [eV]	σ [10^{-16} cm ²]			Energy [eV]	σ [10^{-16} cm ²]
	Cl ₂	ClO ₂	O ₃		
7	40.8	7.85	14.7	1.70	36.2
8	42.5	8.05	15.3	1.8	35.1
9	41.1	8.19	15.9	1.9	34.7
10	39.6 (a3)	8.32	16.5	2.0	35.1

Notes

All the data in Table 6.1.12 are based on TCS measurements with the transmission method from a joint Daresbury and Aarhus laboratories experiment using synchrotron radiation electron sources. The original experimental points have been smoothed and fitted numerically in the present work. Recommended data for C₆H₆ above 0.6 eV are given in Table 6.1.6.

Cl₂ [98Gul3]

ClO₂ [98Gul2]

O₃ [98Gul2]

C₆H₆ [98Gul1]. See Fig. 6.1.7 (p. 6-28).

- (a1) A two-maxima structure, with onset at the threshold of first vibrational level (70 meV) has been attributed in [98Gul3] to a resonant state.
- (a2) No interpretation was attributed in [98Gul3] to a shoulder structure in TCS at about 2.5 eV.
- (a3) Measurements from a trochoidal spectrometer [99Coo1] at 0.3 - 23 eV agree well in shape with those in [98Gul3]; the absolute values coincide at 1 eV while at 10 eV the data in [99Coo1] are 20 % lower. Following a recent review [99Chr1] we have adopted results from [98Gul3] as recommended values.
- (b1) The very large cross-section at low energy most probably arises from rotationally inelastic scattering [98Gul2], see eq. 13 in the introduction.
- (b2) The nature of the maximum at 55 - 60 meV and of a weak shoulder structure at 2 - 3 eV is not clear [98Gul2].
- (c1) The TCS in [98Gul2] at 3 - 10 eV are compatible with the integral elastic cross section measurements [93Shy2], within the declared [93Shy2] error bar.
- (d1) A weak maximum at 0.1 eV remains outside the experimental noise and could correspond to a vibrational excitation through a direct (non-resonant) process (see [75Won1]).
- (d2) A resonant structure, with onset at 1.14 eV, vibrational spacing of 123 meV and -6 mV anharmonicity [75Nen1] was observed in the transmission spectra [72Lar1, 73San1, 75Nen1, 87Bur1]. Measurements in [98Gul1] with 3.5 - 8 meV energy resolution are, to our knowledge, the only results which evidenced such a structure also in TCS.

6.1.12 Alkali metal dimers and alkali halides

Table 6.1.13. Experimental total cross sections for alkali metal dimers and alkali halides.

Energy [eV]	Cross section [10^{-16} cm ²]				
	Li ₂ (1,a)	Na ₂ (1,b)	K ₂ (1,c)	LiBr (2,d)	CsCl (2,d)
0.5	543	305	430		
1	308	242	318		
2	200	195	251		
3	159	175	202		
4		169	174		
5		145	169	350	729
6	133	150	158		
7		127	149		
8		135	138		
9		109	149		
10	98	120	140		
20		100	117	99	178
50		85	97		

Notes

All the data in Table 6.1.13 are based on TCS measurements with a recoil-beam method, see subsect. 6.1.1.2.3.

The main difficulty of this method lies in the determination of the interaction-region geometry. Big discrepancies can be generated from wrong evaluations of these parameters, compare for example [72Sla1, 74Sla1, 83Jad1, 84Jad1].

- (1) The alkali metal dimers are targets with high polarizability values ($\alpha = 34, 30, 60 \cdot 10^{-30}$ m³ for Li₂, Na₂, K₂, respectively [86Wea1]). The classical theory [89McD1] for scattering on a polarization potential predicts an $(\alpha/E)^{1/2}$ scaling of the cross sections. The data in Table 6.1.13 follow this scaling only in a very approximate way (see [96Zec1]).
- (2) The alkali metal halides are targets with high dipole moments D , see [86Wea1]). Various theories, see [78Iti1], predict a (D^2/E) scaling of the cross sections for scattering on polar targets.

Li₂ [82Mil1]

Na₂ and K₂ [73Mil1]

LiBr and CsCl [89Vus1]

- (a) The declared [82Mil1] uncertainty of these data is ± 16 %.
- (b) The declared [73Mil1] uncertainty is 16 % below 4 eV and 14 % above 4 eV.
- (c) The declared [73Mil1] uncertainty is 20 % below 4 eV and 15 % above 4 eV.
- (d) The data for the alkali halides in Table 6.1.13 are from the more recent measurements by the recoil method [89Vus1]. These data show approximately a D^2/E scaling of the TCS [96Zec1]. Earlier data from recoil experiments, for CsF [74Sla1], CsCl [74Bec1], KI [74Sla1] and for CsBr, RbBr, CsCl, RbCl, KI [84Jad1] do not show such an energy dependence, and in the case of CsCl differ by a factor of 4 from the data of [89Vus1].

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