Chapter 15

The IAA Database

> *"A database is never finished, only abandoned."*
>
> — *As was said by many others, in their own wor(l)ds...*

When it comes to cross sections, one could perhaps establish the following hierarchy :

$$\text{Study} \ll \text{Multiple study} \ll \text{Compilation} \ll \text{Review} \ll \text{Database}$$

A study just publishes a set of cross section measurements at various energies, whereas a multiple study presents several ones measured with the same apparatus (for instance elastic along with vibrational or various electronic transitions). A compilation regroups different studies but does not present much critique by comparing data such as in reviews. Finally, a database gives a practical recommendation based on reviews and structures clearly the data into easily transcribable tables and eventually regroups them into a file readily readable by a program.

The purpose of the present chapter is to expose the cross sections assembled in chapter 11 and turn it into a database. Comparison to experimental data and other databases is made in the next chapter 16.

We would like to baptise the present database of electron-molecule cross sections as the "IAA database" in honour of the *Instituto de Astrofísica de Andalucía* which has generously provided its resources to the realisation of the present thesis.
This chapter is devoted to the description of the present – IAA – database which is hosted on the server `https://doi.org/10.5281/zenodo.8190461`.

Our IAA database, is distinguished from other ones in seven respects:

I. – It is mostly *independent* from all other databases but not totally unrelated either.

By this, we mean that we have not directly used the values of the CS featuring in other databases but we gleaned experimentally measured and theoretically calculated CS available in the literature with an emphasis on the most recent ones. The only places where our database coincides exactly point-by-point with another one, is when it relies on theoretically calculated CS for a particular species in a specific energy range from either the BSR calculations of Zatsarinny [1000] or the local-complex-potential resonant CS of Laporta *et al.* [552, 553].

II. – It possesses, in addition to integral cross sections, a grid of differential cross sections (DCS) for *elastic scattering* sampled on angles spanning 0° to 180° with an interval of 0.5° (361 values at each energy).

The energy grid is the union of all energies probed experimentally, with presently made theoretical calculations on a grid of rounded energy values in eV. The only exception is the DCS of argon up to 200 eV for which we resampled the more accurate DCS computed by Zatsarinny and Bartschat [998].

For inelastic scattering, it uses linear interpolation of various experimental data collected into a common file.

III. – The elastic momentum-transfer CS is the product of a three-step chain:

i. Determine the total CS and all inelastic CS (sec. 11.6);
ii. Deduce the residual elastic CS from the subtraction of all inelastic CS (sec. 11.1.5);
iii. Derive the momentum-transfer CS from the average cosine $\langle \cos\theta \rangle$ given by the shape of the DCS (see eq. (11.11)).

This was a choice motivated by the availability of abundant, accurate, well-resolved and updated measurements of the total scattering cross section. The other way around would be physically more relevant, but also unfortunately too risky because of the larger uncertainties and lesser availability of data of elastic momentum-transfer CS.

IV. – It extends on an unequalled wide range of energies from 0 eV to 1 GeV thanks to the extrapolation through relativistically valid analytical formulae.

V. – The extrapolation of the CS at both extremes of the energy range is based on physically meaningful parameters:

◁ At low energies : the scattering length A, static (dipole) polarisability α_d and quadrupole Q (for molecules only)
▷ At high energies : Bethe parameters moments of the oscillator strength distribution for inelastic CS (M^2, $\ln c$) and parameters from a Born expansion for elastic scattering $\tilde{A}$, $\tilde{B}$, $\tilde{C}$ and a cutoff energy K for the Born-scaling.

VI. – The inelastic cross sections are enhanced with more precise information on the electron energy loss such as Franck-Condon factors (or transition probabilities) for discrete vibronic bands of diatomic molecules, distribution over a bump for continuum losses (molecular oxygen) and partial ionisation based on core orbitals and valence-state excitations of the ion.

VII. – It is unadjusted to match transport coefficients when used by a two-term Boltzmann kinetic solver.

In lieu of adjustment, the CS are complemented with an inelastic cross section from unknown losses based on the complementary to the Thomas-Reiche-Kuhn sum rule of oscillator strengths from optically-allowed excitations and ionisation. The big exception is molecular nitrogen, for which the CS had to be complemented with losses from forbidden excitations based on the database of Kawaguchi *et al.* [482].

The known weaknesses of our database depend on each target, but are generally all linked to elastic cross sections at energies below 1 eV because of three reasons:

i) Elastic CS were derived from integral total scattering cross section measurements instead of momentum-transfer cross sections deduced from swarm experiments.

ii) The DCS at very low energies < 1 eV are computed from a too basic model (the MERT described in 10.1.5). The correspondence between integral and momentum-transfer cross sections might thus be inaccurate at low energies.

iii) Because of the two previous limitations, the resolution (number of data points) at low energies is very sparse. Only 3 points are given: 1 meV, 10 meV and 100 meV.

We could not find a reliable way to compute three-body attachment coefficients to molecular oxygen. This process significantly affects transport in O_2 at low electric fields < 100 Td.

For atomic oxygen and nitrogen, the cross section might be very inaccurate, especially elastic scattering due to little availability and lower reliability of experimental data.

Nevertheless, we estimate that the present database reflects electron-molecule interactions in atmospheric gases to the best of our knowledge. The rest of this chapter is divided into two sections. In the first 15.1, we give additional information on how the data was manipulated besides all the explanations given throughout part II. In the second 15.2, we give practical information on how to retrieve and use our data.

15.1 Metadata

In this section, we redirect the reader looking for specific information to the appropriate place in the thesis. Most of the information on how (differential) cross sections were constructed is available in chapter 11, organised in sections according to the collision type. The table 15.1 contains hyperlinks to figures, tables and equations for each target according to the collision type of the cross section. A detailed account of how we used fitting to synthesise data from a large experimental database was given in the previous chapter 13. A commented summary of the results from the physical point of view is presented in section 12.1 organised per gaseous species.

Instructions about how to use our cross sections in Monte Carlo simulations are given in section 15.2 and additional prescriptions in section 4.1. For sampling the outcome or the occurrence of a collision, instructions are given in section 3.2.

An overview of the performance of our cross sections and comparison with other databases is the topic of the next chapter 16.

In the rest of this section, for each target we explain how we dealt with:

A. Outdated experimental data $\Longrightarrow$ **Renormalisation**

B. Missing experimental data $\Longrightarrow$ **Completion**

Renormalisation

Any measurement of a physical quantity requires a calibration of the instrument so as to match the output signal of the instrument to an absolute physically meaningful value. Since a full calibration is such a tedious process, many experimental measurements rely on benchmarks [132] which are a consensus over either very precise experimental values or very accurate theoretical calculations.

Table 15.1: Overview of information about cross sections scattered throughout this thesis for each gaseous target. Next to the number of the section are displayed the page numbers. Both are hyperlinked. To navigate easily back and forth, use `Alt+←`, or check the equivalent shortcut on your pdf browser to come back to this page. In the printed distribution, here is a good page to place your bookmark.

Target		N_2	O_2	NO	Ar	O	N
Anagraph		p.507	p.508	p.508	p.509	p.510	p.510
Transport		fig.16.5	fig.16.10	fig.16.14	fig.16.18	fig.16.21	fig.16.23
References		tab. 16.1	tab. 16.2	tab. 16.3	tab. 16.4		
Total	σ_{tot}	fig.11.51a	fig.11.51b	fig.11.51d	fig.11.51c	fig.11.51f	fig.11.51g
Elastic DCS	$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}$	fig.11.9	figs.11.10,11.12,11.8	fig.11.11	fig.11.2,11.7	fig.11.5	
ICS	σ_{e}			fig.11.13			fig.11.6
MTCS	σ_{m}	fig.11.14a	fig.11.14b	fig.11.14c	fig.11.14d	fig.16.19	
Residual	σ_{re}	fig.16.1	fig.16.6	fig.16.11	fig.16.15	×	×
MTCS	σ_{rm}					×	×
Rotational	σ_{rot}	eq.(11.24)	eq.(11.21b)	eq.(11.21a)			
Vibrational	σ_{vib}	fig.11.19	fig.11.25,11.23				
Attachment	σ_{att}		fig.11.29				
Electronic	σ_{elt}	fig.16.3	fig.16.8	fig.13.17	fig.16.17	fig.13.9	
		tab.11.6	tab.11.7	tab.11.8	tab.11.9	tab.11.10	tab.11.11
		eq.(11.64)	eqs.(11.61),(11.62)			eq.(11.68)	
Ionisation	σ_{ion}	fig.16.4	fig.16.9	fig.16.13	fig.16.16	fig.16.20	fig.16.22
			eq.(11.120) fig.11.45 tab.11.12				
SDCS	$\frac{\mathrm{d}\sigma_{\mathrm{i}}}{\mathrm{d}\varepsilon_2}$	fig.11.46		eq.(11.119)			

Benchmarking serves to bridge the gap between the instrument signal and the measurement value by using a known quantity about a standard object. In scattering experiments, these are typically resonance peaks and cross sections in helium or argon. To know how benchmarks are used to facilitate subsequent measurements of cross sections, please refer to sections 7.3.5&7.3.6. As instrumental or theoretical accuracy improves with time, new benchmarks [e.g. 14] are brought about every decade or so. Therefore, we may say that a set of experimental data becomes outdated when the benchmark it relies on, has been replaced by a more recent one.

One of the great usefulnesses of reviews, is not only to gather information under a coherent ensemble, but also to keep it updated as was done throughout the years [124, 388, 941]. Nonetheless, updating data from someone else's measurements without their assistance is exacting. If original values of the raw measurements are not disclosed, it is all the more risky. This is why, most reviews prefer to update the measurements performed by their group only [941].

In our case, we decided, notwithstanding, to update some of the older sets of measurements based on evidence gleaned from the literature. There are mainly two reasons for this: first, using outdated data to construct a database would compromise the coherence of the database; second, there would be no point in proposing a new database if we decided to overlook this aspect.

For those studies that were not revised for their normalisation to outdated references, we proceeded to a **coarse** renormalisation corresponding to the second case in the equation of point **2**. in section 7.3.5 of the previous part.

By coarse, we mean that instead of properly selecting a benchmark differential cross section (DCS) at each individual energy, calculate all the ratios to the older reference DCS and then applying those ratios to all other concerned DCS (not to mention extrapolation to 0° and 180°); we only proceeded to renormalisation directly from reported integrated DCS (ICS). This assumes that all DCS actually perfectly agree in shape, and that there is only one calibration factor to be adjusted at each energy. This, of course, is not necessarily verified. Nonetheless, normalising through the DCS would require to deal with extrapolation, which may be risky or daunting for the purpose of the present thesis. The renormalisation we present for each target is thus based on an *average* of ICS values.

All experimental which have been renormalised by us are labelled with an asterisk * placed before the author name in our figures.

For instance, data from Zubek [1012] renormalised for N_2 are displayed as "*Zubek (1994)" in figure 16.3.

Completion

An often understated issue of cross section databases is their completeness. It is difficult to obtain a set of cross sections which completely accounts for all the losses endured by electrons in their collisions with molecules. We explain here how we compensate missing cross sections from unknown or unmeasured inelastic processes in our database.

Let us refresh our minds and jump to* figure 11.32a on page 447. Yon figure showed a snapshot of the electron energy-loss spectrum (EELS) for an electron originally at an energy of $\varepsilon_0 = 20\,\mathrm{eV}$ after being inelastically scattered at an angle of 20°. If we were to integrate this spectrum over all angles Ω and all energy-losses ε, we should be able to retrieve the total cross section of interaction:

$$\sigma_{\mathrm{tot}} = \oint_{\Omega} \int_{0}^{\varepsilon_0} \frac{\mathrm{d}\sigma_{\mathrm{EELS}}}{\mathrm{d}\varepsilon\,\mathrm{d}\Omega}\,\mathrm{d}\varepsilon\,\mathrm{d}\Omega\,. \tag{15.1}$$

If we have good spectroscopic knowledge, we may group energy losses according to the (rotationally-broadened) vibronic band pertaining to one identical electronic configuration of an excited state of the molecule. This is a tedious process since, as seen well on figure 11.32a, we would need to fit each peak of a band with a Voigt or Lorentz profile then take the integral value of the fit and sum all integrals to obtain the differential cross section of that electronic excitation at the observed angle of scattering.

Notwithstanding, even with good spectroscopic knowledge, we may not classify all bands; and particularly not those which are drowned in the noise. In relation to this limitation, we would like to quote an astute observation:

Song *et al.* [865]

> “The resultant electronic excitation cross sections, however, should be understood as a whole only to provide realistic energy loss of electrons passing through the gas, and in fact, unique determination of individual cross sections will not be possible as long as there is no additional information.”

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*On a typical .pdf reader press `Alt+←` to promptly navigate back here to the previous page.

This means, that even with the greatest of all care, there will always be a part of the electron energy-loss spectrum unaccounted in our database.

"Completion" of a set of inelastic cross sections is the attempt to include all unidentified losses in the electron energy-loss spectrum into complementary cross sections which may be seen as virtual electronic states at certain average energy levels.
For molecules, completion also comprises the construction of a set of rotational cross sections.

There are essentially three ways to create the complementary cross section:

I. Sum rules: The preferred way is to exploit the Thomas-Reiche-Kuhn sum rule (11.70) when the sum of optical oscillator strengths from dipole-allowed excitations (f_x) and ionisation (f_i) does not amount exactly to the number of electrons (N) in the target molecule. We may then very straightforwardly define a complementary optically-allowed excitation whose oscillator strength f_o is determined by the parameters of our analytical fits from chapter 11:

$$f_o = N - \sum_x M_x \frac{\Delta\mathcal{E}}{\mathrm{Ryd}} - \sum_i Q_i N_i \, . \tag{15.2}$$

[Please mind the notation in the above equation (15.2): x index for discrete excitation, i index for ionisation channel (ground, ionic excitation and/or multiple ionisation). Namely, forgive the potentially confusing notation $N_{\mathrm{i},i} = Q_i N_i$ (roman 'i' subscript stands for **i**onisation, whereas italic i is the index for ionisation channel). The $N_{\mathrm{i},i}$ quantity ("active number of electrons in the ionisation channel i") was defined in (11.93) and more specifically in (11.108). The Q_i and N_i parameters are to be found in each row (indexed by i) of table 11.12.]

If this sum (15.2) is already complete (i.e. $f_o = 0$), then, one must seek for other sum rules or higher moments of the oscillator strength sum rule [319, §IV.C].

II. Total inelastic CS: An alternative way is to derive directly the missing cross section from the difference between the total CS for electronic excitations σ_{exc} and the sum from the CS σ_c in the current database.

$$\sigma_{\mathrm{D}}(\varepsilon) = \sigma_{\mathrm{exc}}(\varepsilon) - \sum_{c \in \mathrm{exc}} \sigma_c(\varepsilon)$$

The disadvantage is that one does not always have access to the total inelastic CS and if so, the accuracy might not be good enough. One then obtains an (ugly) tabulation of the complementary CS whose accuracy is marginal.

III. Blind adjustment : When none of the solutions above are within reach, one must surrender to the ultimate empiricist's tool: *ad hoc* adjustments.

The concept of completion is tightly linked to the adjustment of cross sections so as to match experimental transport coefficients of an electron swarm in a given gas at a certain electric field. The complementary inelastic cross section represents major electron energy losses besides the ionisation which, normally, is well characterised. One may then scale an arbitrarily chosen cross section upwards until the Townsend's first ionisation coefficient α_{i} (or other reaction coefficients) match well the experimental data of electron swarms in discharge gas tubes.

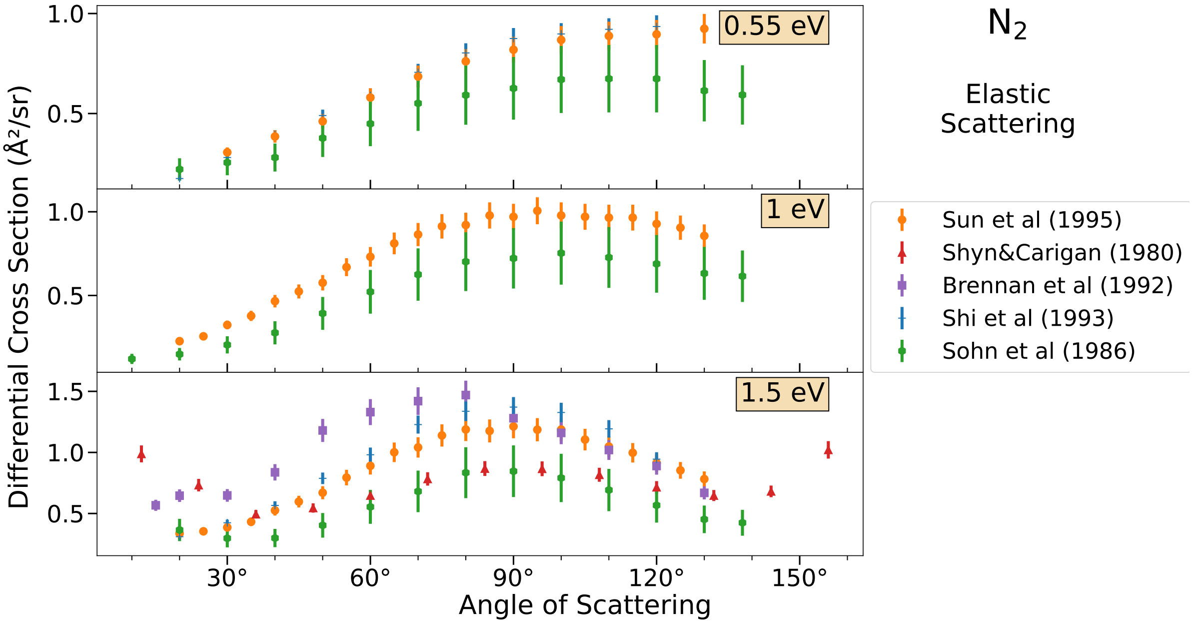

Figure 15.1: Experimental electron elastic differential cross section with N_2 at 0.55, 1 and 1.5 eV. ▲ - Shyn and Carignan [838]; ■ - Brennan *et al.* [105]; •- Sun *et al.* [894]; + - Shi *et al.* [832]; ⬡ - Sohn *et al.* [863]. Earlier data [838, 863] are lower than more recent data [832, 894].

Completion is not a new concept, but its denomination is not standard. Many databases on LXCat possess such a complementary cross section. For instance, for N_2, `Phelps` (and also `IST-Lisbon`) has one named "sum of singlet states" which represents the bulk of all electronic excitations lying beyond $a''\,^1\Sigma_g^+$ at 12.25 eV. `Biagi` also possesses a "sum of singlets" but it is hard to guess which states it comprises because the b, b′, c_3, c_4' and o_3 singlet states are all already present in the database.

We recommend that "completion"* be added as a fourth criterion to the list of Itikawa [435].

15.1.1 N_2 – updates

Renormalisation

The accuracy of elastic DCS of molecular nitrogen improved with time. As an example, several discrepancies [832, fig. 1-2] at low energies got resolved after more recent experiments [894] elucidated the DCS with a deepened comparison with theoretical values and calibration to a well established absolute reference, usually Helium [693, 771]. Such disagreement is shown in 15.1 at 0.55, 1 and 1.5 eV, where the earlier measurements of Sohn *et al.* [863] and Shyn and Carignan [838] are challenged by Sun *et al.* [894] and Shi *et al.* [832].

Although Sohn *et al.* [863] mentioned that all their results were underestimated by calculations and other experimental results, they did not expound their calibration and normalisation procedure. Albeit not systematic, an upward correction by ~1.2, 1.25, 1.3, 1.4 and 1.5 to Sohn *et al.* [863, table 2] at 0.1, 0.35, 0.55, 1 and 1.5eV brings their data into better agreement both with [832, 894] and even the most recent total CS of Kitajima *et al.* [512]. Consequently, we used these factors to scale up all their [863, table 2-3] elastic and vibrational CS.

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[*] "completion of the representation of inelastic losses of electrons in a gas through a discrete set of cross sections".

In the $^2\Pi_g$ resonance region, comparison between theory and experiment and even among different measurements is intricately difficult. This stems from the fact that the energy position of the resonance feature (peaks or dales) varies with the angle of scattering [17, p.3664-5:table 2]. Thus, it is not straightforward to understand whether the energies reported are consistent between different experiments. Instead, it is desirable to take a reverse approach [832, table 2] and compare DCS by adjusting the incident electron energy to remain at the peak position while maintaining the angle fixed [894, 1240-2:table I].

In general, it is observed that Shyn and Carignan [838]'s DCS (also for other molecules [842]) report higher rates of forward and backward scattering than the majority of other experiments [894, figs. 6–8]. This might point toward a systematic contamination of the signal at small and large angles in their apparatus [939, §V:p.82]; a concern that was addressed already many times and that should be reminded to those who use the data for modelling. This is also true for doubly differential cross section from impact ionisation as discussed in section 11.5.4 p.492 in the previous part II (see the triangles ▲ in figures 11.47–11.48).

At higher energies, the agreement between measurements is much better due to an accurate calibration of the absolute DCS [114]. Herrmann *et al.* [397] performed measurements over an extended range of energies (90–1000 eV) but used approximate IAM calculations to normalise their data. They did provided scaling factors [397, table II] to bring their DCS in agreement with Bromberg [114] and Jansen *et al.* [453] on absolute scale. After rechecking those original factors from averaged ratios, we determined that those are valid and should be applied for correcting their reported DCS.

Some measurements published during the 70's were updated due to more accurate results for the values of the DCS used as a reference. This was the case of Cartwright *et al.* [158] and Chutjian *et al.* [181] which were renormalised later by Trajmar *et al.* [941] with the data of Srivastava *et al.* [870] revised. Nevertheless, at the lower energies $\varepsilon < 15$ eV, the latter DCS is higher at small and large angles than more recent measurements as observed in figure 15.2. In contrast, Brunger and Teubner [122, §III.B] relied on the measurements of Shyn and Carignan [838], which they found to lie in better agreement with their own results.

Since the most recent measurements of Linert and Zubek [600] and Allan [17] probed a wide range of angles even up to 180°owing to the magnetic angle changer technique [510], we performed our own quick renormalisation of Cartwright *et al.* [158] DCS using Linert and Zubek [600] below 21 eV and Shyn and Carignan [838] at higher energies. The overall agreement with Johnson *et al.* [463] was slightly improved compared to Trajmar *et al.* [941]. This freshly renormalised set of data was used along with the most recent measurements to obtain fits for the integral cross sections in section 11.4.3 of the previous part.

The difficulty with measurements [910] based on normalisation from the relative ratio to Helium published in Srivastava *et al.* [870, table II] is that they are not guaranteed to be consistently accurate at all angles and all energies. Indeed, uncertainty is introduced twice, when multiplying by the ratio N_2/He and then by the absolute He DCS. In order to obtain newly renormalised sets, one would have to revert the process of normalisation at all angles, multiply by a trusted set of absolute N_2 DCS and extrapolate at small and large angles before finally integrating. We did not choose to pursue this daunting task and decided to simply put less weight on older measurements that could not be renormalised in a straightforward way.

Malone *et al.* [622] reported re-integrated values of Zubek and King [1013] for the $C\,^3\Pi_u$, $E\,^3\Sigma_g^+$ and $a''\,^1\Sigma_g^+$ states. Subsequently, we scaled down Zubek [1012]'s ICS for $C\,^3\Pi_u$ by a factor of 1.28* in order to bring his formerly reported value of $24 \times 10^{-18}\,\mathrm{cm}^2$ at 17.5 eV in agreement with the newly calculated value of $18.8 \times 10^{-18}\,\mathrm{cm}^2$ by Malone *et al.* [622].

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*Malone *et al.* [622, figure 1] had hinted a factor of 1.32

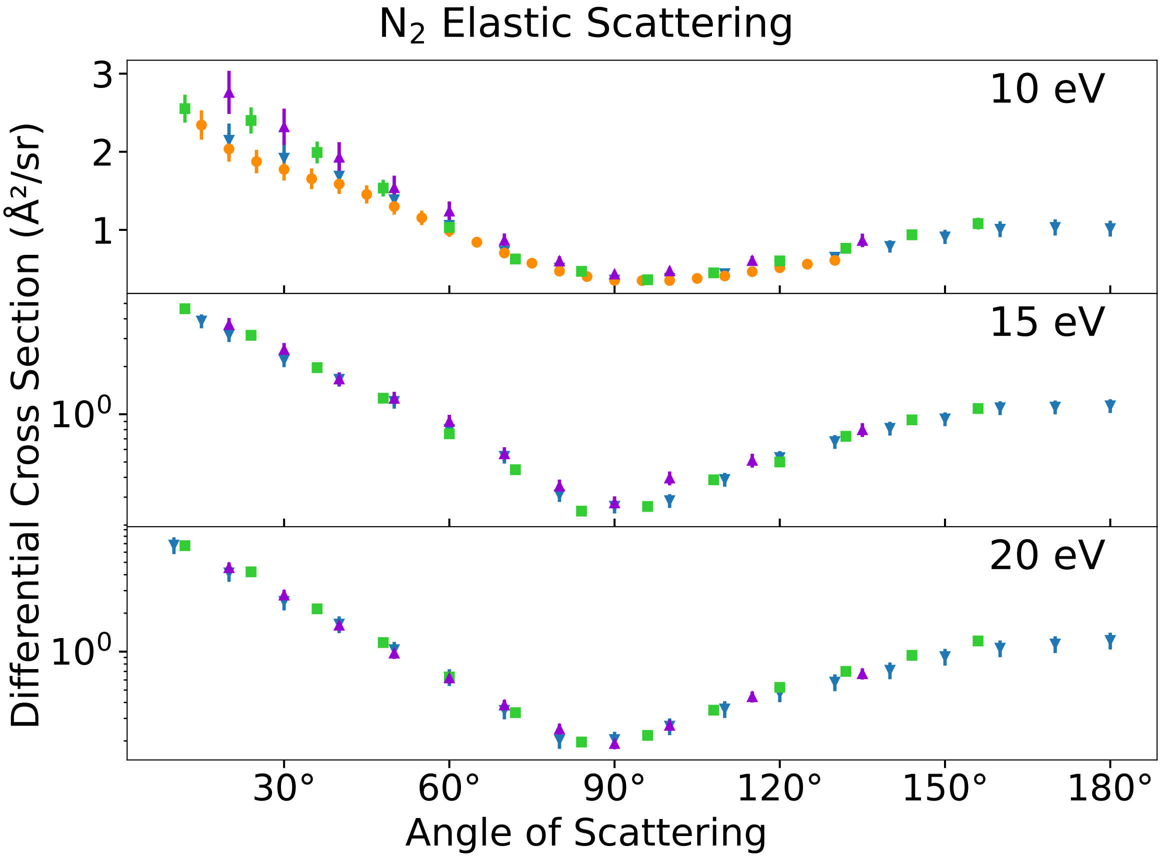


Figure 15.2: Experimental electron elastic differential cross section with N$_2$ at 10, 15 and 20 eV. ▲ - Srivastava *et al.* [870] renormalised by Trajmar *et al.* [941]; ■ - Shyn and Carignan [838]; •- Sun *et al.* [894]; ▼ - Linert and Zubek [600]. At lower energies, the data of Srivastava *et al.* [870] lead to a slight overestimation of the integral cross section.

Completion

Despite the differences between all other databases of N$_2$, what mostly distinguishes our – incomplete – database is that its total inelastic cross section (for N$_2$) lies systematically below any of the other databases as can be seen on the bottom graph of figure 16.2.

We checked that the sum Thomas-Reiche-Kuhn sum amounts to ~14 in our database:

$$\text{OOS completion for N}_2 : \qquad \sum\!\!\!\!\!\!\int_x f_x = \underbrace{\sum_x f_x \frac{\Delta\mathcal{E}}{\text{Ryd}}}_{=1.145} + \underbrace{\sum_i Q_i N_i}_{=12.856} = 14.01 \; ; \tag{15.3}$$

so the difference cannot be imputed to a missing dipole-allowed excitation.

Strangely, we also include the residual dissociation cross section σ_{rd} as defined in (11.65). It is obtained as the remaining dissociation cross section by subtracting the contribution of predissociation to Cosby's [193] cross section for neutral (i.e. non-ionising) dissociation of nitrogen molecules. This "residual" dissociation cross section, together with all other identified electronic states, is also present in the most recently updated database for N$_2$ by Kawaguchi *et al.* [482] but our total inelastic CS is systematically lower than theirs (compare - - - with ··· in fig. 16.2–bottom).

Thus, the only possibility is that we underestimate the cross sections from *forbidden* excitations. This is confirmed by looking at figure 16.3, for four excitation CS of optically-forbidden transitions. Most of the databases show higher peaks, whereas we decided not to follow strictly outlying points in our analytical fits on table 11.6.

We also know from our study of transport coefficients at the end of chapter 4 p. 137, that it is our database which is deficient since it overestimates Townsend's ionisation coefficient α_i by over a factor of 2 (fig. 4.17a–right panel), and the mobility coefficient μ_e by roughly 10 %. Thus, we may reasonably suppose that there are some missing resonance peaks of spin-forbidden excitations which could explain the discrepancy with the ionisation coefficient.

Due to the present lack of information and resources, we opted for the method II. consisting in completing from the total sum of inelastic CS of a known and trusted source. Among the databases listed in the next chapter section 16.1, the "`Muroran`" database of Kawaguchi *et al.* [482] showed the greatest diligence in assembling the cross sections. Therefore, we patched our database with the differences observed between our incomplete (dark blue dashed - - -) database and the dark purple short-dotted curve ··· in figure 16.2–bottom. Then, we split the cross section into two regions: one with a loss at 7 eV and the other at 14 eV. The difference between our incomplete and complete sets can be observed on figure 16.2–bottom, where the complete set is superposed with the purple dotted curve (···) of "`Muroran`" from Kawaguchi *et al.* [482].

Concerning rotational losses relevant at low electric fields <1 Td, we constructed the set of rotational cross section for $J_0 \to J'$, using the sudden-impulse approximation (11.24), with the four elementary transitions: $J = 0 \to 0$, $J = 0 \to 2$, $J = 0 \to 4$ and $J = 0 \to 6$ which we digitised from the figures of Kutz and Meyer [546, fig. 7a].

15.1.2 O$_2$ – updates

Renormalisation

The data from Wakiya [972, 973] and Shyn and Sweeney [845, 847] and Shyn *et al.* [848, 849] were normalised to an elastic cross section that was later found to be in disagreement with more recent and improved experiments [206, 353, 598, 893] as can be seen in figure 15.3. We thus took the initiative of renormalising their data assuming that their DCS overall shape was reasonably correct. Unfortunately, the measurements of Shyn and Sharp [842] showed systematic overestimation at large angles [893, §3:p.4321-2, fig 1&2] and small energies. Brunger and Buckman [124, §3.3.2.2:p.317] believes that this is caused by error contamination of Shyn's measurements at backward angles (> 110°). In addition to this, the data of Shyn and Sharp [842] systematically underestimate DCS at 30 eV in comparison with the data of Sullivan *et al.* [893] and at 200 eV by 30–100 % with those of Daimon *et al.* [206]. This could be due to a bias in the absolute normalisation of the DCS.

The reference data for renormalisation was essentially composed of Linert *et al.* [598] (update of Sullivan *et al.* [893]) at low energies and of Daimon *et al.* [206] at high energies which we extrapolated with our own IAM calculations from the previous part. Currently, there is no other available experimental data from 40–150 eV than that of Shyn and Sharp [842]. Therefore, we have no sound way to assess the accuracy of the DCS and ICS in that range. This discrepancy and uncertainty might somehow affect the inelastic DCS outside of the 10–30 eV range.

The two (original vs. renormalised) are compared in figure 15.3. The data from Shyn and Sharp [842] are all lowered, especially < 10 eV due to spurious backward scattering, whereas Wakiya [972]'s values are all raised in the renormalised version. A dotted line represents the data gathered from other sources [221, 352, 897, 938].

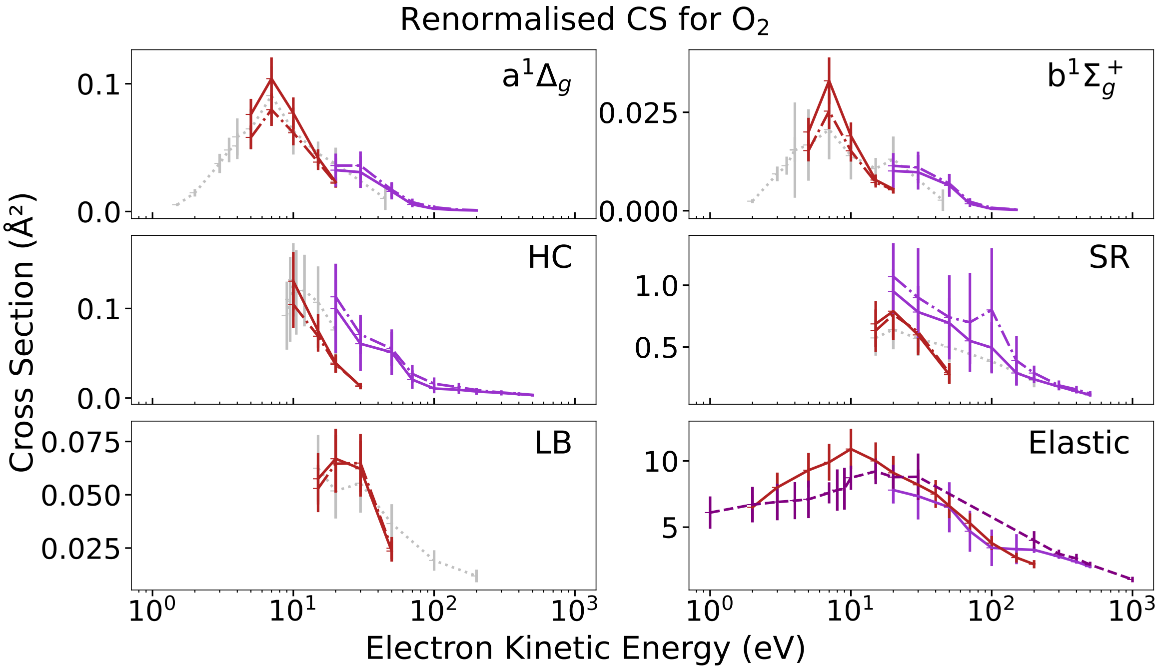


Figure 15.3: Renormalised set of cross sections of Wakiya [972, 973] (in violet) and Shyn and Sweeney [845, 847] and Shyn *et al.* [848, 849] (in red) for electronic excitations of O_2. Solid-dotted (–•–) lines represent renormalised data according to the ratios of the elastic cross sections represented on the bottom right panel. There, the purple dashed (- - -) is our built reference for the integral elastic cross section. Light-grey dotted lines represent data points from other sources in the literature.

Unfortunately, the improvement in experimental concordance with our renormalisation is quite marginal. Wakiya's elastic data was lower than our reference and raising the values actually worsens the trend seen at large energies yielding significant overestimation. A possible cause would be that the inelastic-to-elastic ratios had large uncertainties. A survey of inelastic scattering beyond 50 eV would be desirable in order to check Wakiya [972, 973]'s results. The overlap [599, fig.2] between ground state vibrational levels $v' = 5$ and $a\ ^1\Delta_g$, and $v' = 9$ and $b\ ^1\Sigma_g^+$ could potentially explain a slight overestimation in Wakiya's result below 50 eV but it cannot explain discrepancies above 50 eV, where vibrational losses are typically negligible. Shyn's data are overall brought into better agreement with renormalisation, although the bulk of the data situated in the interval 10–30 eV is luckily in the region where Shyn and Sharp [842]'s elastic CS do not differ much from the reference (cf. fig 15.3 bottom right).

Completion

See the explanation on p.569 about the concept underlying "completion", in particular point I..

If we sum the oscillator strengths from allowed excitations on table 11.7 and from ionisation 11.12, we get:

$$\text{OOS completion for } O_2 : \quad \sum\!\!\!\!\!\!\!\int_x f_x = \underbrace{\sum_x M_x \frac{\Delta\mathcal{E}}{\text{Ryd}}}_{=0.1232} + \underbrace{\sum_i Q_i N_i}_{=15.7828} = 15.906 < 16\ . \tag{15.4}$$

Thus, we took $f_o \approx 0.1$ and $\Delta\mathcal{E}_o = 11\,\text{eV}$. The parameters for (11.61a) are fixed by: $M_o = f_o\text{Ryd}/\Delta\mathcal{E}_o$, $C_o = 3$, $b_o = 1 = c_o$. Hence, we do not make any adjustments on C_o, b_o, c_o. The interested user is invited to do so if he/she finds it convenient.

Another aspect, often tacit, is that inelastic cross sections σ_x associated to a given energy threshold $\Delta\mathcal{E}_x$ might not represent accurately the actual inelastic electron energy loss spectrum (EELS) in the gas. This is particularly true for molecules, whose vibronic bands can extend over several eVs and even more for O_2 because of the broad continuous bumps in the EELS forming the Herzberg pseudo-continuum (HC) and Schumann-Runge (SR) continuum spanning altogether from about 4.5 eV up to roughly 9.7 eV. While in the Monte Carlo approach, we are free to sample the actual energy loss from a discrete (vibronic peaks) or continuous (bump) distribution; this is not (usually) the case of kinetic solvers which are based on a single threshold $\Delta\mathcal{E}$. As a result, it is not correct to set the loss in the HC or SR to the threshold value; rather, one should set it to the *average* value $\mathcal{E}_\text{m}$:

$$\mathcal{E}_\text{m} = \frac{\int_{\Delta\mathcal{E}}^{\mathcal{E}_\text{max}} \frac{\mathrm{d}\sigma}{\mathrm{d}\varepsilon}\varepsilon\,\mathrm{d}\varepsilon}{\int_{\Delta\mathcal{E}}^{\mathcal{E}_\text{max}} \frac{\mathrm{d}\sigma}{\mathrm{d}\varepsilon}\,\mathrm{d}\varepsilon}\,, \tag{15.5}$$

where the upper boundary $\mathcal{E}_\text{max}$ is determined from the EELS (sometimes arbitrarily). Thus, as done in the `Phelps` database, we presently set the centroid $\mathcal{E}_\text{m}$ in the Herzberg pseudo-continuum to 6 eV; whereas in the Schumann-Runge continuum, to 8.6 eV (a small part was left at 6.12 eV for the onset of the SR, which, for practical purposes, can be merged into the HC if one wishes).

For rotational cross sections, we could not find any experimental nor theoretical data. Lacking such information, we used the quadrupole and anisotropic polarisation Born approximation in (eq. 11.21b, p. 412), as given in Takayanagi and Itikawa [908, eq.(38)] from Dalgarno and Moffett [208]. Bluntly put, these rotational cross sections are but a "better than nothing" addition. They are expected to be severely inaccurate since rotational scattering off O_2 should be strongly affected by the O_2^- $^2\Pi_g$ resonance.

In order to fit transport parameters in O_2 from Nelson and Davis [691] below 0.1 Td, Alves *et al.* [24] had to use a value (1.4 a.u.) for the permanent quadrupole Q more than four times higher that the actual experimental value ($Q \simeq -0.29\,\text{a.u.}$). This confirms the invalidity of the quadrupole Born approximation for electron rotational scattering off O_2.

15.1.3 NO – updates

Renormalisation

The elastic cross section used for normalisation [654] was corrected by Brunger *et al.* [120, table 3] before they presented their integrated cross sections (ICS) for electronic excitations. Nevertheless, the value at 50 eV must have been extrapolated because this energy was not measured in Mojarrabi *et al.* [654]. Since the theoretical ICS by Fujimoto and Lee [307, table 1] were all in good agreement with the experimental data at lower energies, Itikawa [441, table 2] recommended to use their results for $\varepsilon \geq 50$ eV. As a result, all values from Brunger *et al.* [120] at 50 eV were presently raised by a factor 7.88/6.444, which, to our relief, improves the agreement of fitted s_{exc} functions at that energy for all cross sections. We interpret this as a clue that the extrapolated [120, table 3] $6.444 \times 10^{-20}\,\text{m}^2$ at 50 eV is underestimated. Sadly, this slight inconsistency was not noticed by any of the most recent reviews [441, 865], we hereby recommend to multiply all the reported ICS at 50 eV by 1.223 for electronic excitations of NO.

Completion

The completion of NO is even more important than for O_2 or N_2. Song *et al.* [865, p.11–2:fig. 13] reports that the sum of all electronic impact excitation CS from Brunger *et al.* [120] is a factor of five below total electronic CS derived from swarm experiments.

This, we confirm from the complementary oscillator strength $f_o = 0.571$ deduced from:

$$\text{OOS completion for NO : } \sum\!\!\!\!\!\!\int_x f_x = \underbrace{\sum_x M_x \frac{\Delta\mathcal{E}}{\text{Ryd}}}_{=0.2587} + \underbrace{\sum_i Q_i N_i}_{=14.17} = 14.429 < 15\ . \tag{15.6}$$

Due to the low ionisation potential of NO at 9.26 eV, we took $\Delta\mathcal{E}_o = 9\,\text{eV}$ giving thus $M_o = f_o \text{Ryd}/\Delta\mathcal{E}_o \approx 0.8636$ and the remaining parameters are fixed as for O_2 ($C_o = 3$, $b_o = c_o = 1$).

When we include this complementary cross section, our complete set agrees better with the swarm results of Song *et al.* [865, fig. 13] and are about a factor of five higher than our incomplete set as observed from the large difference between the solid and dashed dark blue curves in figure 16.12.

NO has a permanent dipole of $D \approx 0.0625ea_0$ [924]. In the Born approximation, rotational excitation CS for NO may be expressed with (11.21a) [442, eq.(39)]. We used this simple formula to compute a set of $J_0 \to J_0 + 1$ cross sections, up to 20 eV, which are the dominant modes of rotational excitation in NO at low energies. Be wary that these cross sections might be inaccurate in the resonance region between 0.2 eV and 1.5 eV.

15.1.4 Ar – updates

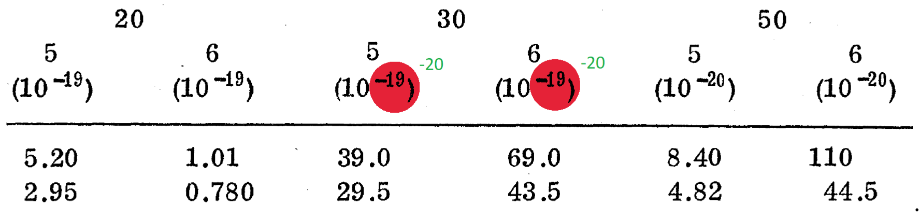
Renormalisation

As with the previous cases, the older data from Chutjian and Cartwright [180] could benefit from renormalisation due to the differences observed between their reference elastic cross section [871] and newer measurements [310, 731]. In his recommendation, Hayashi [388] must have been aware of this because his reported values are much better matched by renormalised data of Chutjian and Cartwright [180]. In his earlier report, Hayashi [387, p.4-5] mentions that he indeed renormalised some of the data with the then recent measurements for elastic scattering with Helium from Register *et al.* [771]. Strangely, Srivastava *et al.*'s measurements were actually normalised on that aforementioned set of Helium data. Perhaps in 2003, another set of reference data was used for renormalisation of subsequent cross section with argon.

Ironically, Srivastava *et al.* [871] in their table IV add a footnote saying that their results from phase-shift analysis are less reliable than from the normalisation, though the former were found in better agreement with all experimental data in those energy ranges [310, p.39-40]. We used the renormalised data based on Furst *et al.* [310] values ≤20 eV and Panajotović *et al.* [731] above, to produce our recommended analytical cross sections. Still today, many sources [313, 319, 383, 491, 1002] do not consider renormalisation when they compare their calculated results. This is probably because no review of argon's CS specifically addressed the daunting task of correctly renormalising DCS and then proceed to integration once more.

Another renormalisation was pointed out in Allan's measurements [14, p.2:bottom right] concerning the most recent data of Khakoo *et al.* [491] for 4s excited states at 15 eV only. They say a division by a factor of 1.45 brings Khakoo *et al.*'s results in agreement with their absolute DCS at 135°. We checked that Khakoo *et al.* [491] DCS at 15 eV indeed show an awkward lump for all four 4s states that is not attributable to a resonance but to the normalisation used. We then used the 1/1.45 reduction for those data (at 15 eV only) in our collected database.

Another important deduction is that the units of DCS at 30 eV in table IV of Chutjian and Cartwright [180] were manifestly mistyped to an order of magnitude larger:



20		30		50	
5	6	5	6	5	6
(10^{-19})	(10^{-19})	(10^{-19}) -20	(10^{-19}) -20	(10^{-20})	(10^{-20})
5.20	1.01	39.0	69.0	8.40	110
2.95	0.780	29.5	43.5	4.82	44.5

This caused Puech and Torchin [760]'s database on LXCat to grow two jolly bumps (cf. figure 13.11 behind) to try to match the erroneous data for $4p[1/2]_1$ and $4p[5/2]_3$ that was fitted in Bretagne *et al.* [106, p.766:table 2].

We surmise that there are two other typographical errors in Chutjian and Cartwright [180]: for the magnitude of level '3' ($^3P_0$) in table III at 100 eV which should be 10^{-22} and level '21' ($(4d')[5/2]2^\circ$) in table IX at 100 eV which should be 10^{-21}. This gives indeed a very good agreement both with the theoretical $1/\varepsilon$ decrease for forbidden transitions but also with Khakoo *et al.* [491] and Chilton and Lin [176] respectively. The first typo could not be identified in Hayashi [388] because no suitable comparison was available at that time.

At the time in 1986, the availability of other databases was scarce and even a typo of an order of magnitude can pass through examination if no comparison can evince the queerness. I used this example in chapter 13 section 13.3 to stress the importance of inspecting thoroughly given information.

Completion

See the explanation on p.573 about the concept underlying "completion", in particular point I..

In case of argon, completion was not obtained through the complementary to the sum of oscillator strengths (OOS). This is because there is almost $f_o = 1$ missing to complete the sum (15.2), which is an implausibly large portion:

$$\text{Missing OOS in Ar}: \quad \sum\!\!\!\!\!\!\int_x f_x = \underbrace{\sum_x M_x \frac{\Delta\mathcal{E}}{\text{Ryd}}}_{=0.505} + \underbrace{\sum_i Q_i N_i}_{=16.532} = 17.037 < 18 \,. \tag{15.7}$$

Furthermore, as we commented in chapter 12 p.509, the RBEQ* model to ionisation could be improved by specifying each particular channel leading to partial ionisation from the $3p$ orbital. Then, the integration of oscillator strength densities from the ionisation continuum could become higher than the actual value (16.53) which corresponds to the minimum reported in Berkowitz [62, p.84:table 3]. We also note that the current Bethe parameter from the RBEQ* fit ($M_{\mathrm{i},Q} = 2.662 < M_\mathrm{i} \simeq 3.52$) is significantly below its reported value M_i. We therefore think that a great portion of the missing (complementary) oscillator strength in Ar is imputable to an imprecise modelling of losses in the ionisation continuum.

In lieu of completion, the complementary oscillator strength in the complete database is obtained from the sum of OOS of allowed excitations to higher states than to $5s$ orbitals (e.g. $4d$, $6s$, etc.) as collected by Gargioni and Grosswendt [319, p.477:table XI].

$$\text{Complementary OOS in Ar}: \quad \sum_{x>5s} f_x = 0.293 = f_o \,. \tag{15.8}$$

These are supposed to encompass loss from 14.7 eV up to the ionisation threshold (15.76 eV). We therefore set $\Delta\mathcal{E}_o = 15$ eV giving $M_o = 0.2678$.

Besides the inclusion of f_o, the complete database for argon is also a finer database in the sense that the excitations to $4p$, $3d$ and $5s$ orbitals are fitted individually, whereas in the “incomplete” database they are grouped together in a singly fitted CS as represented by the gray-shaded lines on table 11.9. Those differences can be observed on the four graphs of figure 16.17, where a true sum of CS (“complete” —) is compared to an overall fit (“incomplete” - - -).

15.1.5 O – updates

Renormalisation

The data of Kanik *et al.* [476] were normalised at each angle and energy based on summed DCS Johnson and Kanik [460] for molecular oxygen, which themselves were normalised based on inelastic excitations of He and Ne. A more recent survey from Suzuki *et al.* [897] probed the same excitation DCS (for O_2) but normalised to the elastic DCS of He. Both sets agree within their uncertainties except at 100 eV where Suzuki *et al.* [897] are systematically a factor of $\simeq 1.25$ higher. Thus, we decided to multiply all values from Johnson and Kanik [460] and Kanik *et al.* [476] by 1.25 at 100 eV. This correction systematically improves agreement with Vaughan and Doering [959, 960]'s measurements.

Completion

See the explanation on p.569 about the concept underlying “completion”, in particular point I..

As for molecular oxygen, the set for atomic oxygen was complete with the complementary oscillator strength:

$$\text{OOS completion for O :}\quad \sum\!\!\!\!\!\!\!\int_x f_x = \underbrace{\sum_x M_x \frac{\Delta\mathcal{E}}{\text{Ryd}}}_{=0.3} + \underbrace{\sum_i Q_i N_i}_{=7.4526} = 17.037 < 8\ , \tag{15.9}$$

giving $f_o = 0.247$. We chose the threshold of 13 eV below ionisation, and thus $M_o = 0.2585$.

Many of these complementary states are auto-ionising and we could have chosen a higher threshold. Nevertheless, when we fitted the RBEQ* on p.488, we only included known (i.e. fitted) auto-ionising states: $3s''\ {}^3P^o$, $2s2p^5\ {}^3P^o$, and $4d'\ {}^3P^o$. Therefore, it is not very clear which auto-ionising states form part of the RBEQ* and which not.

15.1.6 N – updates

Renormalisation

There are not many data about atomic nitrogen, so the discussion about renormalisation is limited. We only detected one potential systematic bias in the data of Doering and Goembel [222, 223] at 30 eV which was normalised to Chutjian and Cartwright [180, table III] excitation to $(4s')[1/2]^o_1$ of Argon, lying about ~1.45 below the more recent Khakoo *et al.* [491, figure 6(d)] and most of the theoretical curves. We multiplied thus Doering and Goembel [222] data at 30 eV by 1.45. Raising this outlying point on Wang *et al.* [975, figure 4-mid] improves the agreement with the most recent theoretical calculations.

Measurements at higher energies were based on the well established values for Helium ${}^1S_0 \to {}^1P$ from Register *et al.* [771], and we could not find any relevant correction applying there.

Completion

The sum rule (15.2) may be applied to any electronically inelastic excitation, including ionisation. In case of atomic nitrogen, we decided to apply the sum rule for completion on the Q parameter of the RBEQ* model instead of fitting it to ionisation CS as was done for the other targets.

This is because, as Kim and Desclaux [506, §III.B] explain, in the experiments of Brook *et al.* [117], the ionisation CS for atomic nitrogen were performed on a mixture including the lowest metastable state $^2D^o$. Thus, if one wishes to derive the ionisation CS for the ground $^4S^o$ state, one needs to adjust also the proportion of the metastable state.

Since we did not wish to make such speculations, we used the known oscillator strengths for electronic excitations from Goldbach *et al.* [338] that pertain to the $\mathrm{N} \to \mathrm{N}^+(^3P)$ channel:

$$\text{OOS completion for N} : f(\mathrm{N} \to \mathrm{N}^+(^3P)) = 1.8 - 0.373 = 1.427 \ ,$$

and ionisation from the $2s$ orbital:

$$\text{OOS completion for N} : f(\mathrm{N} \to \mathrm{N}^+(2s\,2p^3) = 2 - 0.085 = 1.915 \ ,$$

From there, the $Q = N_\mathrm{i}/N$ parameter of the RBEQ* was derived straightforwardly (see explanatory paragraph on page 490).

15.2 Instructions for use

There are essentially two perspectives in which we anticipate our database can be used:

1. Opaque : As input data to electron swarm calculations at moderate to high electric fields.
2. Transparent : As a basis data for future investigation on electron-molecule interaction.

These objectives reflect those of part I and part II of the thesis.

15.2.1 Opaque : pragmatic

If you are looking for raw numerical data of cross sections to be plugged into a kinetic solver or a basic Monte Carlo code, we provide a file available on:

`https://doi.org/10.5281/zenodo.8192503`

which respects the input format of the standard two-term solver BOLSIG+. We advise the users to use a log-log interpolation of the energy and cross sections as explained on p.111, particularly at high energies.

Elastic differential cross sections (DCS) are to be found in separate folders (one per target molecule) at:

`https://doi.org/10.5281/zenodo.8190461`

which also includes our own reading module written in Python for parsing cross sections and differential cross sections in various formats. The interpolation of DCS can in principle be bilinear, nonetheless, we prefer the following scheme:

$$\begin{aligned}\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}(\theta) = &\frac{(S[i,j](x-x[i+1])(y-y[j+1]) + S[i+1,j+1](x-x[i])(y-y[i]))}{(x[i+1]-x[i])(y[j+1]-y[j])}\\ &-\frac{(S[i+1,j](x-x[i])(y-y[j+1]) + S[i,j+1](x-x[i+1])(y-y[j]))}{(x[i+1]-x[i])(y[j+1]-y[j])}\ ;\\ &\text{with } \begin{cases} S[i,j] = \dfrac{\mathrm{d}\sigma}{\mathrm{d}\Omega}(\varepsilon[i],\theta[j])\ ,\\ x[i] = \log(\varepsilon[i])\ ,\\ y[j] = \sin\dfrac{\theta[j]}{2}\ ,\end{cases}\end{aligned}$$

which is a bilinear interpolation in transformed spaces of the electron energy (logarithmic) and scattering angle (sine).

A more robust reader also written in Python, but only for integral cross sections, is included in the package `bolos` (`https://github.com/aluque/bolos`) authored by Alejandro Luque, the director of this thesis.

We list below some important points:

Extrapolation: Cross sections of inelastic processes are typically tabulated up to 1 keV. For extrapolation, you will have to use the analytical formulae given in chapter 11.

Scattering: Electron scattering beyond 10 keV can be safely sampled analytically from the inverse of a single screened Rutherford expression (3.11) on page 94 using the average decay radius $\bar{a}$ tabulated in table 11.4 on page 405.

Rotational Excitations: A common issue for molecules, is to distinguish purely elastic (non-rotational) losses from rotational excitations. The sum total cross section of rotational excitations $J_0 \to J$ varies with the temperature of the gas, because the proportion population of initial rotational states at J_0 changes according to the Boltzmann distribution (see appendix B.2 in part I). The problem is that "elastic" momentum-transfer cross sections are determined experimentally at a given temperature and comprise actually both elastic and rotational losses. They are more formally called "vibrationally elastic" cross sections.

In solvers like BOLSIG+, if you give as input both state-to-state rotational excitations and the elastic momentum-transfer cross section σ_m, there will be a discrepancy because momentum losses will be overestimated due to being counted twice. The solution is to provide an "effective" momentum-transfer cross section which is the sum of σ_m and all inelastic CS. Then, at each gas temperature, the rotational cross sections will be subtracted from the "effective" CS and the remaining CS will determine the momentum-losses which are purely due to elastic scattering.

Thus, for each molecule, we provide an "effective" momentum-transfer cross section that should be used in BOLSIG+. The elastic σ_m is given but in comments.

Resonances: In very narrow resonant scattering, the duration of the collision may have a visible impact on the transport parameters. This is why accurate vibrational cross sections do not entail accurate modelling of electron transport if this "temporal period of attachment" is not considered. We did not investigate this effect in this thesis, but we surmise it should be important in O_2 and NO but negligible in N_2.

In that case, paradoxically, you might wish to use less accurate cross sections that have been adjusted to transport parameters for your needs. Ours have not been adjusted.

Inelastic Losses: The exact position of the energy thresholds for electronic excitations is relatively unimportant compared to the magnitude of the cross section. This is because losses are actually distributions over a discrete band of vibronic states or over a continuum as in molecular oxygen. Ionisation losses are typically underestimated as well, because partial ionisation to excited ionic states may be significantly above the ionisation threshold, albeit the cross section is also much smaller than ionisation to the ground ionic state.

If you are unsatisfied with the accuracy of the cross section database, consider first adjusting the energy threshold of each electronic excitation to the centroid of the vibronic band or continuum.

We did this already for molecular oxygen which makes a significant difference when setting the loss in the Herzberg pseudo-continuum at 6 eV (true threshold is around 4.5 eV) and the Schumann-Runge continuum at 8.1 eV (threshold would be below 7 eV).

In short: tweak the energy loss, not the cross section magnitude.

Atomic oxygen: Oxygen's ground state is split in fine-structure spectroscopy into three very low-lying states: $^3P_2$, $^3P_1$ and $^3P_0$ (separated by some ~20 meV). This is above but still comparable to gaps between rotational states of diatomic molecules. Since oxygen in atomic form appears in gases at high temperatures, oxygen atoms in plasmas must be distributed over their fine-structure states.

From a purely computational perspective, these states may be treated in a kinetic solver just as rotational excitations of molecules, so that their abundance ratio be adjusted according to the temperature. In our database, they are labelled as "ROTATION" (obviously they are electronic excitations). Thus, please do not let yourself be surprised when you check the list of collision types for atomic oxygen.

15.2.2 Transparent : scientific

If you are interested in our cross sections for scientific investigation, in order to improve their accuracy, we recommend you to download the `elmolcs` package on CodeBerg*:

`https://codeberg.org/aschmalz/elmolcs.git`

or the frozen version hosted on a DOI server: `https://doi.org/10.5281/zenodo.8190461`.

With the reader module that we provided, use the routines `loadCS` and `loadDCS` for loading cross section (CS) and differential cross section (DCS) databases respectively.

To load our CS database, use:

```
>>> cs = loadCS('N2','iaa*')
```

and replace `'N2'` by O2, NO, Ar, O or N for other targets. This will load all the analytical fits to electronic excitations and the RBEQ* model for impact ionisation from the `cscoll` module. The `cs` object is a dictionary of cross sections classified according to their collision type:

- `'TOTAL'` : total scattering (integral)
- `'ELASTIC'` : integral and momentum-transfer
- `'EXCITATION'` : only electronic and dissociation

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[*] CodeBerg is an open-source platform for hosting projects, not owned by a private organisation. Feel free to visit it at `https://docs.codeberg.org/getting-started/what-is-codeberg/`

- `'VIBRATIONAL'` : only $v = 0 \rightarrow v' < 4$ transitions
- `'ROTATIONAL'` : elementary $J_0 = 0 \rightarrow J'$ transitions
- `'ATTACHMENT'` : only dissociative attachment
- `'IONIZATION'` : total impact ionisation

To save space, we did not include two copies of our full set of numerical cross sections. For rotational and vibrational cross sections, this means that if you want access to the full numerical values of the CS, you should load:

```
>>> cs = loadCS('N2','iaa')
```

which loads CS from the file presented in the previous section 15.2.1. This is because:

i) Rotational CS are constructed from elementary transitions ($J_0 = 0 \rightarrow J'$) using the sudden-impulse approximation (sec.11.2.2).

ii) Vibrational CS are constructed from the theoretical calculations of Laporta *et al.* [552, 553] which are stored in voluminous files describing rovibrational transitions $J_0, v_0 \rightarrow J', v'$. We decided not to include those files nor the routines to read and process them.

In addition to our database, we provide all the resources from other databases and experiments that we used in our investigation. To load them, replace the `'iaa*'` argument above by any of:

Databases hosted on LXCat

- `'phelps'` : Phelps' database
- `'biagi'` : Biagi's database
- `'ist'` : IST-Lisbon [22]
- `'itikawa'` : Itikawa's reviews (only molecules)
- `'hayashi'` : Hayashi database (only Ar and NO)
- `'flinders'` : Flinders database (only molecules)
- `'bsr'` : BSR database [1000] (only atoms)
- `'muroran'` : from Kawaguchi *et al.* [482] (N_2 only)

Collected experimental data

- `'total'` : Total scattering and ionisation CS
- `'elastic'` : Elastic integral and momentum-transfer CS
- `'excitation'` : Electronic excitations mostly
- `'vib'` : vibrational excitations for O_2 only
- `'rotational'` : Theoretical rotational excitations for N_2 only

If you wish to compare and handle a large database of cross sections together, you can use the `CS_Data` object in the following way:

```
>>> csdata = CS_Data()
>>> csdata.add_database('O2','total')
>>> csdata.add_database('Ar',['hayashi','excitation'])
>>> csdata.add_database(['N2','NO'],'itikawa')
>>> selection,errors = csdata.select(['N2','O2'],['itikawa','Szmytkowski'])
```

This will output two `DataFrame` objects from the `pandas` package, one for the values of the cross sections for the selected criteria (target, source), and the associated uncertainties. All our plots for cross sections were generated using this selection routine.

For differential cross sections, call the routine:

```
>>> dcs,_ = loadDCS('N2','iaa')
```

This will load a `DCS_Data` object in the `dcs` variable of elastic scattering from our database.

As for integral CS, we also made an extensive tabulation of experimental DCS for elastic and inelastic scattering. To access them, call:

```
>>> elast,inel = loadDCS('N2','exp')
```

Elastic DCS (`elast`) are distinguished from all inelastic processes stored in a dictionary of `DCS_Data` objects (`inel`) mapped by keys of the final excitation state of the process. All our DCS were plotted using the `DCS_Data` objects, which stores two `DataFrames`:

```
>>> dcs = elast.data
>>> err = elast.error
```

representing the DCS values and uncertainties respectively on an angle-by-energy array (angles on rows, energies on columns).

Minimal bibliographic information accompanies the data loaded by our routines. If you want to retrieve the original articles, you may either: (1) search for the article (and its DOI link) in the `references.bib` file provided (using a reference management program) or (2) peek into the source files classified in the `Data` folder according to the gas target.

The files are relatively easy to read and contain headers with full bibliographic information and DOI links to the articles. There, you will also find more detailed comments about how cross sections were adapted from experimental data in a given energy range.

If our database receives positive and enthusiastic feedback, we hope to be able to incorporate it to the LXCat server.

Chapter 16

Comparison with Previous Databases

> *"The manipulation of cross-section sets weakens the predictive power of the simulation technique because of its arbitrary nature."*
>
> *— Blevin&co-workers as reported by* Brunger & Teubner*, 1990, Phys Rev A:41-1425*

In the previous chapter we introduced our database of cross sections, overviewed how it has been constructed and gave instructions on how to use it. Here, we are only interested in comparing databases, the creation of which requires a tremendous amount of effort. We make two types of comparisons:

- Direct comparison of cross sections with selected experimental measurements based on our own judgement.

- Comparison of electron transport parameters calculated by the two-term Boltzmann kinetic solver BOLSIG+ [378] which we introduced in part I section 4.3.2 on page 4.3.2.

We do not compare differential cross sections (DCS) because currently, there does exist any proper database of DCS. At best, there are collections of experimental and theoretical data, but no attempt to make a full description of scattering throughout a large scale of electron energies. The consistent modelling of DCS in Monte Carlo simulations is left to the discretion of each author. Instead, in the next chapter 14, we dress a catalogue of analytical DCS expressions based on the first Born approximation to model elastic scattering at high energies.

Most databases presented are hosted by the outstandingly useful LXCat server [732]. Nevertheless, its main focus is for *kinetic solvers* rather than Monte Carlo simulations. As a result, we believe that addition of other databases might significantly enhance the scope of the LXCat project.

A noteworthy example is the cross section set proposed by Kawaguchi *et al.* [482] which we refer to as the `Muroran`[*] database. Its wealthy collection of references prompted us to conduct our own independent assemblage of cross sections (from primary sources), which we described in chapter 11, only to be compared in the forthcoming sections.

Separate from and complementary to the LXCat server is the (Japanese) National Institute for Fusion Science: NIFS [682] which compiles a very wide set of measurements, calculations and evaluations of cross sections for atoms (AMDIS) and molecules (AMOL). The NIFS also hosts the most complete compilation work of collision cross sections between electrons and atoms or molecules which was conducted by Hayashi at the beginning on the new century. This colossal work regroups all the bibliographic references for 17 atoms and 51 molecules from 1906, i.e. since the discovery of the electron, to the beginning of the 21st century. Those reports are available

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[*] It is an unofficial name, we call it thus because the authors are all affiliated to the Muroran institute of technology.

at `http://dpc.nifs.ac.jp/hayashi/`. Furthermore, Hayashi also prepared some recommended sets of cross sections [387] for noble gases, four diatomic molecules and CO_2 readily available as input into Boltzmann solvers or Monte-Carlo codes. Some of them are available on LXCat, whereas others are hosted by the Institute of Electrical Engineers of Japan and are available to download at `http://dpc.nifs.ac.jp/DB/IEEJ/`. Some recommendations have been updated since then.

The rest of this chapter is structured in six sections dedicated to the six atmospheric gas species studied. Comparisons of cross sections and transport parameters are preceded by an introduction and overview of the selected databases.

16.1 N_2

As the most prominent diatomic molecule in atmospheric physics, the database for nitrogen is lush and numerous reviews were published especially in the early 2000. A compilation of cross sections was released as early as 1966 by Takayanagi and Takahashi as cited in Itikawa's 1986 seminal review [436].

Today, a vast number of databases are available on LXCat. They are, however, not all independent works and a certain lineage can be established by looking at table 16.1. We offer a short description of each database below.

`Phelps` The most ancestral database (on LXCat) is the one from Phelps and Pitchford [749] and retranscribed from the JILA report [750]. Some databases (not shown) are direct copies of this data. The CS were adapted from available experimental and theoretical results in order to bring the transport coefficients of the two-term Boltzmann kinetic approach into agreement with experimental data. At low energies $< 7\,\text{eV}$, (elastic) momentum-transfer cross sections are derived from swarm experiments [266]. At higher energies, elastic scattering is derived from integrated DCS of beam experiments. They also derive the integral elastic CS and the average deviation cosine (11.12). Rotational excitations are modelled according to the single-level approximation described in the appendix of Hake and Phelps [381]. Vibrational and electronic excitations from a variety of sources [159, 740, 819] were adjusted so as to yield reaction coefficients in agreement with experimental results.

`IST-Lisbon` We could say that the direct successor of `Phelps` database is the `IST-Lisbon` database whose main differences are (i) interpolation on a finer grid of values, (ii) update of the ionisation cross section with partial ionisation cross section from Isola *et al.* [433] and (iii) extension with a rotational set of quadrupole transition ($\Delta J = 2$) cross sections from Gerjuoy and Stein [323].

`Biagi` This is the most obscure database as it is the least documented of all. There is no publication associated to it and no reference specific to any of the processes included. Its origin comes from the Fortran program of Stephen Biagi [71] called MAGBOLTZ hosted by the CERN. Most probably, it is based on the `Phelps` database, albeit with notable differences.

`Itikawa` Very well documented in Itikawa *et al.* [436] and Itikawa [439] and mostly based on the massive compilation of cross sections in 2003 [434] where Itikawa was the editor. This is the only database on LXCat which has not been adjusted in order to yield good results for the transport parameters calculated by a two-term Boltzmann kinetic solver. When using with BOLSIG+, one needs to ensure to subtract predissociation from the total dissociation cross section.

`Flinders` Comprises only vibrational and electronic excitations as measured by the research group in Flinders' University Campbell *et al.* [141, 142]

`Tabata` Analytical fits by Tabata *et al.* [902], to experimental data mainly from the reviews of Itikawa *et al.* [436] and Majeed and Strickland [620] and the data from Campbell *et al.* [141] as in the `Flinders` database.

`Laporta` Vibrational cross sections exclusively from the N_2^- ($X\,^2\Pi_g$) resonant state using accurate local-complex-potential calculations as published in Laporta *et al.* [554].

`Muroran` Most recently published database in Kawaguchi *et al.* [482] which proposes new fits to the latest experimental studies [463, 622, 624]. It incorporates the calculations of Laporta *et al.* [554] as well.

We owe the authors of this publication the discovery of the most recent references relevant to the cross sections with nitrogen molecules. Our work brings an update to their contribution.

To-date, the databases which give swarm transport parameters most in accord with experimental measurements are the `IST-Lisbon` from Loureiro and Ferreira [609] and the `Muroran` from Kawaguchi *et al.* [482]. The comparison was done in part I, section 4.3.3. It is therefore, very instructive, albeit exhausting, to compare how cross sections sets may differ yet give similar transport parameters when used in a two-term Boltzmann kinetic solver (see p. 81 and sec. 4.3.2).

Comparisons

Using the renormalised data when applicable (all preceded by an asterisk when labelled in legends as : " *Zubek "), we now display comparisons of cross section sets against experimental measurements. At the very end, in figure 16.5, we compare the transport coefficients obtained for each (complete) database when used by the two-term kinetic solver BOLSIG+ [378].

Elastic CS fig. 16.1

1. At very low energies < 0.1 eV, we both need to improve the momentum-transfer cross section given from the MERT method (see sec.10.1.5) and use swarm-derived measurements such as Haddad [374].

2. In the N_2^- $^2\Pi_g$ resonance region ($2\,\text{eV} < \varepsilon < 4\,\text{eV}$), the "`Muroran`" momentum-transfer CS has been scaled upward [482, p.4] so as to closely match the electron-drift experimental measurements in the 1—100 Td region.

3. At intermediate energies above the N_2^- $^2\Pi_g$ resonance region ($4\,\text{eV} < \varepsilon < 15\,\text{eV}$), there are two classes of measurements, those of Shyn and Carignan [838] and Srivastava *et al.* [870] of higher momentum-transfer and the more recent from Linert and Zubek [600] about 10–20 % lower. The databases tend to either follow one set or the other with a crossing point at 15 eV where the trends revert (overestimate $\rightleftharpoons$ underestimate).

Table 16.1: Databases of electron collision cross sections with molecular nitrogen. First half represents the ones hosted on LXCat, the second half are incomplete or separate databases. Names in quotes are unofficial denominations. In the columns we regroup the references to the experimental data upon which the database are constructed. If it exists, the reference to the publication which describes each database is under the column "Origin".

Database	Year	Origin	Total	Elastic	Vibrational	Electronic	Ionisation
IAA (Present)	2023	11	[124, 317, 488, 512, 699, 894, 900]	[344, 600, 684, 700, 832, 863, 894]	[554, 600, 863, 910]	[123, 407, 463, 622, 624, 1012]	[768, 831, 888]
Phelps	1985	[749]	[266]	[113, 288, 453, 838, 870]	[819]	[159, 1011]	[768, 814]
Itikawa	2006	[436, 439]	[478, 488, 699, 894]	[105, 232, 832, 838, 863, 870, 894]	[105, 863, 894, 910]	[123, 141, 289, 333, 633, 757, 941, 1013]	[768, 888]
Biagi	2012						
IST-Lisbon	2014	[22]	[749]		[609, 819]	[159, 1011]	[433, 768]
Flinders	2001-4				[142]	[141]	
"Tabata"	2006	[902]	[105, 316, 405, 699, 705]	[105, 436, 832]	[436]	[9, 123, 159, 289, 452, 1012]	[768, 888, 932]
Laporta	2014	[554]					
"Muroran"	2021	[482]	[512]	[232, 600, 684, 838, 863, 870, 894]	[554, 600, 863, 910]	[141, 407, 463, 622, 624]	[888]

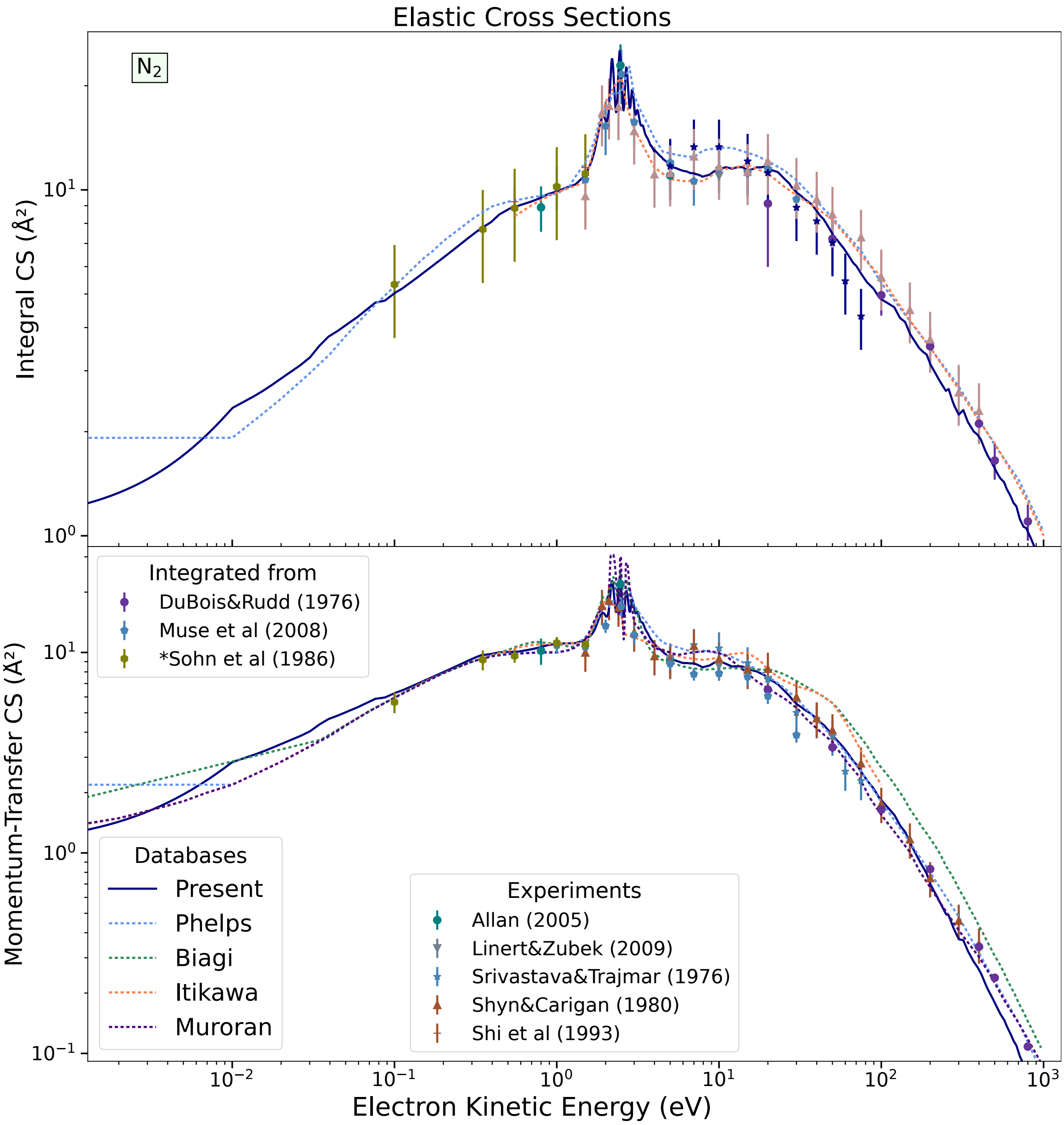

Figure 16.1: Comparison of elastic integral and momentum-transfer cross sections for molecular nitrogen.

Inelastic CS fig. 16.2

- Vibrational CS : $\sum_{v'} \sigma_{v=0\to v'}$

  1. First resonance $^2\Pi_g$ 2–4 eV: similar for all databases except Itikawa [439], who purposefully recommended only the $v = 0 \to 1$ transition, since updated experimental data for all other transitions is missing.
  2. Second resonance $^2\Sigma_u^+$ $\sim$23 eV [600, p.6] (broad shape resonance): two sets of measurements, the former from Tanaka *et al.* [910] and more recent from Linert and Zubek [600], explain the difference between our and other databases.
  3. Outside resonances: databases manage the CS differently. Some use linear-linear interpolation which creates the skipping aspect of the pink ··· and green ··· dotted curves on figure 16.2-top; when a database uses linear interpolation instead of logarithmic (power-law) interpolation to between sparse data points.

- Electronic CS : $\sum_{a'} \sigma_{0\to a'}$

  △ Resonance peaks of spin-forbidden transitions < 12 eV : most databases have higher peaks near threshold, in particular `Flinders` and `Itikawa` (orange ··· and beige ··· dotted curves on fig 16.2-bottom) because they follow Campbell *et al.*'s [145] measurements as seen on the individual electronic CS in figure 16.3.

  △ Missing tail : at energies above 30 eV our incomplete cross sections (- - -) are systematically below the others. We did include the residual dissociation CS $\sigma_{\rm rd}$ obtained from eq. (11.65); i.e. fitted to the data of Cosby [193] after subtracting all contributions from predissociation (see p. 445). Notwithstanding, the uncertainty on the total dissociation into neutral products is large as seen from the error bars on fig. 16.2-bottom. Also, our incomplete (- - -) CS intersects with the total dissociation CS at the last measurement at 200 eV, which should not be the case since some excitations do not lead to dissociation.

  This missing tail is the reason why we decided to patch our database with the remaining difference to "`Muroran`" curve (purple dotted ···) from Kawaguchi *et al.* [482].

Electronic CS fig. 16.3

1. In general, the measurements of Campbell *et al.* [145] (comprised in the `Flinders` database) tend toward indicating the presence of tall peaks of dipole- and spin-forbidden transitions near threshold. Most databases try to follow those peaks, except ours which used resonance profiles only for well-resolved measurements as, for example, from Zubek [1012] for the C $^3\Pi_u$ state (fig. 13.8).

2. The high-energy decaying tail is not well constrained in any of the databases, except in ours (from the imposed integer d in (11.61) determining the $\sim 1/\varepsilon^d$ decay) and in `Muroran` [482]. This has however no observable effect on the swarm transport coefficients.

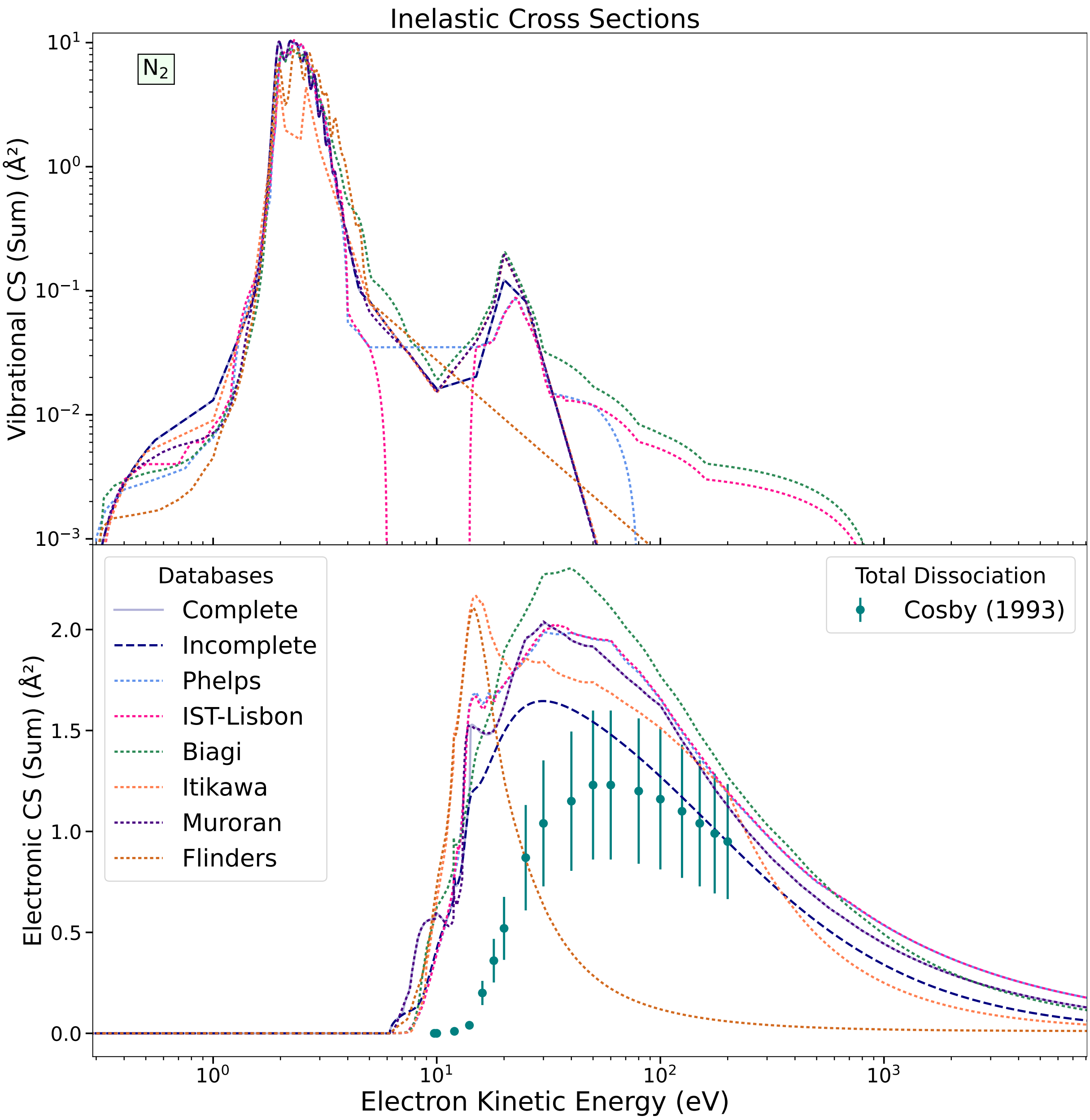

Figure 16.2: Comparison of the sum of vibrational and electronic impact excitation cross sections for molecular nitrogen. The "Complete" curve is superposed with the dotted purple curve labelled "Muroran".

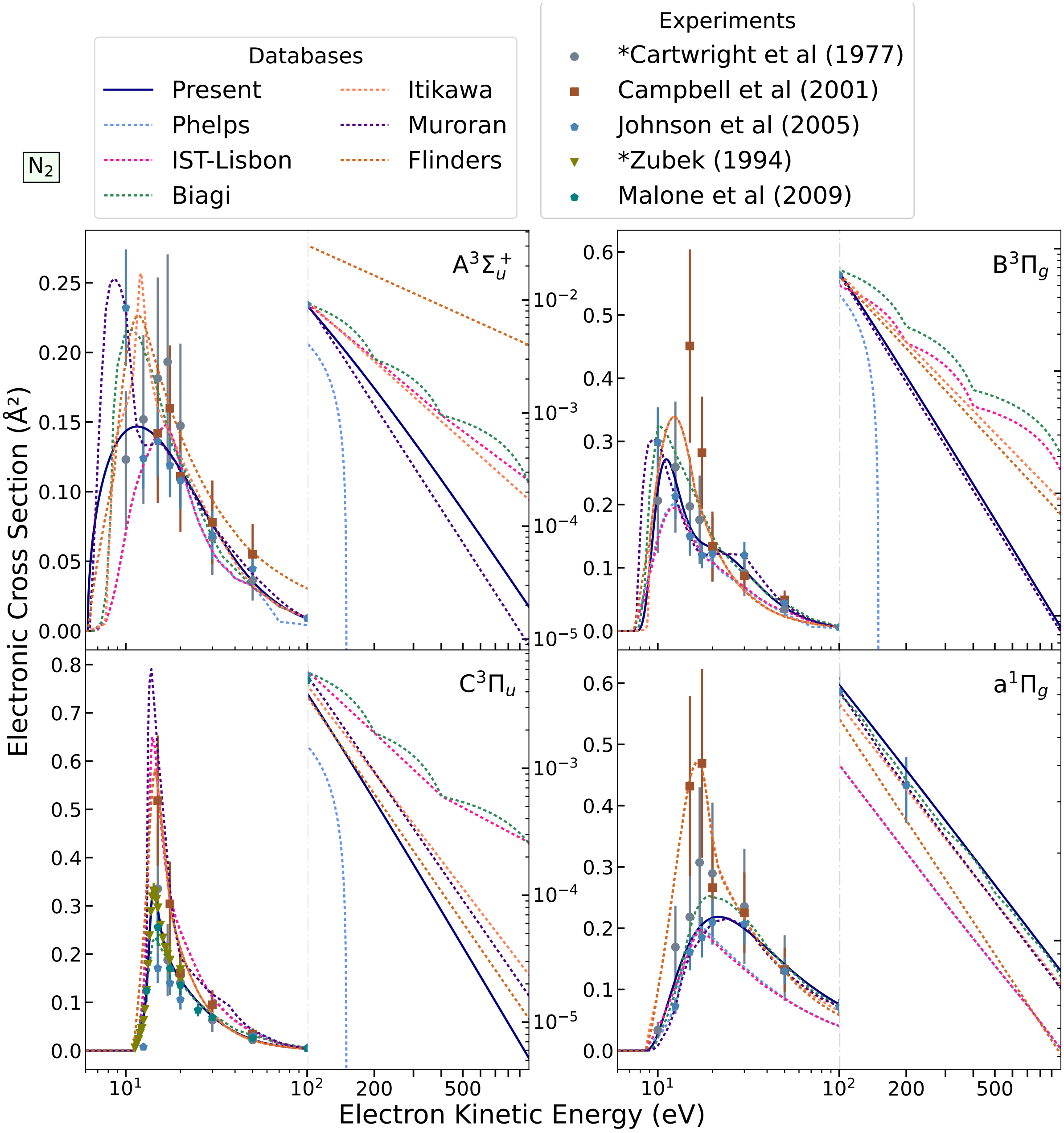

Figure 16.3: Comparison of selected electronic impact excitation cross sections for molecular nitrogen.

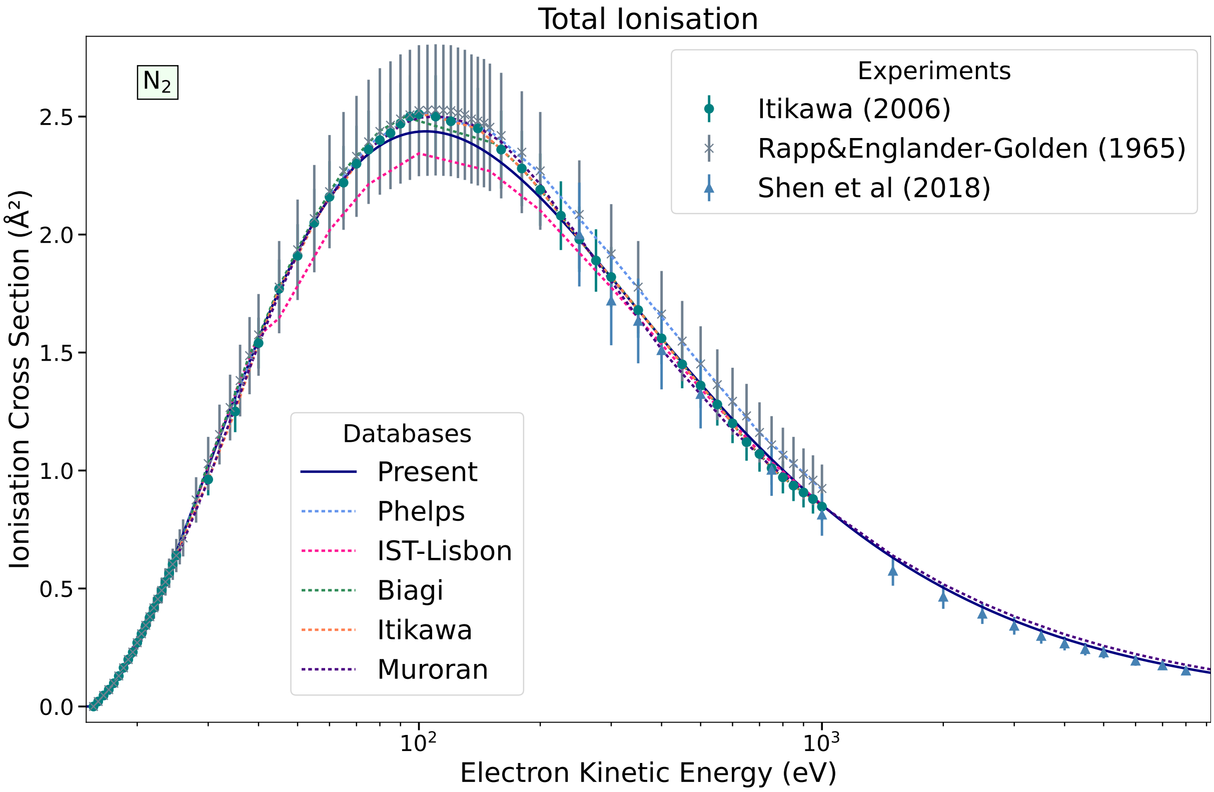

Figure 16.4: Comparison of impact ionisation cross sections for molecular nitrogen.

Ionisation CS fig. 16.4

- All databases follow the measurements of Rapp and Englander-Golden [768] below 50 eV and the values of Straub *et al.* [888] (renormalised in Lindsay and Mangan [596]) at higher energies.
- Our analytical RBEQ* fit misses about ~3 % on the peak.
- The data of `IST-Lisbon` [433] are surprisingly lower than the rest. This is due to retraction of the N_2^+ $B\,^2\Sigma_u^+$ ionic excitation, which is treated separately, but even when included, does not sum to the total ionisation.

Transport Coefficients fig. 16.5

- Below < 2 Td : Transport is dominated by rotational excitation. Both sets of Gerjuoy and Stein [323] in `IST-Lisbon` and of Kutz and Meyer [546] in our `IAA` database bring mobility into accord with experiments. For diffusion in particular, the set in our database gives more accurate results. The influence of rotational cross sections on transport in N_2 was elaborated in Ridenti *et al.* [774].

  Note that the comparison with `Muroran` is not fair because we did not include the rotational set. Nevertheless, the results are practically identical to `IST-Lisbon` below 0.5 Td so that the difference between `IST-Lisbon` (---) and `Muroran` (---) highlights the importance of rotational excitations.

- Between 0.6–6 Td : we predict a mobility about 10 % higher than most experiments (except Pack and Phelps [727] which is lying above). This difference is hard to explain but we surmise that it is because our elastic MTCS is lower than for other databases in the energy region 0.1–1 eV surrounding the characteristic energy $\langle\varepsilon\rangle$ and especially at the onset of the resonance region at 1.5 eV. Part of this difference could also be due to rotational excitations but this does would affect only values below ~ 5 Td. `Muroran` has an even lower elastic CS, but then compensates with a MTCS scaled upwards in the resonance region. Given the very close similarity of our `IAA` database with `Muroran`, we attribute our overestimation of the mobility to an underestimation of momentum loss in particular in the resonance region.

- Between 5–100 Td : The average electron kinetic energy $\langle\varepsilon\rangle$ is nearing toward the N_2 $^2\Pi_g$ resonance region. The separation of `Itikawa` transport curves is due to the absence of vibrational excitations higher than the $v = 0 \to 1$ transition in that set.

- α_i : Ionisation coefficient in decreasing order `IAA`>`Muroran`> `IST-Lisbon`> `Phelps`> `Itikawa`. `Biagi` crosses from first to last as the electric intensifies. This is explained by a late but higher loss of energy in electronic excitations (fig. 16.2). `Itikawa`'s lowest α_i is due, on the contrary, to an early peaked electronic inelastic CS (at lower energies).

16.2 O_2

In comparison to N_2, molecular oxygen is much less studied. As a reactive gas, it is difficult to make accurate measurements. An early review of cross sections was done, again, by Itikawa *et al.* [438] and updated two decades later [440].

Because of its high electron affinity (see sec. 11.3, fig. 11.18), the electron interaction with O_2 at low sub-eV energies is sprouted with a series of sharp narrow and very tall resonance peaks from the $O_2^-(X\,^2\Pi_g)$ symmetry (fig. 11.25). Proper visualisation of those peaks require precise and highly resolved measurements which became possible only recently [128, 714].

Those peaks seem to be better characterised now. Nonetheless, according to the most recent survey of Szmytkowski and Możejko [901, fig. 4], there is an ongoing "disaccord" of measurements beyond 1 eV in the total scattering cross section.

An overview of the principal databases for O_2 is laid out in table 16.2, for each of which we give an individual description below.

`Phelps` This database predates the one for N_2 and was described in the appendix C of Lawton and Phelps [566] and tabulated in Phelps and Pitchford [751]. The elastic momentum-transfer of Hake and Phelps [381] was modified below 1 eV so as to yield good results in agreement with Nelson and Davis [691] at electric fields < 1 Td, together with the single-level approximated rotational cross section at a loss of 20 meV (as for N_2). Three-body attachment cross section are adapted from Spence and Schulz [868] with regular peaks coinciding with the shape resonance of the O_2^- ($^2\Pi_g$) anion. Dissociative attachment was adapted from Schulz [818]. Apart from the two lowest electronic states $a\,^1\Delta_g$ and $b\,^1\Sigma_g^+$, electronic excitations of higher states are grouped into losses at 4.5 eV, 6 eV and 8.4 eV.

`Itikawa` Documented in depth in Itikawa [440] which updates the former review [438]. The cross sections are principally taken from the massive compilation of Itikawa [434]. The major difference with our database is that Itikawa privileged data from Shyn *et al.*'s laboratory [842, 845, 846, 848, 849], whereas we shunned those data due the availability of more recent results and also to Brunger and Buckman's observation in Brunger and Buckman

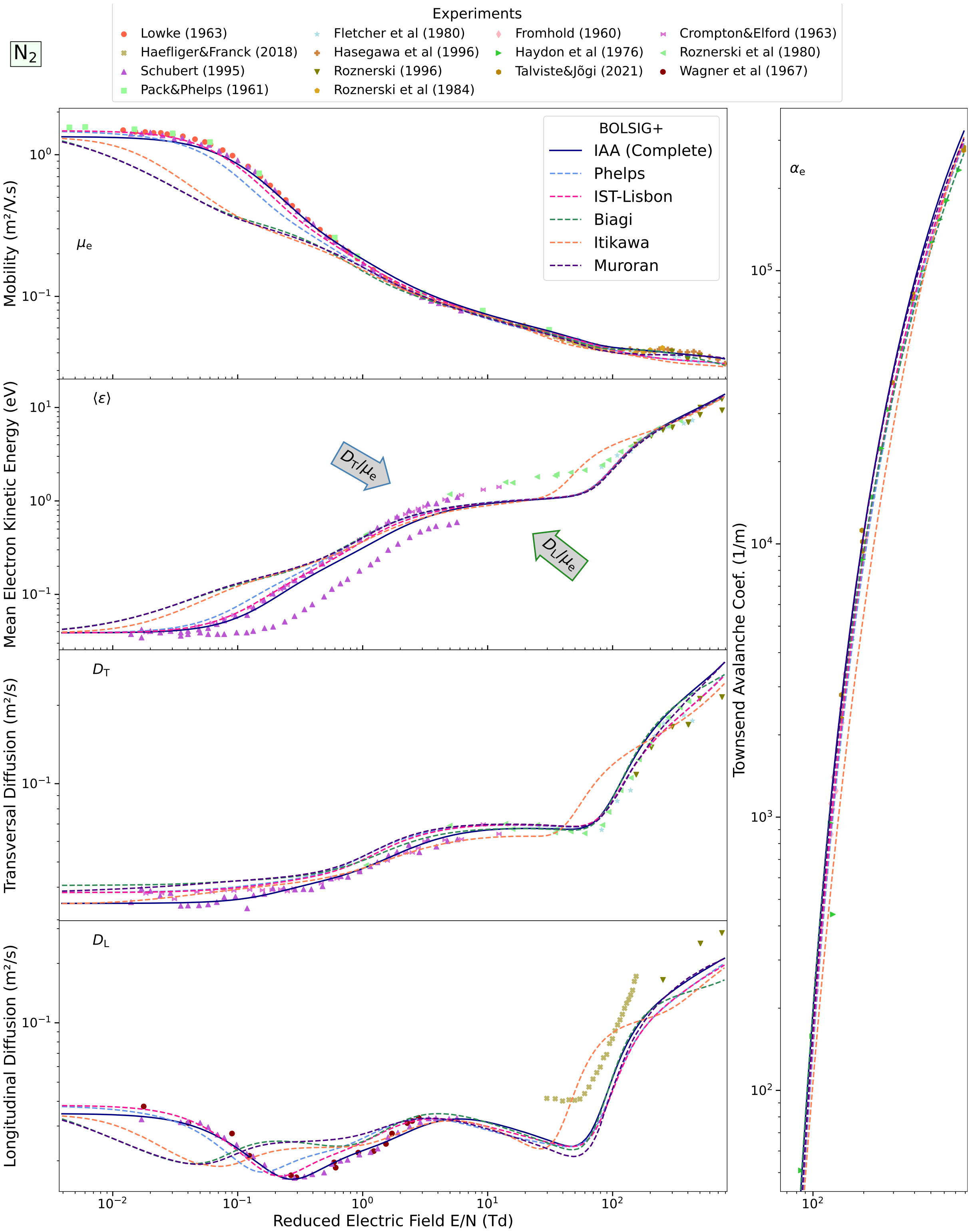

Figure 16.5: Transport coefficients in molecular nitrogen as calculated by BOLSIG+ for different cross section sets and compared with a variety of experimental data.

Table 16.2: Databases of electron collision cross sections with molecular oxygen. Middle rows represent the ones hosted on LXCat, the last rows are incomplete databases. In the columns we regroup the references to the experimental data upon which the database are constructed. If it exists, the reference to the publication which describes each database is under the column "Origin".

Database	Year	Origin	Total	Elastic	Vibrational	Electronic	Ionisation	Attachment
IAA (Present)	2023	11	[207, 315, 477, 714, 900, 1003]	[353, 598, 893]	[552]	[352, 845, 848, 897, 972, 973]	[768, 814, 815, 888]	[558]
Phelps	1978	[566]		[381]	[593, 987]	[593] …	[917]	[818, 868]
Itikawa	2009	[438, 440]	[205, 207, 477, 798, 890, 900, 1003]	[598, 842, 893, 938]	[12, 401, 599, 846]	[845, 848, 849]	[888]	[767]
Biagi	2012							
IST-Lisbon	2016	[24, 346]	same as `Phelps` + 14 eV exc.					
Flinders	2014				[467]	[897]		
Laporta	2013	[552]		[552]	[552]			[558]

[124, p.317]. Careful that the energy thresholds for the longest (LB) and second (2B) as re-transcribed on LXCat should be modified to 9.97 eV and 10.29 eV respectively (instead of put 6.12 eV which is for the Schumann-Runge continuum). Also, do not use the total dissociation cross section when input to BOLSIG+.

`Biagi` See note for N_2 in the previous section 16.1.

`IST-Lisbon` It is practically the same as the `Phelps` database, except that it includes an additional electronic excitations lumped together at a loss of 14 eV as the last table in the report of Phelps and Pitchford [751]. Also, in Alves *et al.* [24], it was extended with a set of rotational cross sections as calculated with the quadrupole Born approximation of Gerjuoy and Stein [323], albeit with a highly contrived value of the quadrupole $Q = 1.4\,\mathrm{e}a_0^3$ which is more than four times the actual value $Q = -0.29$ a.u. reported in Khristenko *et al.* [498, p.81]. This was changed in order to fit closely the transport coefficients of Nelson and Davis [691] at low energies.

`Flinders` Vibrational and electronic excitations as reported in the cross-beam measurements of Jones *et al.* [466] and Suzuki *et al.* [897].

`Laporta` Resonant vibrational excitation and attachment cross sections from local-complex-potential calculations of Laporta *et al.* [552, 558] and used in Laporta *et al.* [559] to estimate vibrational relaxation in oxygen plasmas.

Comparisons

Elastic CS fig. 16.6

1. Very low energies < eV : no data from beam experiments, only swarm data [e.g. 381], though they have been modified in `Phelps` [566, Appendix C:(1)] so as to match transport coefficients from Nelson and Davis [691]. Our values directly result from Okumura *et al.*'s measurements [714] scaled by $1 - \langle \cos\theta \rangle$ from the MERT DCS (cf. fig. 11.1).

   Also, hard to determine is the momentum-transfer CS in the resonance peaks.

2. Low-to-intermediate $1\,\mathrm{eV} < \varepsilon < 30\,\mathrm{eV}$: our momentum-transfer CS and `Itikawa` faithfully meander between the two most trusted results of Linert *et al.* [598] and Sullivan *et al.* [893], whereas the other databases go through a "roller-coaster" of over-then-under-estimations.

3. Intermediate $30\,\mathrm{eV} < \varepsilon < 200\,\mathrm{eV}$: unadjusted angular-momentum close-coupling calculations (see chapter 9). We know from Brunger and Buckman [124, §3.3.2.2:p.317] and our own observations that Shyn and Sharp's results [842] most probably have a systematic error, so that we cannot rely on those. The same is true about Trajmar *et al.* [938] as noted by Lawton and Phelps [566, p.(1065):§C(1)]. Systematic errors could be due to contact potential changes* since O_2 is a reactive gas as Green *et al.* [353] say so in their conclusion.

4. High energies > 200 eV : our CS dashes (accompanied by the hopping `Biagi` CS) between the beam measurements of Daimon *et al.* [206] and Iga *et al.* [418], whereas `IST-Lisbon` and `Phelps` go their own clearly distinct way.

Inelastic CS fig. 16.7

- Vibrational CS : $\sum_{v'} \sigma_{v=0\rightarrow v'}$

  1. First resonance $O_2^-\ {}^2_{\Pi}g < 1.2\,\mathrm{eV}$: our tall skewed peaks come entirely from Laporta *et al.* [552]. Of very important note :

     > The first vibrational resonance peak strongly affects the electron mobility in O_2 between 1—10 Td. Reducing this peak both in our and `Biagi`'s CS would considerably improve agreement with experimental mobilities (see fig. 16.10).

     What about modelling the delay in electrons resonantly scattering from O_2? This could also lower the discrepancy observed in the mobility while keeping the CS intact.

  2. Second broad resonance (mainly ${}^4\Sigma_u^-$) 7—14 eV : we follow theoretical calculations, whereas other databases interpolate experimental measurements [846, 938, 987].
  3. Between resonances 1.2—4 eV : participation of other electronic configurations to the excitation to higher vibrational levels [552, p.6:§5]

- Electronic CS : $\sum_{a'} \sigma_{0\rightarrow a'}$

  △ Schumann-Runge (SR) $\gtrsim 8.6\,\mathrm{eV}$: cliff discontinuity for `IST-Lisbon` and `Phelps` because they do not include losses to the SR below 8.6 eV. Overestimation due to Wakiya [972], see fig. 16.8-left-bottom.

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[*] I am not an experimentalist, so behold my words like an umbrella repelling rain.

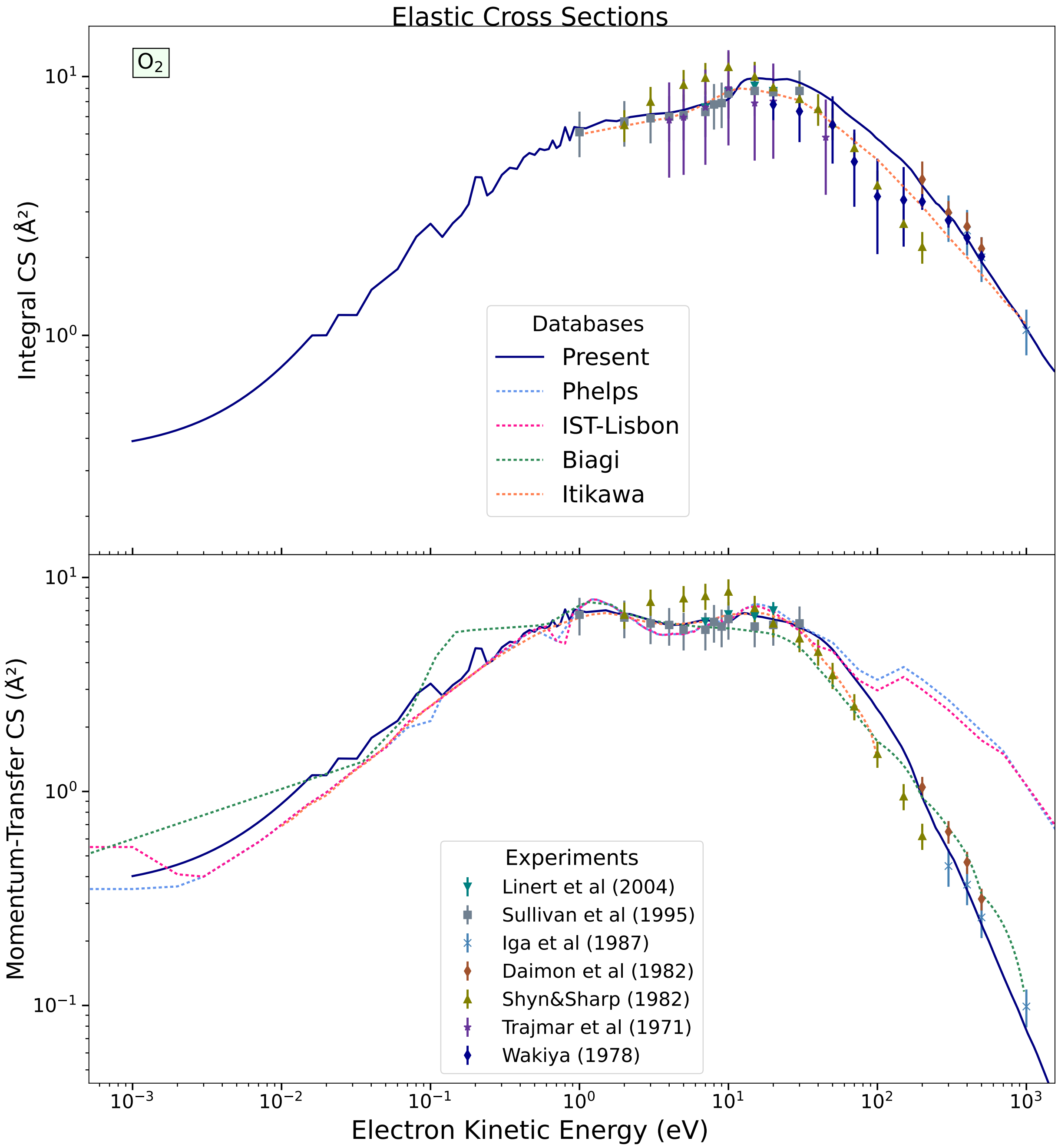

Figure 16.6: Comparison of elastic integral and momentum-transfer cross sections for molecular oxygen.

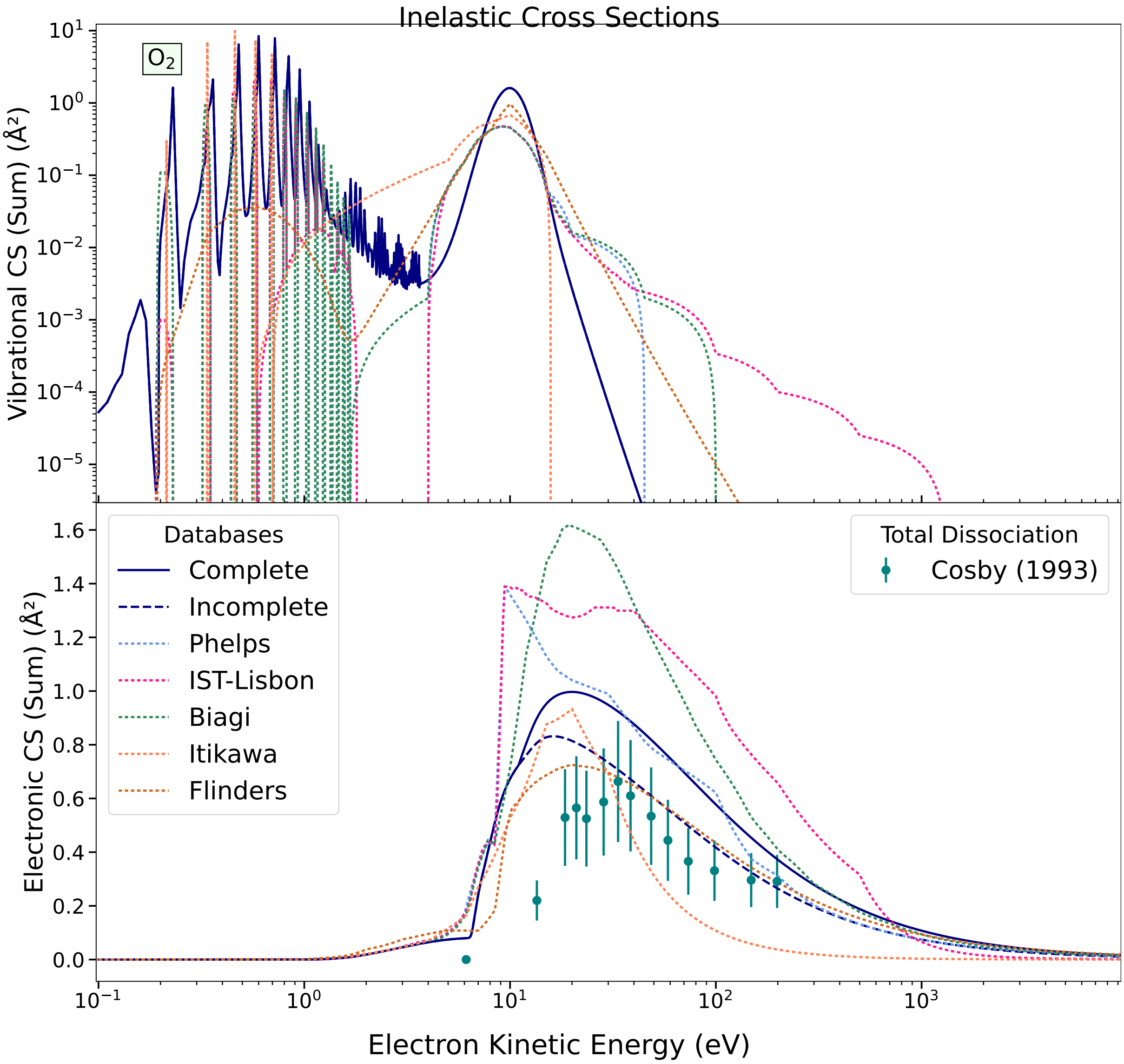

Figure 16.7: Comparison of the sum of vibrational and electronic impact excitation cross sections for molecular oxygen.

△ Losses beyond the SR > 10 eV : Our incomplete CS (---) are complemented with an unknown loss from an optically allowed excitation of $f_o = 0.1$ oscillator strength which increases the total CS to the solid dark blue curve —.

It is very unlikely that the states from the complementary CS would not predissociate. Nevertheless, these losses are not part of the neutral dissociation of Cosby [194]. Therefore, we think that these losses are most probably from *auto-ionising* excitations not comprised in the ionisation RBEQ* model.

`Itikawa`'s database does not provide extrapolation beyond 50 eV (which is why the tail drops at high energies).

Supplementary losses in `IST-Lisbon` and `Biagi` are unreasonably overestimated.

Electronic CS fig. 16.8

1. Forbidden low-lying a$^1\Delta_g$: the peak is sharper than our fit can follow.
2. Herzberg Pseudo-continuum (HC) : `Phelps, IST-Lisbon` and `Biagi` overestimate the peak but underestimate the tail.
3. Schumann-Runge continuum (SR) : Wakiya's results [972] are about twice the values of Suzuki *et al.* [897] and Shyn *et al.* [849], this is the first cause of too high CS of `Phelps, IST-Lisbon` and `Biagi`.
4. Longest and Second bands (LB+2B) : origin of overestimation same as for SR.

Ionisation CS fig. 16.9

- More recent : `Itikawa` and our database following Straub *et al.* [888] and Schram *et al.* [814, 815].
- Older : `Phelps, Biagi` following Rapp and Englander-Golden [768]
- Outlying : `IST-Lisbon` below 200 eV overestimates the ionisation CS for no apparent reason. It is supposed to be identical to the `Phelps` database [346].

Transport Coefficients fig. 16.10

- Three-body Attachment : Only included in `Biagi`'s curve. The effect is high below 20 Td and extreme at any field below 0.7 Td. This effect is only shown for illustration of the importance that three-body attachment has at low electric fields.
- Dissociative Attachment : Our and `Ititkawa`'s CS for dissociative attachment are identical. The differences in the reduced Townsend coefficient $\eta_{\mathrm{a}} = \nu_{\mathrm{a}}/v_{\mathrm{d}}$ for attachment are thus entirely due to the differences in the electron energy distribution function. The same can be said about the ionisation coefficient α_{i}.
- Below < 5 Td : The good matching between `IST-Lisbon` and Nelson and Davis [691] is due to an adjustment of the rotational set of cross sections calculated in the Born approximation setting the quadrupole of O_2 to a value of 1.4 atomic units which is more than 4 times its true value. Our rotational cross sections were calculated with the experimental value $Q = -0.29$ atomic units and are manifestly too small. The adjustment of Q serves as a scaling factor of the rotational CS which are mostly flat. This indicates that rotational scattering off oxygen ought to be strongly enhanced by low-energy resonant scattering, of which a proper study would be highly valued.
- Between 0.5–15 Td : Region dominated by vibrational resonant collisions linked to O_2^- $^2\Pi_g$ (lowest threshold ~20 meV). This can be seen by the glitchy behaviour of `Itikawa` curves (μ_{e} and D_{L}) whose vibrational CS are very sharp and very tall (fig. 16.7–top). The wider the peaks, the smoother the curve is, but the larger the deviation. Our and `Biagi`'s transport coefficients are strongly affected by the resonant vibrational CS which are wider and taller than used in `Phelps` and `IST-Lisbon`.

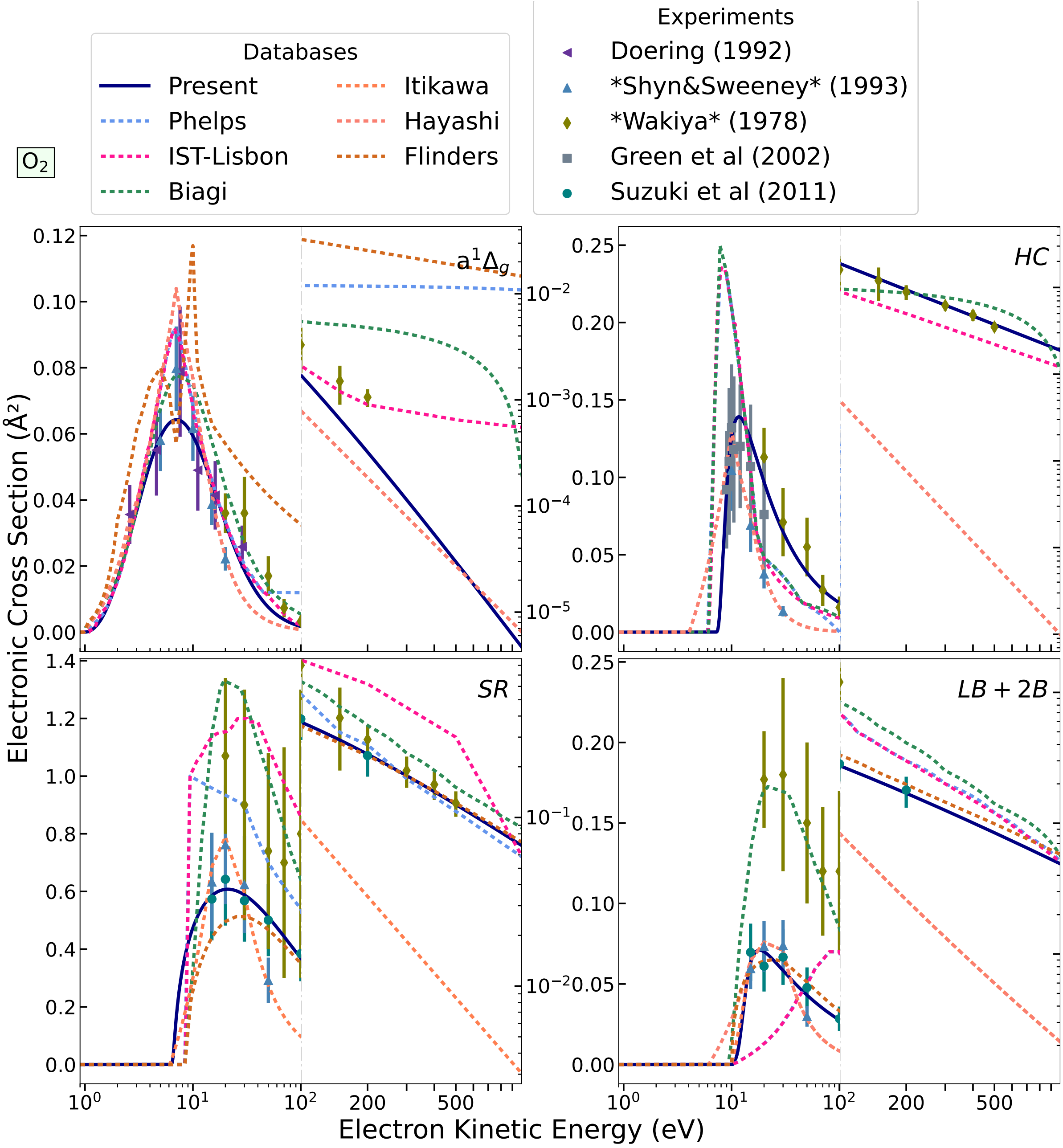

Figure 16.8: Comparison of selected electronic impact excitation cross sections for molecular oxygen.

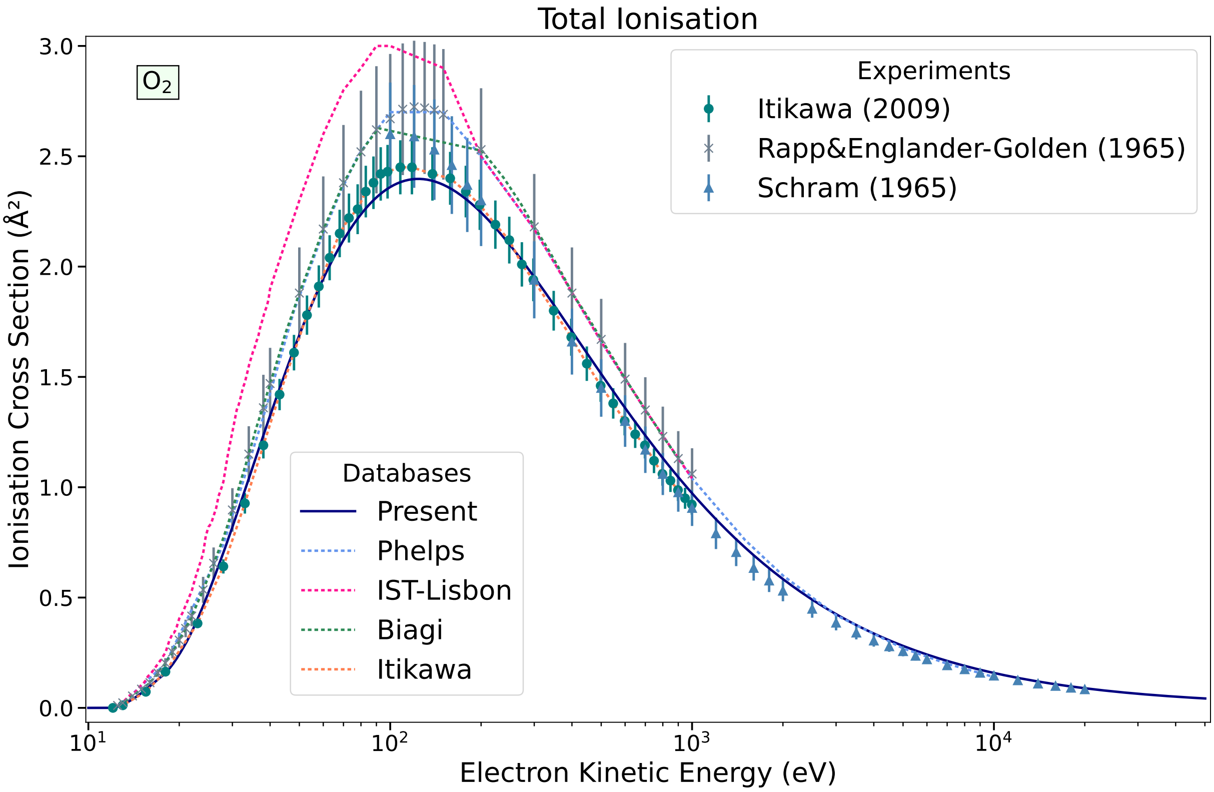

Figure 16.9: Comparison of impact ionisation cross sections for molecular oxygen.

- Above 200 Td lowest inelastic losses in electronic excitations in `Itikawa` (fig. 16.7) explain why transport and ionisation are enhanced at higher electric fields.
- α_i : Ionisation coefficient in the following order : `Itikawa>IAA>Phelps>IST-Lisbon`. `Biagi` crosses through. This can be explained by initially low elastic MTCS (fig. 16.6) and low inelastic CS (fig. 16.7). Then, the ionisation rate decreases as the inelastic losses in electronic excitations rise and peak highest than all other databases.
- `IST-Lisbon` : has the lowest α_i but highest σ_{ion}. This is because it has to compensate for the overestimation of losses in electronic excitations (fig. 16.7).

16.3 NO

Interest in nitric oxide is more recent than for other diatomic molecules since it is absent in the list of recommended CS of Hayashi [387]. In the near past, the interest in studying NO has been spurred due to its presence in auroral emissions from the Earth's ionosphere where it is formed by recombination of nitrogen and oxygen atoms as dissociated products from UV radiation [144]. More recently, it received further attention due to its production in discharges [743], or as a byproduct of fossil fuel combustion, in order to assess its climatological impact.

It has been reviewed twice in recent years. Once by Itikawa [441] which was then extended by Song *et al.* [865] about three nitrogen oxides. Nitric oxide is usually included in studies of electrons scattering off diatomic molecules together with the unmissable hydrogen, nitrogen and oxygen diatomic molecules. [207, 768, 900].

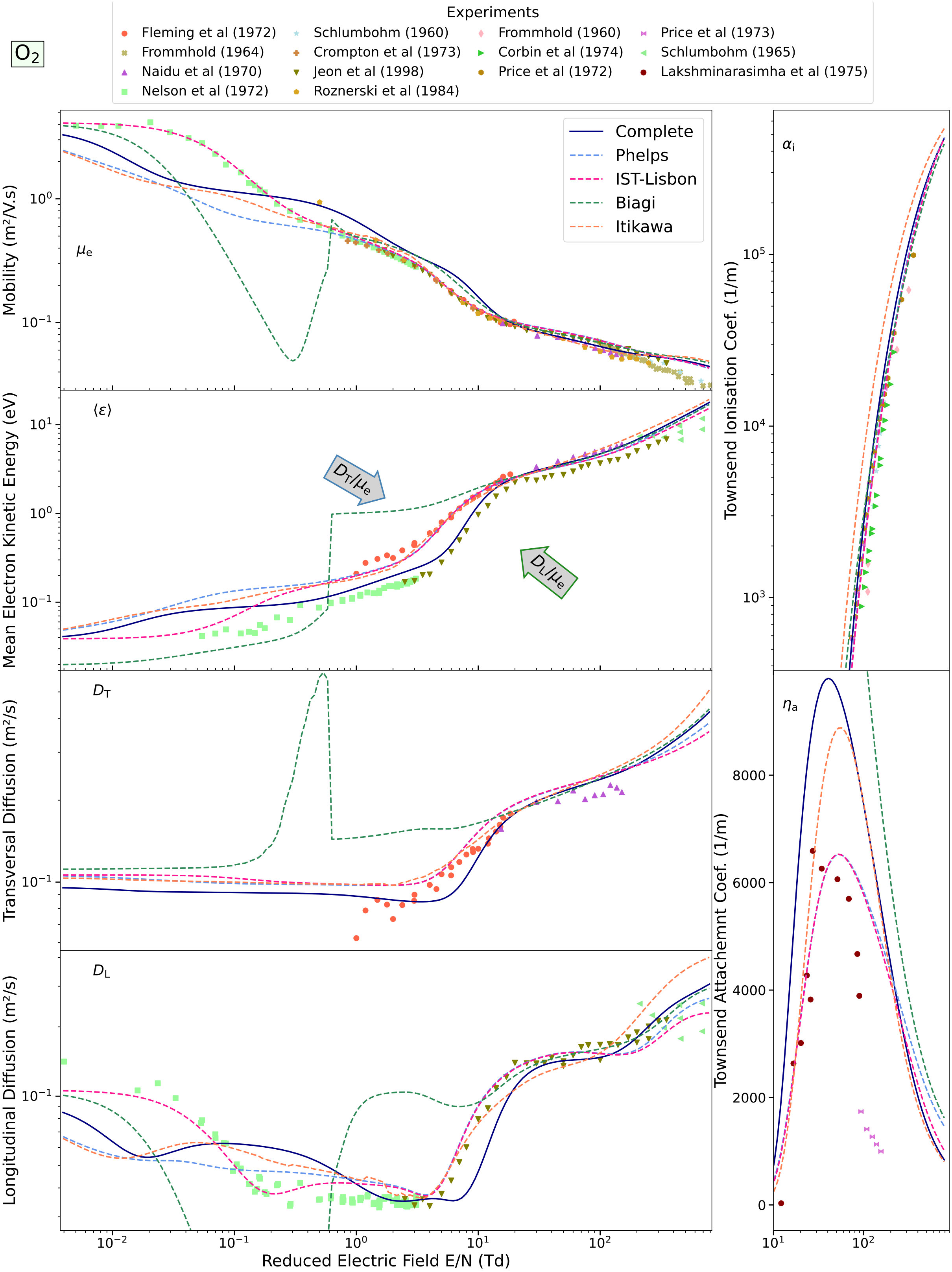

Figure 16.10: Transport coefficients in molecular oxygen as calculated by BOLSIG+ for different cross section sets and compared with a variety of experimental data.

Nevertheless, the database of elastic and inelastic scattering of electrons off NO is nearly reduced to the studies from the group of Brunger *et al.* [120]. In particular, the database of elastic DCS for NO is restricted to the single study of Mojarrabi *et al.* [654]. We could not access the measurements of Kubo *et al.* [541], though they lie roughly in agreement with Mojarrabi *et al.* [654, figs. 2–3]. Also, at low energies below 1.5 eV, there is a strong resonant structure in electron-NO scattering [944, figs. 1–2], which makes the establishment of elastic DCS prohibitive there.

In table 16.3, we offer an overview of current databases of cross sections with NO, which we briefly describe below.

`Phelps` This database seems to be even older than the one from N_2 and O_2. It has been updated only once for its ionisation cross section from Lindsay and Mangan [596, p.5-60]. The documentation regarding the determination of the remaining cross sections is unavailable.

`Hayashi` Database from Hayashi's massive compilation of electron-molecule cross sections. It was privately communicated to the JILA centre.

`Itikawa` From the recent review of Itikawa [441]. The cross sections are principally taken from the massive compilation of Itikawa [434]. For inelastic (vibrational and electronic) excitations, the cross sections are the same as in the `Flinders` database.

`Flinders` Vibrational and electronic excitations as constructed in Campbell *et al.* [144] from the cross-beam measurements of Cartwright *et al.* [157], Jelisavcic *et al.* [456], and Mojarrabi *et al.* [654].

`Laporta` Resonant vibrational excitation and attachment cross sections from local-complex-potential calculations of Laporta *et al.* [553, 555, 556] and used in Laporta *et al.* [557] to investigate electron transport in non-equilibrium nitrogen-oxygen plasmas.

"`Song`" Most recent review in Song *et al.* [865] principally based on the previous review from Itikawa [441]. The main differences are (i) the total scattering cross section has been corrected at high energies to follow the Born-Bethe scaling, (ii) the elastic momentum-transfer has been updated from swarm measurements, (iii) the electronic excitations are completed with Born-scaled analytical fits as described in Kim [505]. Also, (iv) the new review includes transitions between the fine-structure spin-orbit split states of the ground configuration $^2\Pi_{1/2}$ and $^2\Pi_{3/2}$ from Allan [15].

This latest review served as a basis for the creation of the present set of cross sections.

Comparisons

Elastic CS fig. 16.11

1. Resonance region $NO^- \, ^3\Sigma^- < 1.5\,\mathrm{eV}$: vibrationally-elastic data of Laporta *et al.* [557].

2. Low to intermediate energies 2–50 eV : cross-beam ICS from Mojarrabi *et al.* [654] (corrected in [120, tab. 3]). Our ICS are taken from the total CS recommended by Song *et al.* [865, table 2] and the subtraction of the sum of all inelastic CS. The inclusion of the complementary inelastic CS improves the agreement with the measured ICS below 20 eV but is underestimated beyond.

Table 16.3: Databases of electron collision cross sections with nitric oxide. Middle rows represent the ones hosted on LXCat, the last rows are incomplete databases. In the columns we regroup the references to the experimental data upon which the database are constructed. If it exists, the reference to the publication which describes each database is under the column "Origin".

Database	Year	Origin	Total	Elastic	Vibrational	Electronic	Ionisation	Attachment
IAA (Present)	2023	11	[865]	[654]	[557, 654]	[120]	[597]	[555]
Phelps	1969		unpublished					
Hayashi	1987							
Itikawa	2016	[441]	[207, 899, 900, 1005]	[654]	[456, 654]	[120]	[597]	[767]
Flinders	2004				[144]	[157, 655]		
Laporta	2013	[553]		[553]	[553]			[555]

3. Momentum-transfer CS : The complete database lies systematically in better agreement with the momentum-transfer CS integrated from the DCS of Mojarrabi *et al.* [654] and the recommendation of Song *et al.* [865, fig. 6]. The data recommended by Itikawa [441] are somewhat lower than the rest.

   The data of `Phelps` are outdated (and were actually never published).

4. Above 500 eV : the lowering correction from the tail of the complementary inelastic cross section is too strong and could be reduced.

Inelastic CS fig. 16.12

- Vibrational CS : $\sum_{v'} \sigma_{v=0\to v'}$

  1. Below 2 eV : vibrational excitation CS from Laporta *et al.* [557] mainly from NO$^-$ $^3\Sigma^-$ (0.2–1.5 eV) resonant state.
  2. Between 5–15 eV : double peak is an artifact due to the mismatch in the position of the dominant $^3\Pi$ resonance between theoretical calculations [557] (~ 8 eV) and measurements (~ 15 eV) [144, 654] synthesised by the `Flinders` database (light brown dotted ···).

- Electronic CS : $\sum_{a'} \sigma_{0\to a'}$

  △ A significant portion of the electronic excitation CS is missing from the survey of excitations by Brunger *et al.* [120]. The total sum of inelastic CS for electronic excitations must be completed with four times its value in order to bring calculations from a kinetic solver in agreement with experimental swarm transport parameters [865, §2.7].

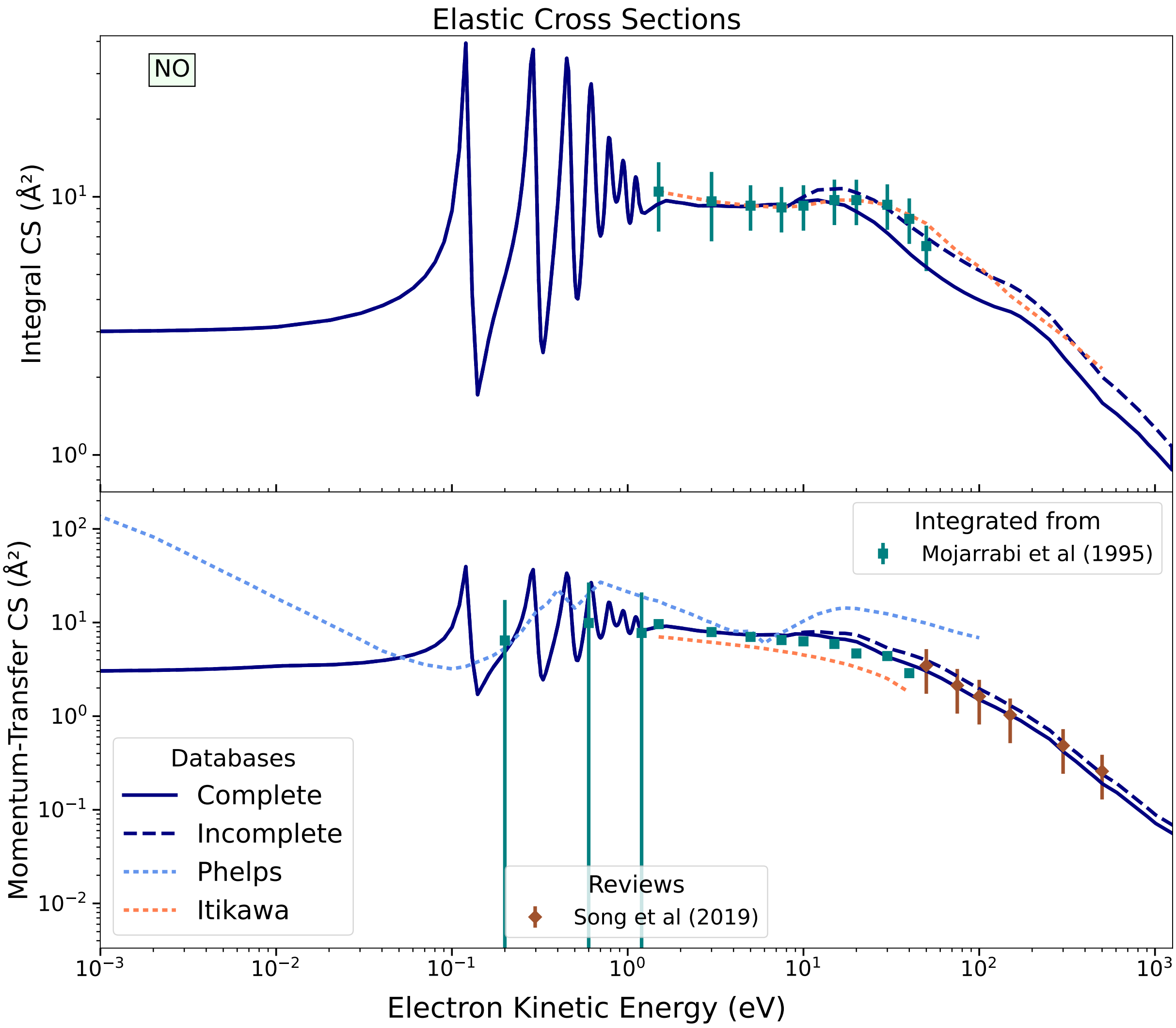

Figure 16.11: Comparison of elastic integral and momentum-transfer cross sections for nitric oxide. No curve could be obtained from `Hayashi` because the subtraction of inelastic CS from the reported ‘total’ cross section gives negative values above 10 eV.

△ The significant difference between the complete (—) and incomplete (- - -) CS might be due to the non-ionising dissociation CS of NO which is expected to be large, although concrete experimental data is missing [865, §2.8].

Ionisation CS fig. 16.13

Transport Coefficients fig. 16.14

- Our and `Itikawa` sets differ substantially, it is therefore not surprising to see almost a complete discord among the calculated transport coefficients.
- The effect of rotational cross sections at electric fields <1 Td is very strong and completely governs the transport of electrons in that region. This was already observed in CO by Vialetto *et al.* [961]. NO’s dipole is about 1.5 times stronger than CO’s.

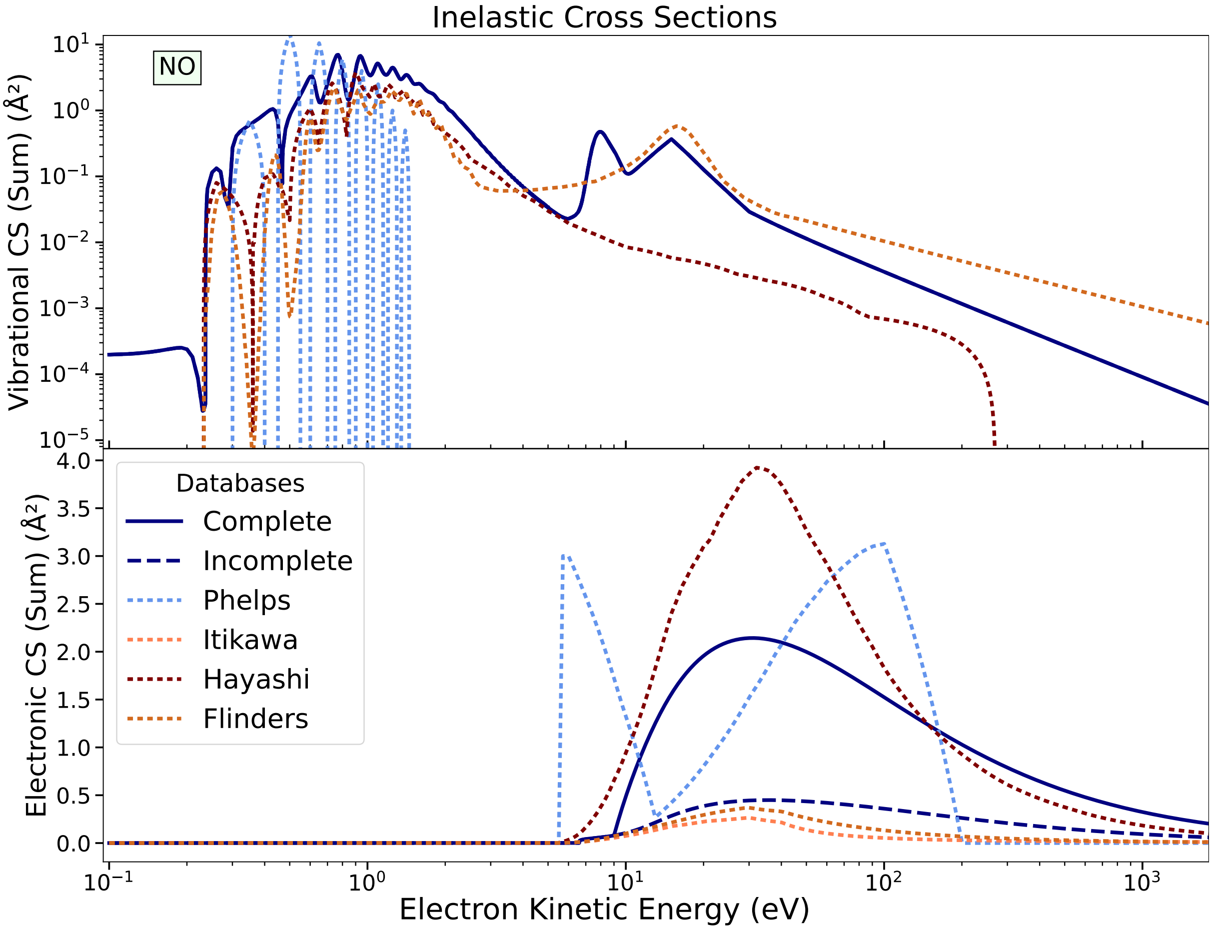

Figure 16.12: Comparison of the sum of vibrational and electronic impact excitation cross sections for nitric oxide.

- Below < 40 Td : Transport in `Hayashi` is eased by a lower vibrational CS (fig. 16.12–top) and absence of the $^3\Pi$ resonance around ~ 8—12 eV.
- Above > 40 Td : Inversion of trends due to acute inelastic losses in `Hayashi` total electronic CS (fig. 16.12–bottom).

16.4 Ar

There are many reviews about noble gases in general. Argon is the second most studied noble gas after helium. An early set of recommended cross sections was given in Hayashi's report [387]. Later came many other reviews, which sometimes cover also other noble gases. Brusa *et al.* [125] gave analytical fits to elastic, electronic excitation and ionisation cross sections of electrons colliding with noble gases.

Most recently, Boffard *et al.* [89] reviewed electron-impact excitations of noble gases including from metastable states. Then, Gargioni and Grosswendt [319] performed a more detailed review specific to argon including the verification of the consistency of optical oscillator strength measurements and sum rules. The construction of our database was mainly based on the information reviewed in those two recent studies [89, 319].

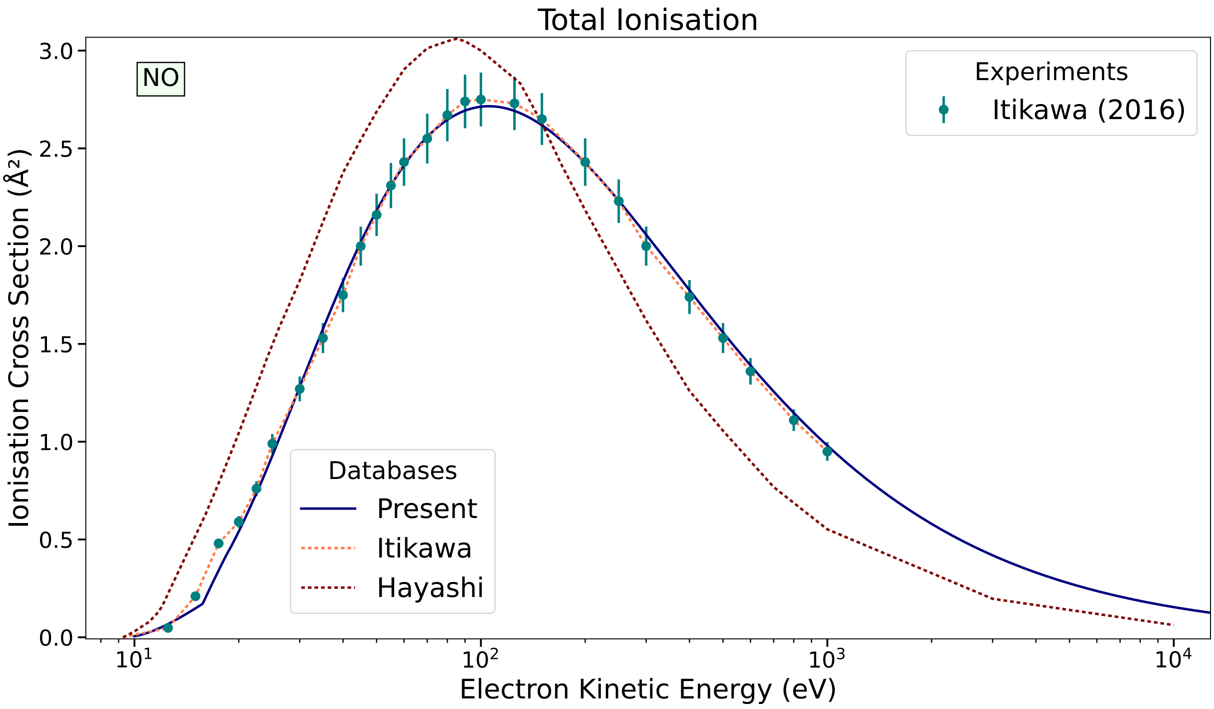

Figure 16.13: Comparison of impact ionisation cross sections for nitric oxide. We exclusively follow the recommendation of Itikawa [441] from the review of Lindsay and Mangan [596]. Data in `Hayashi` database were communicated privately to the JILA centre and are available on LXCat only.

Regarding cross section databases, argon is perhaps one of the targets most replete with sets of data. A review and comparison of databases hosted on LXCat for argon was conducted by Pitchford *et al.* [752]. It is actually the first of the review trilogy for noble gases continued in Alves *et al.* [23] and Bordage *et al.* [95]. Extensive comments to each database of LXCat are given in appendices of that review [752], we invite the reader to consult them there and offer only a tabular overview, for practical purposes, of the argon database in table 16.4 below.

Comparisons

Elastic CS fig. 16.15

1. Very low energies < 0.01 eV : the elastic cross sections of each database converge to a difference value $\sigma_\text{e}(\varepsilon = 0) = \pi A^2$ corresponding to the scattering length A. Ours is based on the value most recently deduced by Kurokawa *et al.* [545, p.7:table II].

2. Low energies < 10 eV : Purely elastic scattering, ICS identical to total CS of Kurokawa *et al.* [545] the `BSR` calculations of Zatsarinny and Bartschat [998] are slightly different.

3. Momentum-transfer (MT) : obtained from ICS with the $\langle\cos\theta\rangle$ given by the `BSR` DCS. Thus, the differences in σ_m between our and all other databases are a consequence of the slight mismatch between the `BSR` and the ICS. The calculated average cosine $\langle\cos\theta$ is too large in the Ramsauer-Townsend minimum at ~ 0.23 eV

4. From 10–100 eV : our ICS and MTCS are closer to the values of DuBois and Rudd [232] and Panajotović *et al.* [731] than all other database.

NO

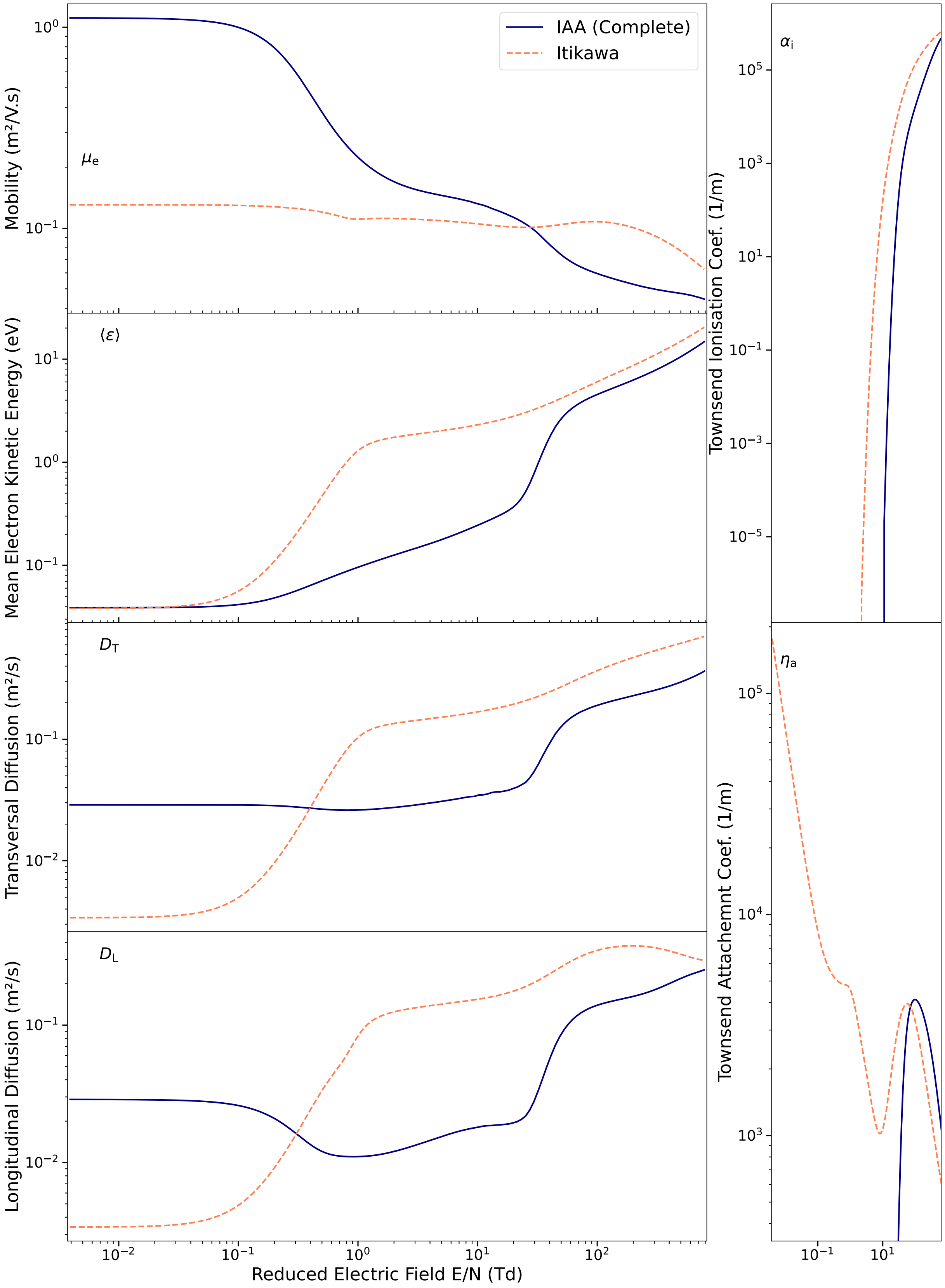

Figure 16.14: Transport coefficients in nitric oxide as calculated by BOLSIG+ for different cross section sets. We could not retrieve any experimental data in NO, consult Laporta *et al.* [557, fig.9] on which our set is based.

Table 16.4: Databases of electron collision cross sections with argon hosted on `https://www.lxcat.net/`. In the columns we regroup the references to the experimental data upon which the database are constructed. If it exists, the reference to the publication which describes each database is under the column "Origin".

Database	Year	Origin	Elastic	Electronic				Ionisation
				$4s$	$4p$	$3d$, $5s$	other	
IAA (Present)	2023	11	[129, 278, 545, 701, 708, 891, 900, 1004]	[8, 180, 282, 283, 491]	[180]	[180]	[319]	[321, 768, 814, 815, 869]
Phelps	1983	[306, 903]	[295, 650]	Schaper and Scheibner [809]				[861]
Puech	1986	[760]	[306, 650]	[106, 107, 180]				[106]
Hayashi	1991	[388]	Hayashi [388, p.200–9]					
IST-Lisbon	2005	[993]	[991]	[491]	[175]	[388]	[568, 977]	[768]
Biagi	2011	[752, app.A]	[689, 746]	[14, 319, 504, 505]				[768, 888]
BSR	2014	[998]	Zatsarinny *et al.* [1002]					

5. Above $> 100\,\mathrm{eV}$: the trends inverse. Our database lies closer to `Hayashi`'s and `BSR`, whereas `Biagi` and `IST-Lisbon` are lower.
6. At $1\,\mathrm{keV}$: All database intersect and coincide with the last measurement of Iga *et al.* [418] except `Phelps` which has been straying away from $150\,\mathrm{eV}$.
7. Completion : the complete database has a roughly constant correction ratio of $-8\,\%$.

Inelastic CS fig. 16.16

- Electronic CS : $\sum_{a'} \sigma_{0\to a'}$
  - △ Below $< 200\,\mathrm{eV}$: All databases peak differently. `Hayashi` and `Biagi` have a broad and tall peak, `BSR` has a flat and low plateau, `IST-Lisbon` and our incomplete database have sharper peaks, and `Phelps` has a tall pointy peak with only one excitation at $11.55\,\mathrm{eV}$
  - △ Above $200\,\mathrm{eV}$: our complete database is well in agreement with `Hayashi, Biagi, BSR` and `Phelps IST-Lisbon` coincides with our incomplete database.
- Ionisation CS :
  - Below $< 100\,\mathrm{eV}$: All databases follow Rapp and Englander-Golden [768] except `BSR` [1002] which misses a large portion. Ours analytical fit cannot swerve awkwardly between 50–70 eV.
  - Above $> 100\,\mathrm{eV}$: Two groups:

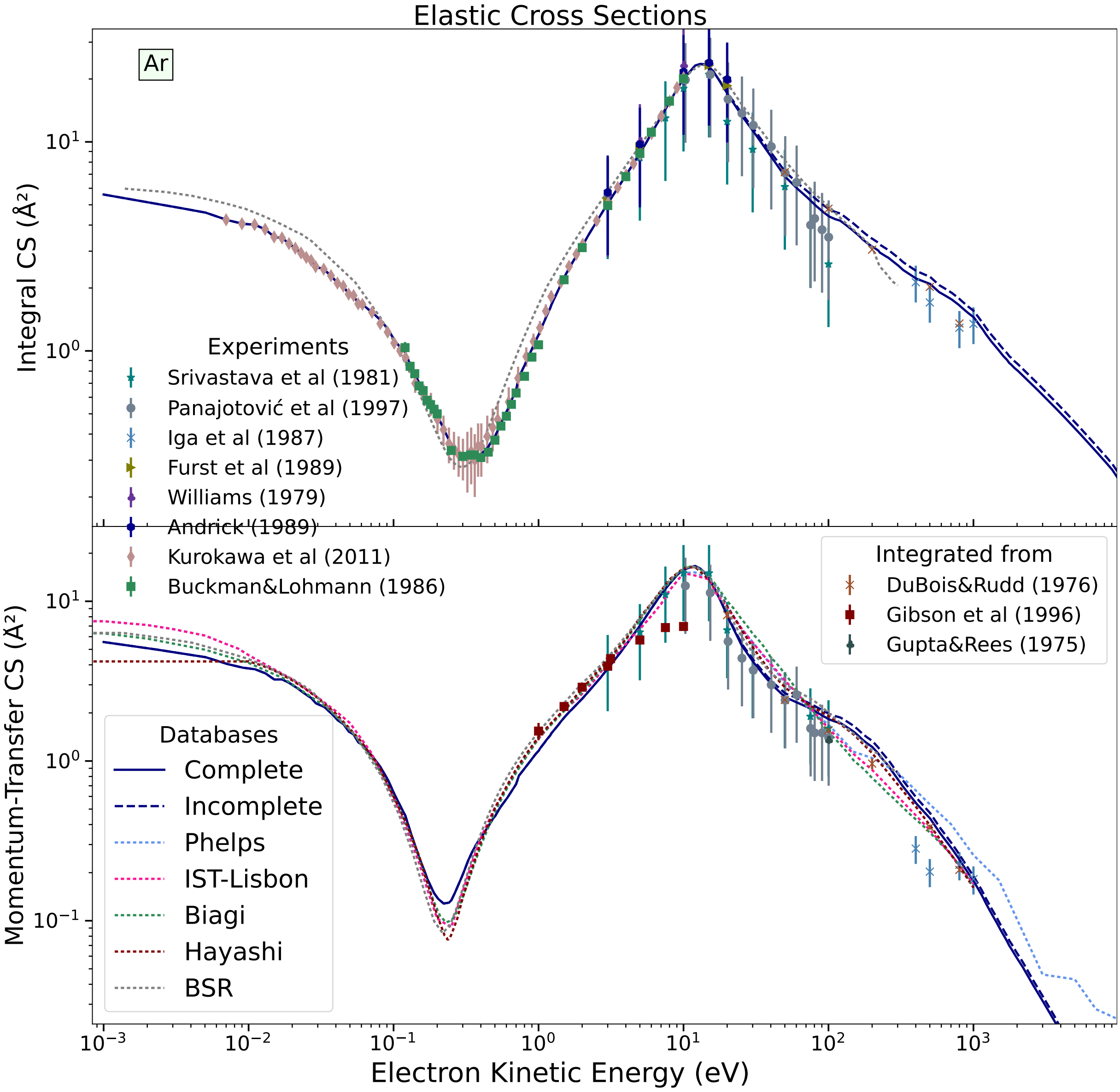

Figure 16.15: Comparison of elastic integral and momentum-transfer cross sections for argon.

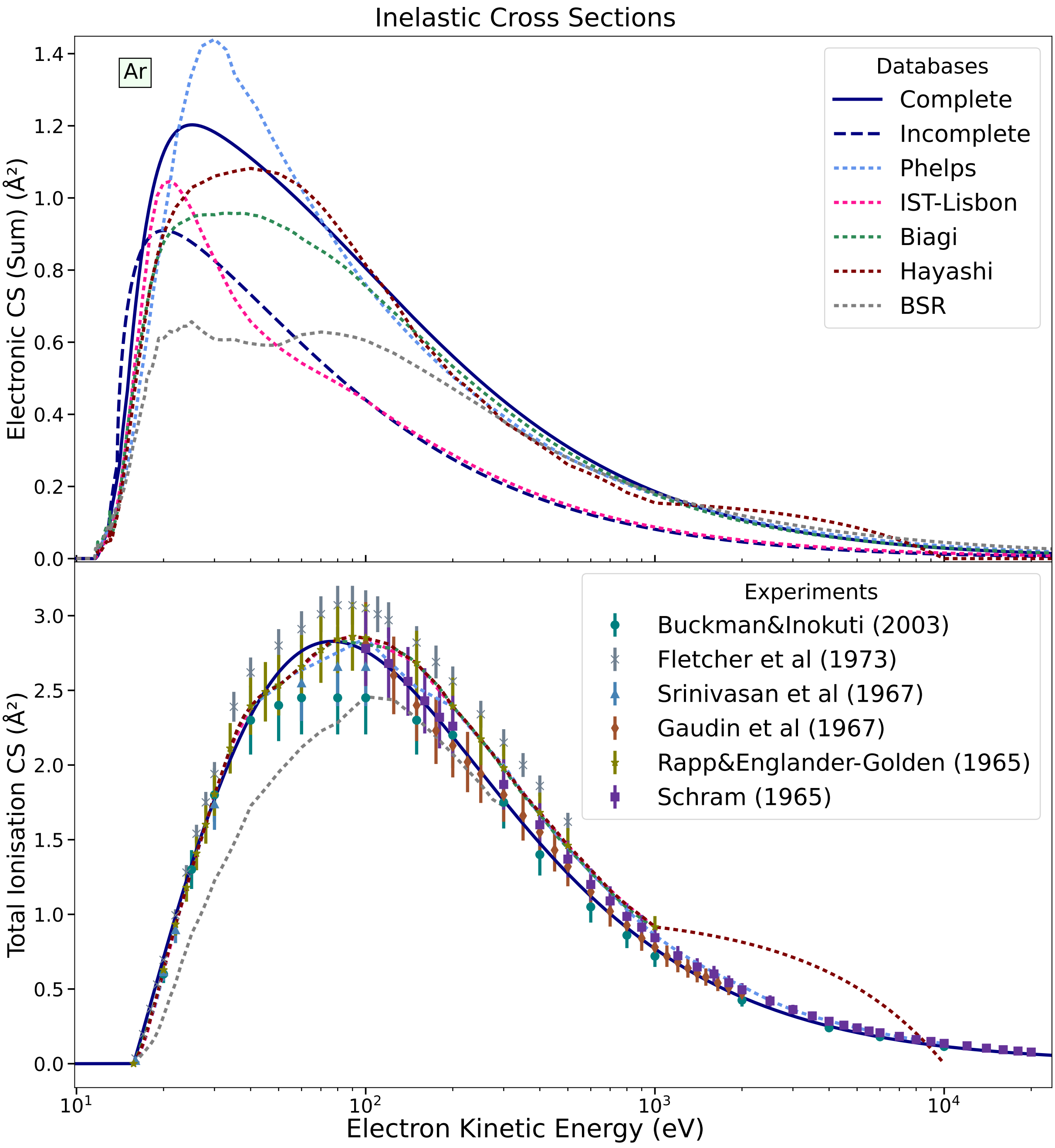

Figure 16.16: Comparison of the sum of electronic impact excitation and ionisation cross sections for argon. The weird bump on the `Hayashi` curve is due to a linear interpolation from 1 keV to 10 keV where the CS is forced to zero.

A. Followers of Rapp and Englander-Golden [768] : `IST-Lisbon`, `Phelps`, `Biagi` and `Hayashi`.

B. Followers of Gaudin, Albert and Hagemann, Robert [321], Inokuti *et al.* [425], and Schram *et al.* [814] : our database (`IAA`) and `BSR`.

Electronic CS fig. 16.17

1. Completion : The dashed curves “incomplete” --- are direct fits to the data plotted, whereas solid curves — and dotted curves **cdots** are sums over the states mentioned.

2. Allowed $4s$ ($^3P^o_1$ and $^1P^o_1$) : When renormalised, Chutjian and Cartwright [180] and Filipović *et al.* [282] seem to indicate the presence of a peak between 40–50 eV, which is only followed by `Hayashi`. The most recent cross-beam measurements of Khakoo *et al.* [491] show the opposite. Theoretical `BSR` [1002] calculations follow neither trends, and `IST-Lisbon` is about half the updated CS estimate.

3. $4s$ forbidden ($^3P^o_0$ and $^3P^o_2$) : peaked CS in the following order : `IST-Lisbon` > Present > `Hayashi` > `BSR`. Our CS follow most Khakoo *et al.* [491] and Filipović *et al.* [283]. `Hayashi` follows Chutjian and Cartwright [180] when renormalised, we suspect he did his own renormalisation when constructing his recommended data in Hayashi [387].

4. $4p$ (9 dipole-forbidden + 1 pure spin-forbidden): `IST-Lisbon` follows closely Chilton *et al.* [175], whereas we and `Hayashi` preferred to follow Chutjian and Cartwright [180] after renormalisation. The `BSR` database misses a significant portion of the CS below < 100 eV.

5. $3d + 5s$ (mixture of allowed, dipole forbidden and spin-forbidden transitions, 12 in total) : Here is where lumping together the cross sections in a single fit (‘Incomplete’: ---) is inaccurate compared to a sum of individual fits (‘Complete’: —). `IST-Lisbon` is practically superposed with `Hayashi` which is located between Chutjian and Cartwright [180] when renormalised and Chilton and Lin [176]. Our full curve is a fit to individual CS from various sources: Chilton and Lin [176] and Stewart *et al.* [883] and Chutjian and Cartwright [180] renormalised. One can see in the inflexion points of the curve, the regions where forbidden and allowed transitions dominate respectively. Again, `BSR` underestimates the CS in the peak region.

Transport Coefficients fig. 16.18

See Pitchford *et al.* [752] for a detailed comparison of transport in argon and explanation of each cross section database. Here, we only highlight differences with the present database.

- Below < 5 Td : Differences are entirely imputable to the momentum-transfer CS (fig. 16.15–bottom).
    - 0.005–0.1 Td : Diffusion coefficients governed by the depth of the Ramsauer-Townsend minimum at 0.23 eV. Our MTCS is certainly less accurate in that minimum than all other databases.
    - D_L at 3 Td : Two groups in the sharp bend: `IST-Lisbon, Phelps` and all others. This demarcation may only be explained by the lower elastic MTCS for those two databases between 5–12 eV (fig. 16.15).
- Above > 10 Td : mean kinetic energy $\langle\varepsilon\rangle \gtrsim 5$ eV, influence of electronic excitations starts building up.
    - μ_e around ~ 10 Td : Difference in the mobility is probably also due to the elastic MTCS; separation again of `Phelps, IST-Lisbon` from the rest (fig. 16.15).

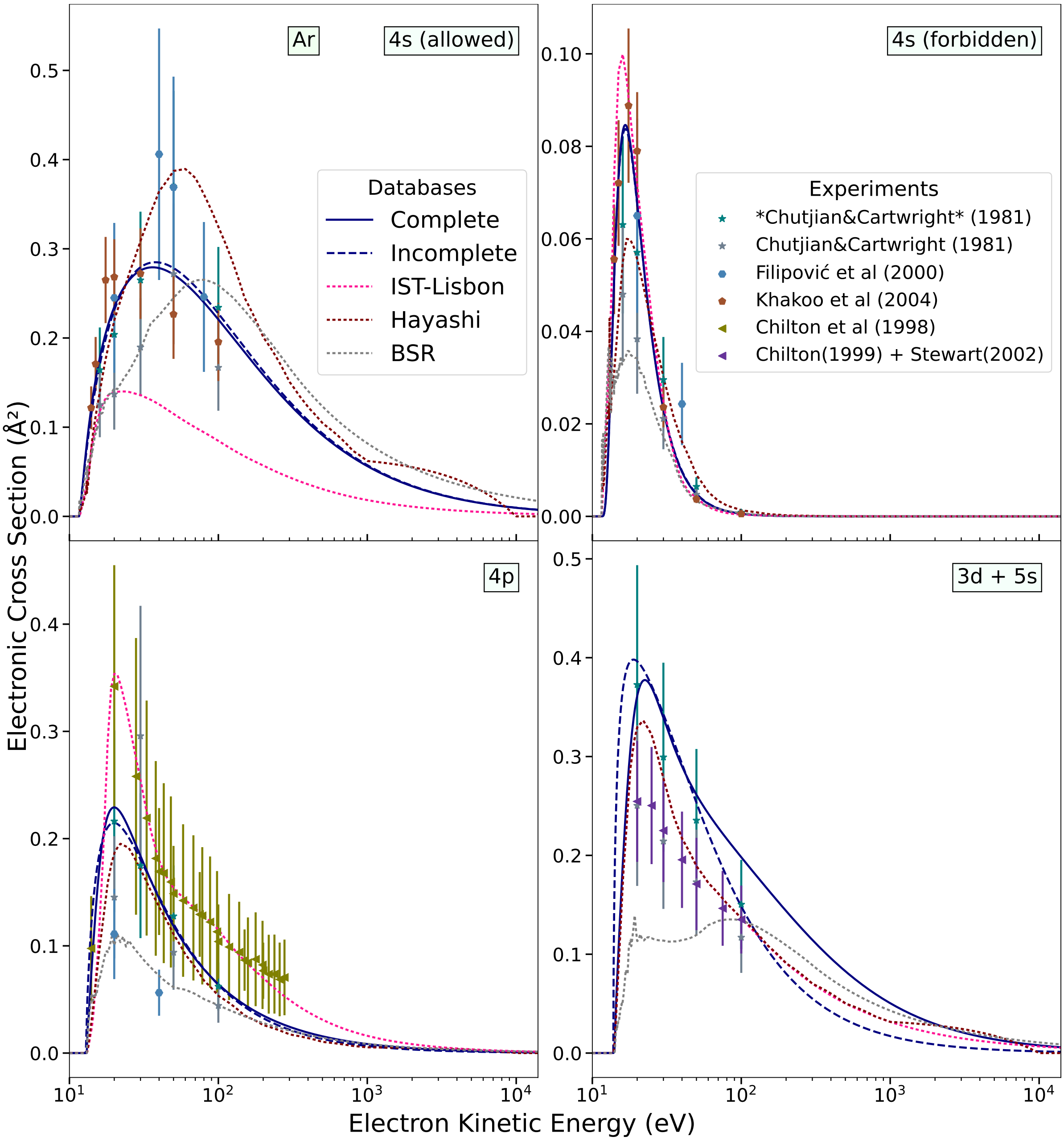

Figure 16.17: Comparison of selected electronic impact excitation cross sections for argon.

  - α_{i} : neatly ordered values of the ionisation coefficient from highest to lowest: `Phelps` > `Hayashi` > `Biagi` ~ `BSR` > `IST-Lisbon` > `IAA`.

    It is very probable that our RBEQ* to the ionisation CS is too low at the peak around ~100 eV and should be raised. This is not obvious from the experimental data shown on figure 16.16–bottom.

- Above 100 Td : difference in transport of the `BSR` database due to underestimation of inelastic losses (fig. 16.16).

16.5 O

Atomic oxygen was mainly studied by Vaughan and Doering in a series of articles [220, 227, 958–960].

More recently, Johnson *et al.* [462] made a survey of the available experimental and theoretical cross sections for O.

Two databases exist for atomic oxygen: `IST-Lisbon` who reinterpolated the data reported in the former survey of Laher and Gilmore [549] and `BSR` from the calculations in Tayal and Zatsarinny [921]. The latter are unfortunately not disclosed on LXCat, so we could not compared our results to `BSR`.

Comparisons

Elastic CS fig. 16.19

1. Below < 0.5 eV : our CS are calculated with the MERT (sec. 10.1.5).
2. Between 0.5 $10 eV$: we closely stick to the only experimental results available of Williams and Allen [984].
3. Above 10 eV : all our CS are obtained from partial wave calculations off the optical potential. They differ significantly from the ones of `IST-Lisbon` for increasing energies.

Inelastic CS fig. 16.20

- Electronic CS : $\sum_{a'} \sigma_{0 \to a'}$
  - △ Below < 20 meV : our CS are dominated by superelastic collisions between the fine-structure states of O: $^{3}_{P}0^{o}$, $^{3}_{P}1^{o}$ and $^{3}_{P}2^{o}$ (ground). These were obtained by pure conjecture based on the theoretical calculations of Berrington [63] and scaled according to the Boltzmann distribution at 300 K.
  - △ From > 20 meV : we see two bumps due to excitations from the ground to fine structure states.
  - △ At > 2 eV we see excitations to the two lowest spin-forbidden excitations to valence states: $2p^4\ {}^1D$ and $2p^4\ {}^1S$ (fig. 13.9), which are a bit lower in `IST-Lisbon` from Laher and Gilmore [549].
  - △ Beyond > 10 eV : Large bump due to all other electronic excitations. The complementary cross section is significant and its relevance is supported by the tall peak seen in `IST-Lisbon`.

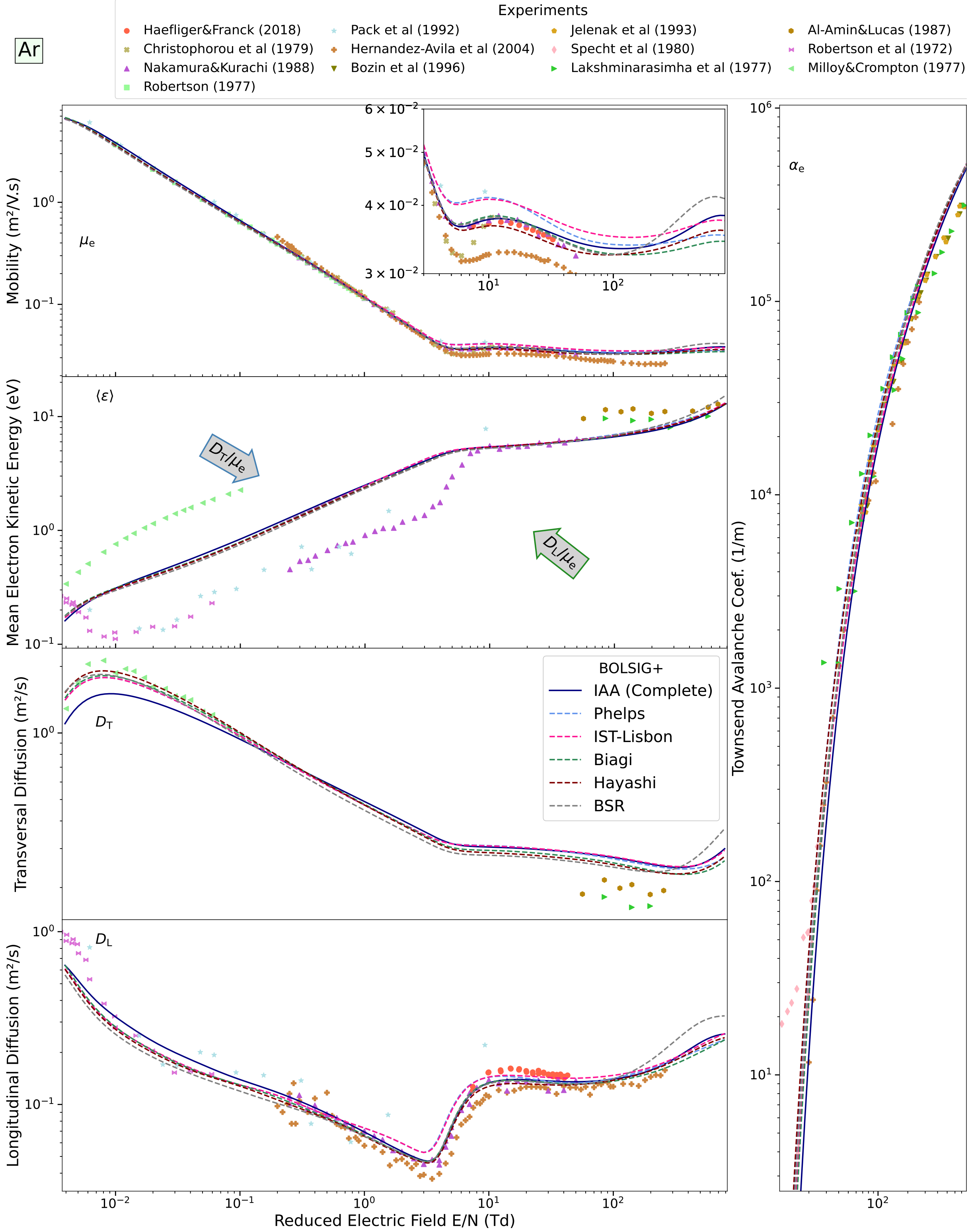

Figure 16.18: Transport coefficients in argon as calculated by the two-term Boltzmann solver BOLSIG+ for different cross section sets and compared with a variety of experimental data.

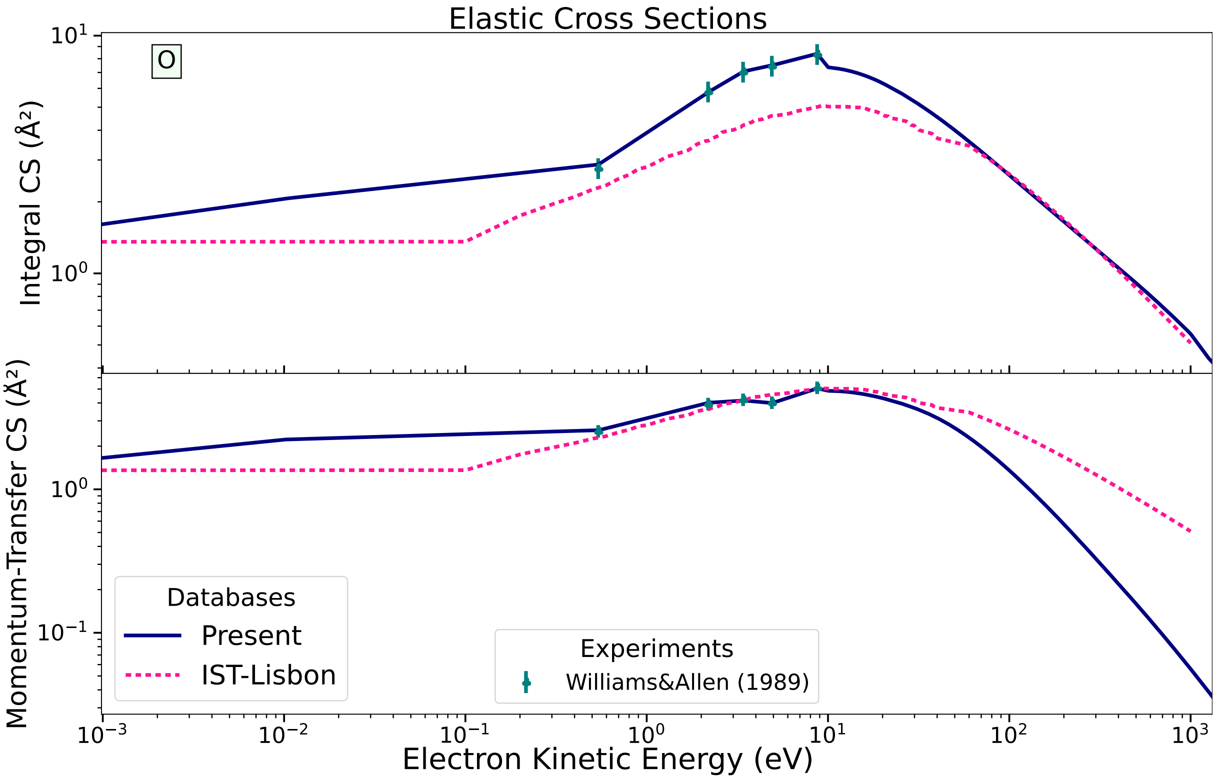

Figure 16.19: Comparison of elastic integral and momentum-transfer cross sections for atomic oxygen.

- Ionisation CS : The main difference between our database and `IST-Lisbon` is that we treat three auto-ionising states ($3s''\ {}^3P^o$, $2s2p^5\ {}^3P^o$, and $4d'\ {}^3P^o$) separately from the total ionisation cross section. This explains why our CS is lower that experimental measurements.

Transport Coefficients fig. 16.21

- Below < 1 Td : Electron transport is dominated by the inelastic spin-forbidden transitions between the fine-structure spin-orbit states of O : ${}^{3}_{P}2$, ${}^{3}_{P}1$ and ${}^{3}_{P}0$.

  Trick : when given as input to BOLSIG+, these three inelastic transitions are treated as 'rotational' excitations, so that the program scales the superelastic transitions according to the temperature (300 K).

- Between 0.5–50 Td : Mean kinetic energy of `IST-Lisbon` is higher due to lower inelastic CS (fig. 16.20) higher ionisation rate due to higher ionisation CS.

- Above > 100 Td : Transport trends inverse, probably due to the difference in ionisation and perhaps also due to CS divergence of momentum-transfer CS between `IST-Lisbon` and our database above 20 eV (fig. 16.20).

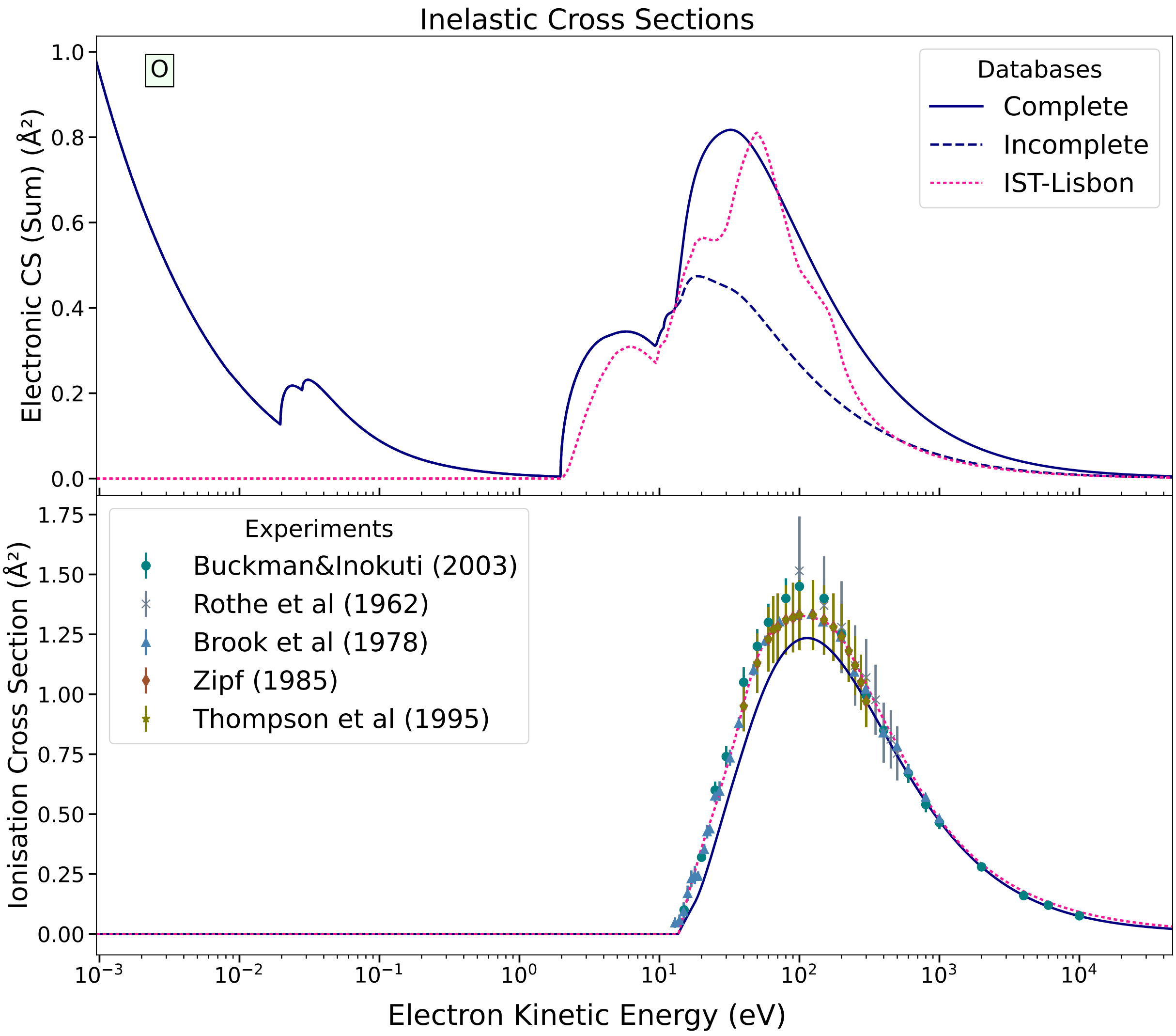

Figure 16.20: Comparison of the sum of electronic impact excitation and ionisation cross sections for atomic oxygen.

16.6 N

Cross sections for atomic nitrogen were mainly measured by the group of Doering and Goembel [222, 223, 992].

From the theoretical perspective, the most recent calculations were conducted by Wang *et al.* [975] from which two databases derive : the `BSR` and the `IST-Lisbon` which can be seen as reduced and reinterpolated version of the former.

Comparisons

Elastic CS fig. 11.6

- Below 140 eV : we use calculations from Wang *et al.* [975] (`BSR` database)
- Beyond 140 eV : our calculations of partial wave from the optical potential merge smoothly with the `BSR` data.

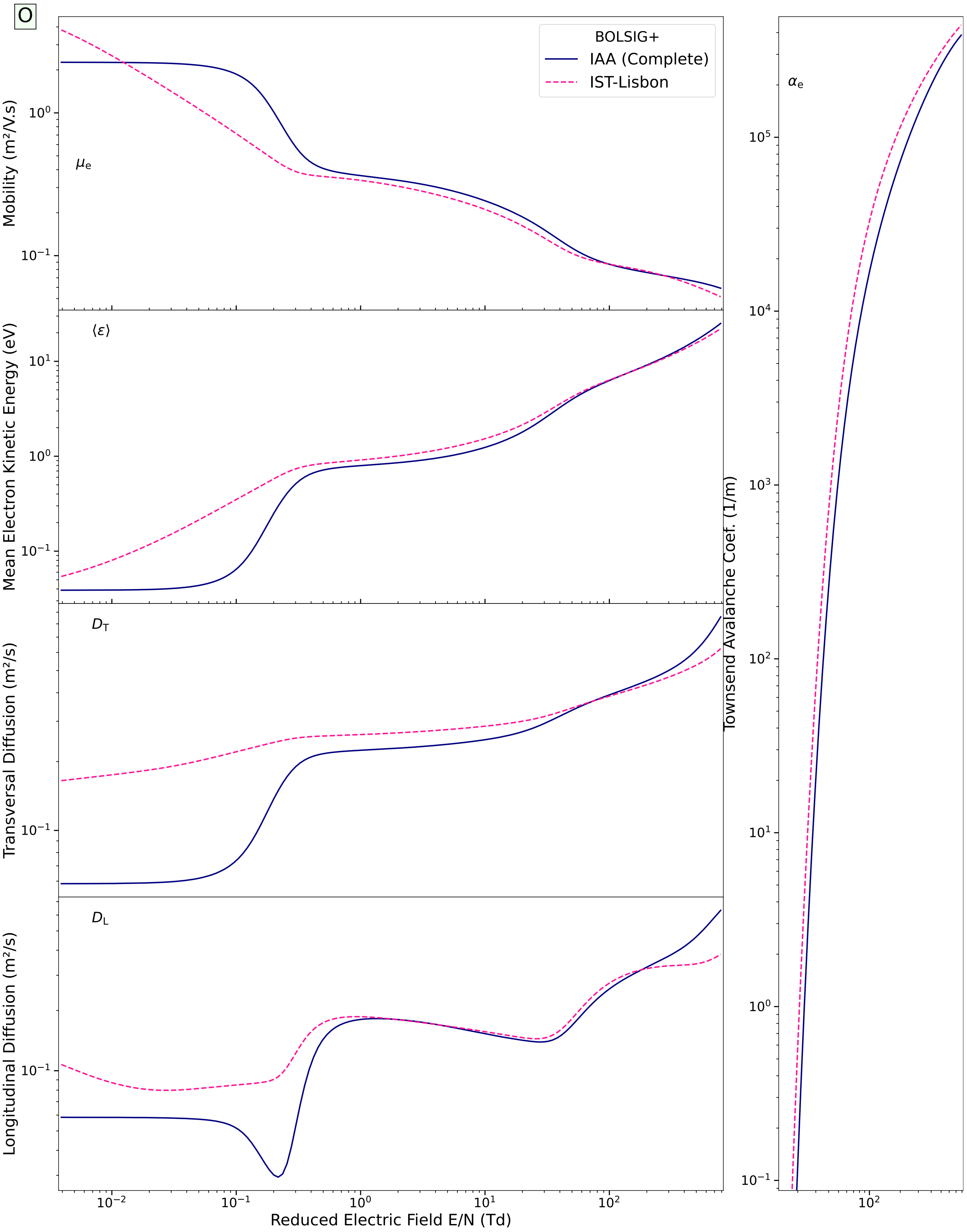

Figure 16.21: Transport coefficients in atomic oxygen as calculated by the two-term Boltzmann solver BOLSIG+ for different cross section sets at a temperature of 300 K.

Inelastic CS fig. 16.22

- Electronic CS : $\sum_{a'} \sigma_{0\to a'}$, three peaks :
  - △ First peak < 10 eV : due to spin-forbidden low-lying excitations ($2p^3\ ^2D^o$ and $2p^3\ ^2P^o$). The `BSR` calculations predict a sharp rise, whereas we fitted a curve rising more slowly to the data of Yang and Doering [992].
  - △ Middle peak ~ 12 eV : mainly from $2s\,2p^4\ ^4P$ allowed excitation and a small participation from $3p$ dipole-forbidden states.
  - △ Third peak > 40 eV : mostly from allowed $3s\ ^4P$ excitation and small participation of higher allowed excitations ($4s$ and $3d$).
  - △ In `BSR`, the two last peaks are merged into a mound. We find this a more 'natural' shape for the electronic CS in nitrogen.
  - △ `IST-Lisbon` does not include higher states than the lowest two spin-forbidden from `BSR`.
- Ionisation CS : We recall that we did not perform a fit with the RBEQ* model but derived the Q parameter based on the sum rule of oscillator strengths (see previous page 580). Worthy to note, the `BSR` calculations [975] seem to fit well the ionisation of Brook *et al.* [117] without taking into account metastable states, whereas Kim and Desclaux [506] obtained a good fit corresponding to a 70:30% ratio of $\mathrm{N}\,^4S^o$:$\mathrm{N}\,^2D^o$. To be continued…

Transport Coefficients fig. 16.23

- Below < 1 Td : Electron transport is identical in all databases since most is due to elastic scattering.
- Above > 1 Td : Mean kinetic energy and ionisation in our database is superior to the `BSR`, as expected from the higher electronic CS of the latter.
- Above > 100 Td : The effect of higher excitations than forbidden states (second bump on figure 16.22–top) is significant as can be seen by the divergence of the `IST-Lisbon` from the `BSR` database. Since the former does not include higher electronic excitations.

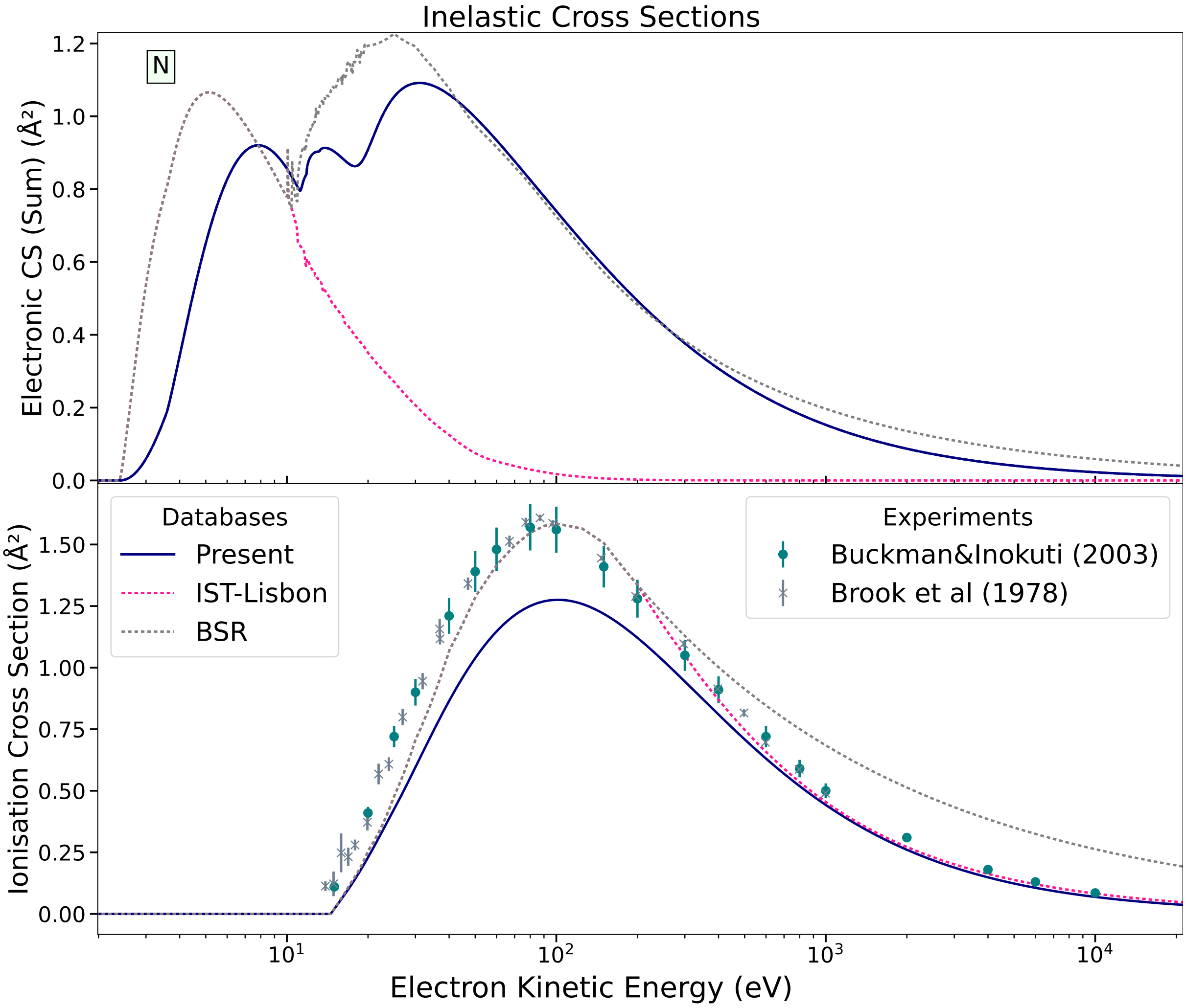

Figure 16.22: Comparison of the sum of electronic impact excitation and ionisation cross sections for atomic nitrogen.

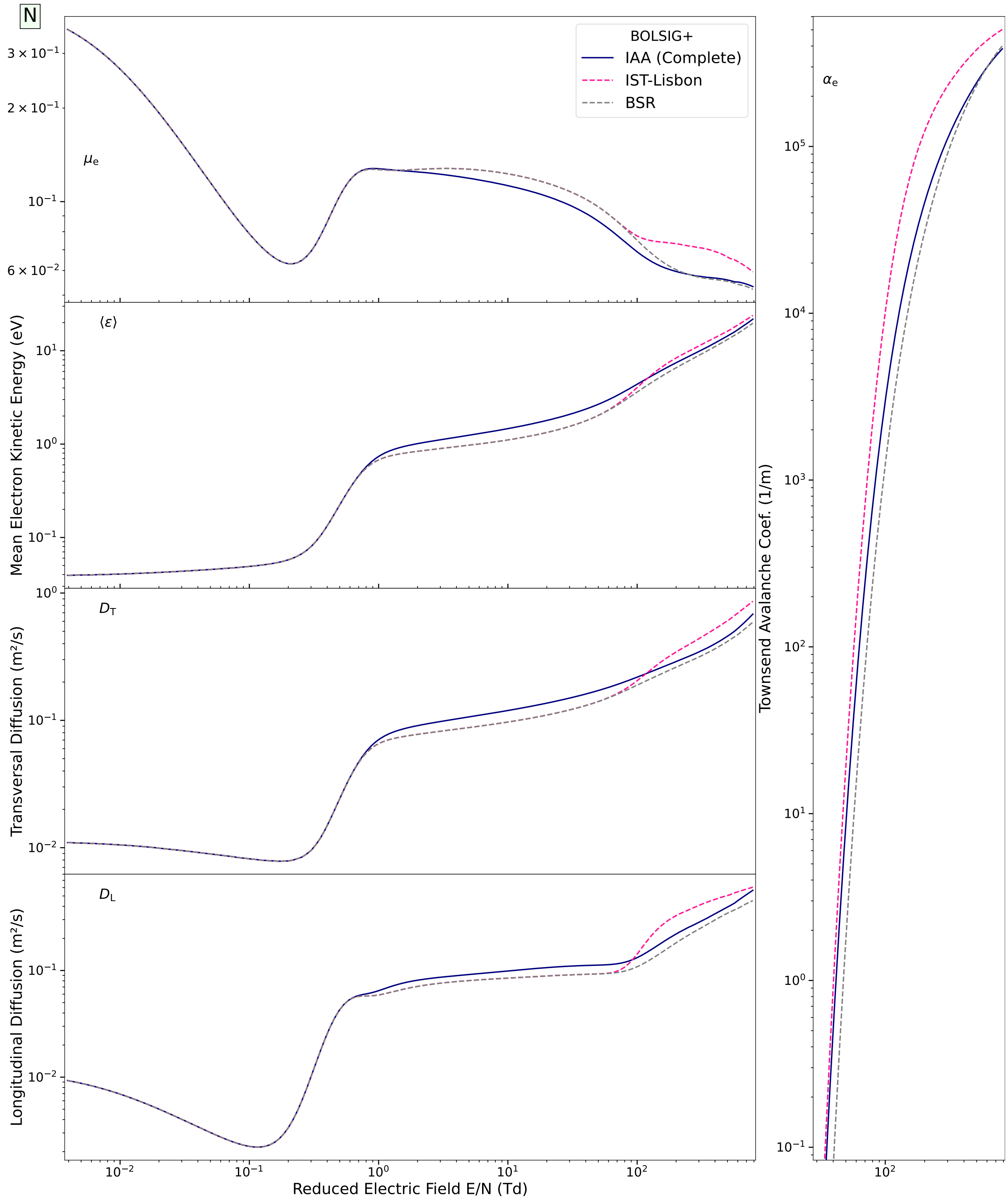

Figure 16.23: Transport coefficients in atomic nitrogen as calculated by the two-term Boltzmann solver BOLSIG+ for different cross section sets at a temperature of 300 K.

Electron-Molecule Collisions (Part II)

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