## Database for Inelastic Collisions of Sodium Atoms with Electrons, Protons, and Multiply Charged Ions

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#### Abstract

The available experimental and theoretical cross section data for inelastic collision processes of ground (3s) and excited (3p, 4s, 3d, 4p, 5s, 4d, 4f) state Na atoms with electrons, protons, and multiply charged ions have been collected and critically assessed. In addition to existing data, electron-impact cross sections, for both excitation and ionization, have been calculated using the convergent close-coupling approach. In the case of proton-impact the database was enlarged by new atomic-orbital close-coupling calculations. Both electron-impact and proton-impact processes include excitation from the ground state and between excited states (n = 3 - 5). For electron-impact also ionization from all states is considered. In the case of proton-impact electron loss cross sections (the sum of ionization and single-electron charge transfer) are given. Well-established analytical formulae used to fit cross sections, earlier published by Wutte et al. and Schweinzer et al. for collisions with lithium atoms, were adapted to sodium. The "recommended cross sections" for the considered processes have been critically evaluated and fitted using the adapted analytical formulae. For each inelastic process the determined fit parameters are tabulated. We also present the assessed data in graphical form. The criteria for comprehensively evaluating the accuracy of the experimental data, theoretical calculations, and procedures used in determining the recommended cross sections are discussed.

#### 1. Introduction

The work on this database is motivated not only by the fundamental interest in the matter, but also by the need for reliable cross sections for the evaluation of plasma edge diagnostics in magnetically confined fusion plasmas by means of active neutral sodium beam spectroscopy. The basic experimental, theoretical, and computational concepts are based on and refer to the earlier work on neutral lithium beam diagnostics [1]–[8]. Similar to lithium, injection of a fast neutral sodium beam into the edge of a magnetically confined plasma is able to deliver diagnostic information such as radial electron density profiles and spatially and time resolved impurity ion concentrations [9]–[11]. A series of recent experiments at the tokamak ASDEX Upgrade and their preliminary analysis have shown that sodium beams are even better suited for this purpose than lithium. The interpretation of the emission line Na(3p-3s) of injected atoms, which provides information on the plasma edge density, requires a good knowledge of all involved inelastic collision processes. Therefore, the success of this plasma edge diagnostic method strongly depends on the availability of reliable cross sections of inelastic collisions of sodium atoms with plasma particles namely electron, protons, and multiply charged impurity ions.

The scope of the presented cross section database for collision processes of sodium atoms is mainly determined by the requirements of the Na-beam diagnostics. For the modeling of the diagnostic Na beam eight bound Na states, 3s, 3p, 4s, 3d, 4p, 5s, 4d, 4f are sufficient. The inelastic collision processes involving these eight Na states, are electron-impact target excitation, electron-impact target ionization, proton-impact target excitation, and proton-impact target electron loss. In the following chapters data for these processes will be presented. Sorting according to quantum numbers nl will be applied.

For many processes no cross sections could be found in the literature. Therefore we used advanced theoretical methods in this work to derive accurate cross sections for all inelastic processes involving collisions with Na atoms, see chapter 2. These theoretical results are critically assessed by comparing them with the most reliable experimental data available. In all cases good or at least satisfactory agreement between experiment and theory is found. Thus it is

plausible to have a comparable level of confidence in the theoretical cross sections were experimental validation is not feasible.

The recommended cross sections for the considered processes are a product of either a critical assessment of available experimental and theoretical data or these new calculations alone. They are presented by giving their analytical fit expressions and tabulating the values of all parameters entering these analytic fits. We also present the recommended cross sections in graphical form together with the cross section data used for their generation.

## 2. Basic Description of the Applied Theoretical Methods

2.1. Convergent Close-Coupling for Electron-Impact Collisions

In the past twenty years there has been an enormous progress both in theoretical description of electron-atom scattering and the computational adaptation of these theories. The latter is of course strongly supported by the more and more powerful computational resources which allow large closecoupling basis sets. Here we use the convergent close-coupling method (CCC) developed by Bray and Stelbovics [12]. Briefly this method uses a set of square-integrable basis states, obtained by diagonalizing the target Hamiltonian in an orthogonal  $L^2$ Laguerre basis, to expand the total wave function of the system. For the sodium target we assume that the frozen-core Hartree-Fock Hamiltonian is a sufficiently accurate representation. Hence, we treat sodium as essentially a one-electron target and electron-sodium scattering as a three-body problem.

The CCC method has already been extensively tested for inelastic electron-sodium scattering [13]. It reproduces closely the very detailed measurements of 3p excitation and the total ionization cross section. Thus, we have very good reasons to believe in the accuracy of the CCC method in evaluating integrated cross sections for all discrete transitions at all energies. The key issue is obtaining convergence for the transitions of interest with increasing number of expansion states [14]. Generally, the smaller the cross section, the larger the calculation necessary to obtain an accurate result. In practice, we choose a sufficiently large set of states to obtain accurately the most important transitions of interest.

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#### 2.2. Atomic-Orbital Close-Coupling for Ion-Impact Collisions

For ion-impact cross section calculations, we adopted the semiclassical impact-parameter formalism of the close-coupling (CC) method, assuming straight line trajectories for the projectiles [15]–[17]. The time-dependent electronic wave function is expanded in projectile- and target-centered traveling orbitals which need not necessarily be eigenstates of the corresponding atomic Hamiltonian. Thus, in addition to atomic-orbital (AO), so-called pseudostates (PS) are also included in our two-center expansion model. While AO represent the bound spectrum of the separated atoms of relevance for the considered inelastic collision process, PS are chosen to account for the formation of transient molecular orbitals as well as to represent ionization channels. The CC calculation always starts from a linear combination of states which result from diagonalization of the atomic Hamiltonians within the given set of basis states on each center.

The interaction between the core electrons and the "active" electron is described by a model potentials. The experimental energy level diagram of Na  $(n \leq 5s)$  is accurately reproduced by the eigenvalues of the model potential in. One-center couplings between projectile states induced by the electric field of the  $Na^+$  core are calculated in good approximation by assuming a pure Coulomb interaction potential.

For collisions of H<sup>+</sup> with Na(nl) cross sections for single electron capture (SEC), target excitation (EXC), and ionization (ION) are mainly derived from AO calculations involving 44 states centered on the proton core and 83 states (AO44\_83) centered on the Na<sup>+</sup> core. This main basis set is used for calculations with initial Na target states 3s, 3p, 3d, 4s, and 4p for impact energies between 1 and 500 keV. On both centers atomic states with principal quantum numbers  $n \leq 5$  are represented in the calculations. All other states are PS, which are orthogonal to the included atomic states of the basis and thus will overlap with higher excited bound states as well as with continuum states. The projection of such discrete non-bound pseudo-states on the continuum is the basis for the calculation of ionization cross sections. Another basis set AO70\_29 is used to check the convergence of results as well as to extend the impact energy range towards 0.2 keV. In addition to the two-center calculations, pure one-center calculations without projectile centered states (AO0\_83) were also performed. These calculations were used to derive EXC and ION cross sections at impact energies of 200–1000 keV with considerable less computational effort. In this high-impact-energy region the EXC and ION process is completely decoupled from electron capture, and thus results from AO0\_83 do not differ from those of the much more elaborate calculation AO44\_83.

Cross sections for target electron loss (ELOSS, that is SEC + ION) are obtained by summing over all cross sections for population of projectile-centered states and the direct ionization cross section of the Na atom. Results for ELOSS from the AO44\_83 calculations are believed to be convergent for impact energies of 1–15 keV. For higher impact energies the ELOSS cross section is dominated by the ionization process, which is not sufficiently well described in the basis set applied here. Therefore, at high impact energies ELOSS cross sections are underestimated by our AO calculations. This was taken into account in the process of establishing recommended cross sections (see section 3.3).

In general, the coupled equations are solved along straight line trajectories R = vt + b (R being the internuclear distance and v the velocity) from  $vt = -300a_0$  to  $vt = 300a_0$  ( $a_0$  being the Bohr radius) and for impact parameters b from 0.3 to 50  $a_0$ . However, for dipole-allowed EXC cross sections with small  $\Delta E$  values much larges meshes had to be used.In particular, the AO0\_83 calculations were done between  $vt = -800a_0$  and  $vt = 800a_0$  with impact parameters up to  $200a_0$ .

Similar calculations were performed for  $He^{2+}$  and  $Be^{4+}$  colliding with Na(3s,3p). Results from these calculation were used to check the behavior of EXC and ELOSS cross section with respect to the projectile charge q (see section 3.4).

### 3. Presentation of the Data

## 3.1. General Remarks on Credibility and Weighted Fitting

The most important excitation and ionization cross sections induced by the collisions of both electron and proton impact on sodium have been subject to a large number of experimental and theoretical studies. Obviously, the various methods imply different margins of error. For a comprehensive evaluation of the cross sections it became necessary to judge the credibility and to weight

the cross sections accordingly in the fit leading to recommended cross section. The following general guidelines were applied to this process. First, it is a known fact that First-Order Plain Wave Born Approximation (PWBA) cross sections excellently predict the asymptotic cross sections in the high energy tail and but show a large discrepancy in the low energy region. Thus, PWBA cross sections were weighted strongly above a certain energy limit and very poorly below this limit. Second, the better the data were compatible with the general trend of all collected cross sections of one transition the stronger they were weighted in the fit. Third, data predating 1980 were generally considered to be not as accurate as more recent ones.

#### 3.2. Collisions with Electrons

The presented database consists of comprehensively evaluated data found in the scientific literature. The quality and reliability of the database is further enhanced by including the CCC calculations into the critical data assessment process. All calculations are performed in the impact-energy range from the excitation threshold up to 10 keV.

Experimental data exist for electron-impact excitation (EXC) processes from the ground state to 3p, 3d, 4s, 4p, 4d, and 5s. Additionally experimental data for  $e^- + Na(3p) \rightarrow e^- + Na(3d)$  is available.

Representation of the cross sections is achieved by applying the Levenberg-Marquardt method for non-linear fits [54] implemented in gnuplot [55] and using the following analytic expression with seven parameters  $(A_1, \ldots, A_7)$ :

$$\begin{split} \sigma_{e^-}^{EXC}(e/eV)[cm^2] &= \frac{A_7 \cdot 10^{-16}}{E} \left[ \frac{E - \Delta E}{E} \right]^{A_6} \cdot \\ &\cdot \left[ \sum_{j=1}^4 \frac{A_j}{(E/\Delta E)^{j-1}} + A_5 \cdot \ln \left( \frac{E}{\Delta E} \right) \right] \\ &\forall E > \Delta E \end{split}$$

where  $\Delta E$  is the excitation threshold energy. The fitting functions were chosen to assure asymptotically correct behavior both at low and high impact energies. The behavior in the low energy region is mainly implemented by the second factor. It is thus essentially necessary that parameter  $A_6$  does not take negative values. As a typical example for the quality of the fitting procedure the result of the CCC

calculation for a single EXC process  $(Na(3s \rightarrow 3d))$  is presented in Fig.1 together with the fit parameters according to Tab.1. Deviations of the fit from the defining data points are in general below a few percent. In some cases there are data available for energies just above, but very close to the excitation threshold energy. The fits, though, all converge toward zero at threshold.

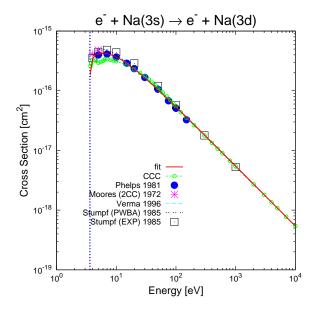


Fig. 1. Results from the CCC calculations for the  ${\rm Na}(3s\to 3d)$  electron-impact excitation in comparison with experimental and other theoretical data and the analytic fit (see Eq.(1) and Tab.1)

The collections of cross sections including the present CCC calculations are visualized in graphs in section 8.1. In these graphs the excitation threshold energy of the corresponding transition is displayed by a vertical blue single-dashed line. The accuracy of the experimental and theoretical data is limited according to the terms in chapter 3.1.

The collection of electron-impact target ionization (ION) cross sections includes additional data only for ground state and first excited state ionization. Again, the deviations of the fit and the data points are essentially below a few percent, except very close to the threshold. This gave rise to the introduction of the low energy limit  $E_{low}$ , below which the fit cannot predict the trend of the cross section anymore. Thus, the final form of the used analytical fit formula for electron-impact target ionization with seven fit parameters  $(A_1, \ldots, A_7)$  is

(1)

		Electron	-impact target	excitation	
Transition	Name	Published in	Referenced in	Weight in fit	Comment
$3s \rightarrow 3p$	Buckman 1979	[18]	[19]	Low	Experiment
	Enemark 1972	[20]	_	High	Experiment
	Gould 1970	[21]	[22]	Low	Calculation
	Karule 1970	[23]	[22]	Low	Experiment
	Kim 2001	[24]	_	Moderate	Below 100 eV: very low
					Calculation
	Mitroy 1987	[19]	_	Low	Calculation
	Moores (2CC) 1972	[22]	_	Low	Two center close-coupling calculation
	Moores (4CC) 1972	[22]	_	Low	Four center close-coupling calculation
	Phelps 1981	[25]	_	High	Experiment
	Srivastava 1980	[26]	_	Moderate	Experiment
	Zapesochnyi 1976	[27]	[28]	Very low	Experiment
$3s \rightarrow 3d$	Moores (2CC) 1972	[22]	_	Low	Two center close-coupling calculation
	Phelps 1981	[25]	_	High	Experiment
	Stumpf (PWBA) 1985	[29]	_	Moderate	Born approximation calculation
	Stumpf (EXP) 1985	[29]	_	High	Experiment
	Verma 1996	[30]	_	Low	Calculation
$3s \rightarrow 4s$	Moores (2CC) 1972	[22]	_	Low	Two center close-coupling calculation
	Phelps 1981	[25]	_	High	Experiment
	Srivastava 1980	[26]		Moderate	Experiment
$3s \rightarrow 4p$	Phelps 1981	[25]	_	High	Experiment
$3s \rightarrow 4d$	Phelps 1981	[25]	_	High	Experiment
$3p \rightarrow 3d$	Stumpf 1985	[29]	_	Moderate	Experiment

Table A

Used publications for electron-impact target excitation cross sections. The columns contain the following information: (1) transition in question. (2) name of the data in the graphs. (3) original reference. (4) if applicable the publication where the used data were taken from. (5) weight in fit according to assigned credibility. (6) comment.

	Electron	n-impact targ	get ionization			
Ground state	Name	Published in	Referenced in	Weight in fit	Comment	
3s	Bates 1965	[31]	[32]	Low	Calculation	
	Fujii, Srivastava 1995	[33]	_	Very high	Experiment	
	Johnston 1995	[34]	_	Moderate	Experiment	
	McGuire 1971	[35]	_	Low	Calculation	
	McGuire 1997	[36]	_	Moderate	Calculation	
	Rakstikas 2001	[37]	_	High	Calculation	
	Tan 1996	[38]	_	High	Experiment	
	Zapesochnyi 1968	[39]	[38]	Low	Experiment	
3p	Tan 1996	[38]	_	High	Experiment	

Table B

Used references for electron-impact target ionization cross sections. For description of column contents see Table A.

$$\sigma_{0,e^{-}}^{ION}(E/eV)[cm^{2}] = \frac{A_{7} \cdot 10^{-13}}{E \cdot I_{nl}} \cdot \left[ A_{5} \cdot \ln \left( \frac{E}{I_{nl}} \right) + A_{6} \cdot \exp \left( -\frac{E}{I_{nl}} \right) + \right]$$

$$+ \sum_{j=1}^{4} A_{j} \cdot \left( 1 - \frac{I_{nl}}{E} \right)^{j-1}$$

$$\forall E \geq E_{low}$$

$$(2)$$

Neither this fit formula nor the CCC calculations take into account that at impact energies above the binding energy of the 2s and 2p subshells inner-shell ionization possibly occurs. We proceeded in the following way: first the available cross section data were collected and fitted and then the contribution of inner-shell ionization was added to the fitting curve. We used the Lotz-Formula (Eq.(3)) that provides an analytical evaluation of inner-shell ionization [56]. In this case the Lotz-formula is outlined explicitely as follows:

$$\sigma_{2p}^{ION}(E/eV)[cm^{2}] = q_{2p} \cdot L_{1} \cdot \frac{\ln(E/I_{2p})}{E \cdot I_{2p}} \cdot \left\{ 1 - L_{2} \cdot \exp(-L_{3}(E/I_{2p} - 1)) \right\}$$

$$\sigma_{2s}^{ION}(E/eV)[cm^{2}] = q_{2s} \cdot L_{4} \cdot \frac{\ln(E/I_{2s})}{E \cdot I_{2s}} \cdot \left\{ 1 - L_{5} \cdot \exp(-L_{6}(E/I_{2s} - 1)) \right\}$$

$$(3)$$

The input parameters to Eq.(3) according to [57] are:  $I_{2p} = 34$  eV and  $I_{2s} = 67$  eV, the binding energies of 2p respectively 2s electrons,  $q_{2p}=6$  and  $q_{2s} = 2$ , the number of equivalent 2p respectively 2s electrons, and  $L_1, \ldots, L_6$  are sets of individual constants for the 2p respectively 2s subshell.

The overall formula for electron-impact target ionization now presents as

<b>2</b> p	electr	ons	2s electrons			
$a_2$	$a_2$ $b_2$		$a_3$	$b_3$	$c_3$	
3.49	0.81	0.087	10.8	0.46	1.5	

Table D

Parameters for the Lotz formula, Eq.(3. The values vary slidely from the ones presented by Lotz [56], but represent the experimental values excellently.

$$\sigma_{e^{-}}^{ION}(E/eV)[cm^{2}] =$$

$$\forall \quad E_{low} \le E \le I_{2p}$$

$$= \begin{cases} \sigma_0^{ION} & \forall E_{low} \leq E \leq I_{2p} \\ \sigma_0^{ION} + \sigma_{2p}^{ION} & \forall I_{2p} \leq E \leq I_{2s} \\ \sigma_0^{ION} + \sigma_{2p}^{ION} + \sigma_{2s}^{ION} & \forall E \geq I_{2s} \end{cases}$$

$$(4)$$

The constants in Eq.(3) have to be determined either by experiment, theory, or reasonable guesswork [57]. We were able to gather experimental data on ionization from the ground state in the energy region were inner-shell ionization occurs, see [33]. We now used Eq.(2 to fir ionization of the valence electron without considering inner-shell ionization. This led to the red line curve in Fig.2. Now the parameters  $A_1, \ldots, A_7$  remained constant and we used

$$\sigma_{\text{core}}^{ION}(E/eV)[cm^2] = \begin{cases} \sigma_{2p}^{ION} & \forall I_{2p} \leq E \leq I_{2s} \\ \sigma_{2p}^{ION} + \sigma_{2s}^{ION} & \forall E \geq I_{2s} \end{cases}$$
(5)

with variable parameters  $L_1, \ldots, L_6$  to fit the inner-shell contribution. The obtained parameters, see Tab. D, vary slidely from the original parameters presented by Lotz [56], but represent the experimental values excellently. We therefore used these new t parameters, see Tab. D, to derive the core corrections in all ionization cross sections. In this way not only ionization including the core-correction but also pure valence ionization is represented for all transitions.

Fig.2 presents ground state electron impact ionization. It shows very clearly that the contributions from the core electrons are substantial in the high energy region and cannot be neglected.

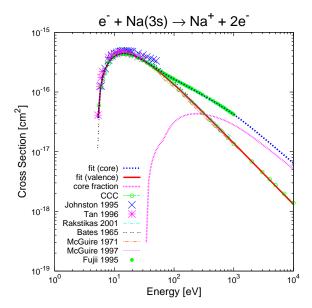


Fig. 2. Electron-impact target ionization from Na(3s). The fit of the valence is plotted according to Eq.(2) and Tab.2. The fit containing inner shell ionization ("fit with core") is plotted according to Eq.(4), where the core correction is added to Eq.(2) according to Eq.(3)) and Tab. D. The core fraction represents the contribution of inner-shell ionization according to Eq.(5) and Tab. D.

#### 3.3. Collisions with Protons

If the velocities of relative motion are the same, and are sufficiently high, the cross sections for proton-atom collisions are equal to the cross sections for the corresponding electron-atom collision. The electron-impact cross sections need to be scaled according to the formula [58]

$$E_{H^{+}}[\text{keV}] = 0.9165 \cdot E[\text{eV}] \cdot \left(1 - 0.5 \cdot \frac{\Delta E}{E} + \sqrt{1 - \frac{\Delta E}{E}}\right)$$
(6)

This scaling is appropriate in the asymptotic region at high energies where Born approximation cross sections for  $\mathrm{H^+}$  and  $\mathrm{e^-}$  are the same at the same relative velocity of collision partners, since in this region the mechanism of direct excitation is the same for electrons and protons, see Fig.3. In the graphs depicting proton-impact target excitation cross sections, these scaled electron-impact cross sections are labeled "scaled CCC".

When the impact energy of the incident proton is lowered, a change from direct excitation to the forming of a quasi-molecule takes place. In this energy

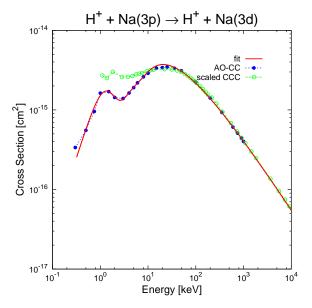


Fig. 3. Results from atomic-orbital close-coupling calculations for the Na(3p  $\rightarrow$  3d) excitation process in collisions of H<sup>+</sup> with Na(3p) in comparison with the corresponding fit (Eq.(7), Tab.3 & 4) and with the scaled electron impact cross section. The latter has been derived from the new CCC calculations by applying the scaling relation from [58] (Eq.(6))

region the scaling relation (6) is no longer valid and single electron charge transfer becomes the dominant process. Originating from this interference of SEC and EXC channels the cross sections show oscillations. Due to this more complex behavior a formula with twelve fit parameters has to be used for proton-impact target excitation.

$$\sigma_{H^{+}}^{EXC}(E/keV)[cm^{2}] =$$

$$A_{1} \cdot 10^{-16} \left\{ \frac{e^{-A_{2}/E} \cdot (A_{12} + \ln(A_{11} + A_{3}E))}{E} + A_{4} \cdot \frac{e^{-A_{5}E}}{E^{A_{6}}} + A_{7} \cdot \frac{e^{-A_{8}/E}}{1 + A_{9} \cdot E^{A_{10}}} \right\}$$

$$\forall E \geq E_{low}$$

$$(7)$$

The fit parameters for EXC processes  $Na(nl \rightarrow n'l')$  in collisions with  $H^+$  are listed in Table 3 & 4. The theoretical data defining the fit for the Na(3p  $\rightarrow$  3d) EXC cross section are presented in Fig.3 together with the fitted curve and the scaled electron-

impact cross section derived from CCC results by using the scaling relation from [58] (Eq.(6)). The AO data from Na(nl  $\rightarrow$  n'l') EXC processes with n=3-5 and n'=3-5 are shown in Graphs in section 8.3 together with the fits and compared with experimental and other theoretical data where available and the scaled CCC cross sections; the comparison will be further discussed in the next section.

Proton-impact target electron loss (ELOSS) is the sum of proton-impact ionization and proton-impact single electron capture (SEC). There are no ELOSS data available in the literature. But there are data for both proton-impact SEC and ION. Fig.4–6 show, using the ground state Na(3s) as an example, how our new AO-CC calculations predict both SEC and ION cross sections excellently and how the SEC and ION fits if added together agree excellently with our AO-CC calculation of ELOSS. ION and SEC cross sections were fitted using the same formula.

$$\sigma_{H^{+}}^{ION,SEC}(E/keV)[cm^{2}] =$$

$$= A_{1} \cdot 10^{-16} \left\{ \frac{e^{-A_{2}/E} \cdot (A_{12} + \ln(A_{11} + A_{3}E))}{E} + A_{4} \cdot \frac{e^{-A_{5}E}}{E^{A_{6}}} + A_{7} \cdot \frac{e^{-A_{8}/E}}{1 + A_{9} \cdot E^{A_{10}}} \right\}$$

$$\forall E \geq E_{low}$$

$$(8)$$

with the fit parameters  $A_1 - A_{12}$ , tabulated in Tab.5, and  $\mathbf{E}_{low}$  again the energy limit in the low energy region.

Finally the combined cross section, i.e. target electron loss, was fitted using the following formula:

$$\sigma_{H^+}^{ELOSS}(E/keV)[cm^2] = A_1 \cdot 10^{-16}$$

$$\left\{ \frac{e^{-A_2/E} \cdot \ln(1 + A_3 E)}{E} + A_4 \cdot \frac{e^{-A_5 E}}{E^{A_6}} \right\} \tag{9}$$

$$\forall E \geq E_{low}$$

where  $A_1 - A_6$  are the fit parameters, see Tab.5, and  $E_{low}$  the limit of the validity of the fit in the low energy region.

The data for ELOSS involve processes with initial Na(nl)  $\forall n \leq 5$ . They have been compared with

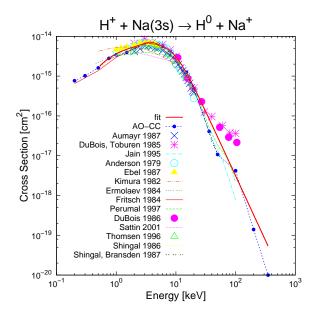


Fig. 4. Proton-impact single-electron capture cross sections from Na(3s). For references see Tab. F.

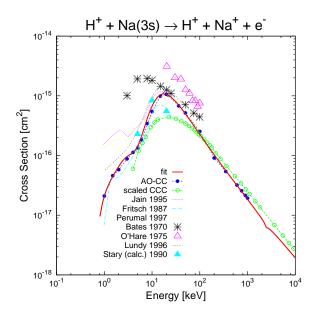


Fig. 5. Proton-impact target target ionization cross sections from Na(3s). For references see Tab. G.

scaled CCC calculation of electron-impact ionization cross sections. The agreement between these data is expected to be good in the energy region above  $\approx 100$  keV where ionization is the dominant process in ELOSS. Unfortunately, the agreement is not always as good as hoped. This is due to the insufficient representation of ionization channels in the

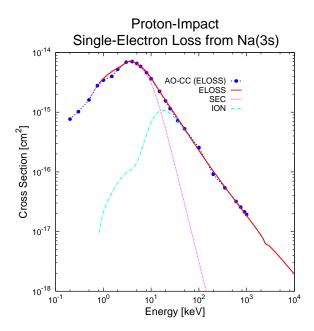


Fig. 6. Proton-impact target electron loss cross sections from Na(3s). AO-CC (ELOSS): present AO-CC calculations. ELOSS: fit for electron loss (Eq.(9)). SEC: fit for single-electron capture (Eq.(8)). ION: fit for ionization (Eq.(8))

AO-CC calculations. Furthermore the AO calculations neither include SEC from Na inner shells nor ionization of the latter.

# 3.4. Scaling Relations for Collisions with Multiply Charged Ions

A realistic fusion plasma is always polluted by a certain amount of impurity ions. Thus, to achieve satisfactory quality in simulations, it is necessary to include sodium - impurity ion collisions. The behavior of EXC cross sections with respect to a rescaling relation with projectile charge state q and mass m (in amu), derived from a three-state close-coupling dipole approximation [71] [72]. This scaling formula with respect to the electron binding energy  $E_b$  of the initial state of the target sodium and the charge of the fully stripped projectile has been derived for single electron charge transfer from excited hydrogen atoms H(n) in a wide impact energy range. The same reduced impact energy and cross section are introduced for target excitation [17]

$$E_{\text{red.}}^{\text{EXC}} = \frac{E}{q}, \qquad \sigma_{\text{red.}}^{\text{EXC}} = \frac{\sigma}{q}$$
 (10)

and for single electron capture [17]

$$E_{\rm red.}^{\rm ELOSS} = \frac{n^2 \cdot E}{\sqrt{q}}, \qquad \sigma_{\rm red.}^{\rm ELOSS} = \frac{\sigma}{n^4 q}$$
 (11)

where n is the principal quantum number of the sodium target with respect to the binding energy  $(n = (2E_b)^{-1/2})$  [17]. These well approved scaling relations have been applied to collisions involving He<sup>2+</sup>, and Be<sup>4+</sup> projectiles. Fig. 7 shows calculated excitation cross sections (Na(3s)  $\rightarrow$  Na(3p)) by ion impact, whereas Fig.8 shows the corresponding reduced cross sections (in terms of Eq.(10)). In the energy region above reduced energies E/q of about 3 keV/amu, the fit of the proton-impact cross section (Eq.(7), Tab.3 & 4) represents the other reduced cross sections well. A similar behavior can be observed for excitation from Na(3p) to Na(3d) and to Na(4s), see Fig. 9 and Fig. 10, respectively. The qscaling typically breaks down below reduced energies E/q < 3 keV/amu. In this low impact energy range no general behavior of EXC cross sections with respect to q can be expected.

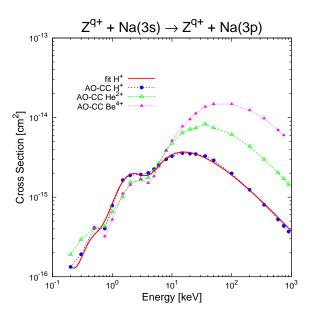


Fig. 7. Cross sections of collisions of Na with  $H^+$ ,  $He^{2+}$ , and  $Be^{4+}$  ions for the transition Na(3s)  $\rightarrow$  Na(3p). The fit is for proton-impact excitation in terms of Eq.(7) and Tab.3 & 4

Fig.11 and 12 show reduced ELOSS cross sections from Na(ns) and Na(np) initial states, respectively. In the reduced energy region below 10 keV/amu reduced ELOSS cross sections from Na(ns) become almost independent from the energy of the incident particle, except for the  $\rm H^+$  - Na(3s) case (see Fig.11). The behavior of the latter is typical for a

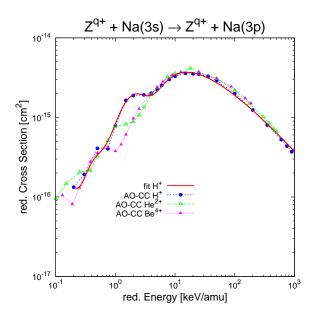


Fig. 8. Reduced cross sections  $\sigma/q$  of collisions of Na with H<sup>+</sup>, He<sup>2+</sup>, and Be<sup>4+</sup> ions for the transition Na(3s)  $\rightarrow$  Na(3p). For reduced energies  $E/q > 3 \frac{\text{keV}}{\text{amu}}$ , the reduced cross sections of He<sup>2+</sup> and Be<sup>4+</sup> follow the proton-impact cross section very well. The fit is for proton-impact excitation in terms of Eq.(7) and Tab.3 & 4

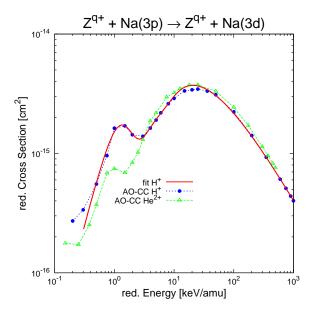


Fig. 9. Reduced cross sections  $\sigma/q$  of collisions of Na with H<sup>+</sup> and He<sup>2+</sup> ions for the transition Na(3p)  $\rightarrow$  Na(3d). The fit is for proton-impact excitation in terms of Eq.(7) and Tab.3 & 4

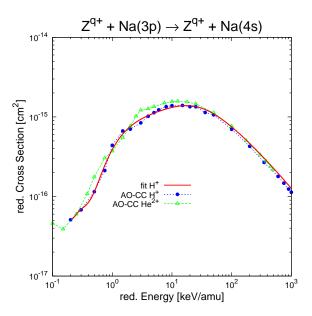


Fig. 10. Reduced cross sections  $\sigma/q$  of collisions of Na with H<sup>+</sup>, He<sup>2+</sup>, ions for the transition Na(3p)  $\rightarrow$  Na(4s). The fit is for proton-impact excitation in terms of Eq.(7) and Tab.3 & 4

non-resonant SEC, whereas all other collision systems are close to resonance (H<sup>+</sup> - Na(4s,5s)) or are quasi-resonant ( $\mathbb{Z}^{q+}$  - Na(ns)). Therefore the fitted (Eq.(9)) reduced He<sup>2+</sup> ELOSS cross section represents a general curve from which cross sections for any projectile of higher q and initial Na(ns) can be derived. In the case of initial Na(np) the situation is similar and again the fit to the He<sup>2+</sup> data serve as the general curve from which all cross sections for higher charged projectiles can be derived. Tab.8 shows the corresponding fit parameters. For even higher excited initial Na(nl) the scaling relation (Eq.(11)) can be directly applied to the fit of H<sup>+</sup> - Na(nl).

		Proton-impa	ct target excita	ation	
Transition	Name	Published in	Referenced in	Weight in fit	Comment
$3s \rightarrow 3p$	Allen 1988	[40]	[41]	Very high	Experiment
	Aumayr 1987	[42]	_	Very high	Experiment
	Fritsch 1987	[43]	[44]	High	Calculation
	Howald 1983	[45]	_	Low	Experiment
	Jain 1995	[46]	_	High	Calculation
	Jitschin 1986	[47]	_	Low	Experiment
	Lavrov 1983	[48]	[49]	Low	Experiment
	Shingal (AO) 1986	[50]	_	High	Atomic-orbital calculation
	Shingal, Bransden 1987	[44]	_	Low	Calculation
	Stary 1990	[51]	_	Moderate	Calculation
	Theodosiou 1987	[49]	_	Very low	Calculation
$3s \to 3d$	Anderson 1979	[52]	_	Moderate	Experiment
	Anderson 1985	[53]	_	Moderate	Experiment
	Jain 1995	[46]	_	High	Calculation
	Shingal, Bransden 1987	[44]	_	High	Calculation
	Theodosiou 1987	[49]	_	Low	Calculation
$3s \rightarrow 4s$	Theodosiou 1987	[49]	_	Low	Calculation
$3s \rightarrow 4p$	Theodosiou 1987	[49]	_	Low	Calculation
$3s \rightarrow 4d$	Theodosiou 1987	[49]	_	Low	Calculation
$3s \rightarrow 4f$	Theodosiou 1987	[49]	_	Low	Calculation

Table C

Used references for proton-impact target excitation. For description of column contents see Table A.

	$\mathbf{E_{low}}$	$\mathbf{A_1}$	$\mathbf{A_2}$	$\mathbf{A_3}$	$\mathbf{A_4}$	$A_5$	$\mathbf{A_6}$	$A_7$	$A_8$	$\mathbf{A_9}$	$A_{10}$	$A_{11}$	$A_{12}$
ION	1	8.389	8.83	$-7.95 \cdot 10^{-4}$	-0.179	0.4266	-2.554	1.13	2.095	$1.52{\cdot}10^{-3}$	1.998	2.02	21.21
SEC	0.5	24.21	1.0	0	$1.68 \cdot 10^{-3}$	5.02	-18.34	3.342	0.798	$8.155 \cdot 10^{-4}$	3.25	1.0	0

Table E

Fit parameters for proton-impact target ionization (ION) and single-electron capture (SEC) from Na(3s)

	Proton-im	pact single-ele	ectron capture		
Ground state	Name	Published in	Referenced in	Weight in fit	Comment
3s	Anderson 1979	[52]	[46]	High	Experiment
	Aumayr 1987	[42]	_	Very high	Experiment
	DuBois, Toburen 1985	[59]	_	Very high	Experiment
	DuBois 1986	[60]	_	Moderate	Experiment
	Ebel 1987	[61]	_	Moderate	Experiment
	Ermolaev 1984	[62]	[61]	Moderate	Calculation
	Fritsch 1984	[63]	_	Very high	Calculation
	Jain 1995	[46]	_	Very high	Calculation
	Kimura 1982	[64]	[61]	Low	Calculation
	Permual 1997	[65]	_	Moderate	Calculation
	Sattin 2001	[66]	_	Very low	Calculation
	Shingal 1986	[50]	_	High	Calculation
	Shingal, Bransden 1987	[44]	_	High	Calculation
	Thomsen 1996	[67]	[66]	High	Experiment

Used references for proton-impact single-electron capture cross sections. For description of column contens see Table A

		Proton-im	pact target ion	nization	
Ground state	Name	Published in	Referenced in	Weight in fit	Comment
3s	Bates 1970	[68]	[65]	Low	Experiment
	Fritsch 1987	[43]	[46]	High	Calculation
	Jain 1995	[46]	_	Moderate	Calculation
	Lundy 1996	[69]	_	Moderate	Calculation
	O'Hare 1975	[70]	_	Low	Experiment
	Perumal 1997	[65]	_	Moderate	Calculation
	Stary (calc.) 1990	[51]	_	Low	Optical potential calculations

Table G

Used references for proton-impact target ionization cross sections. For description of column contents see Table A

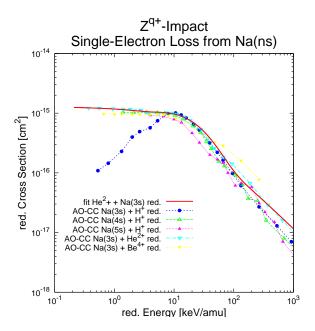


Fig. 11. Reduced cross sections of collisions of Na(ns) with  $\rm H^+, He^{2+}$ , and  $\rm Be^{4+}$  ions resulting in Na electron loss. Eq.(9) was fitted to the reduced  $\rm He^{2+}$  cross section. For parameters see Tab.8.

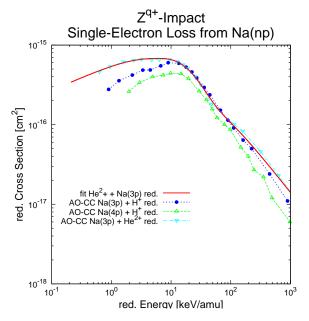


Fig. 12. Reduced cross sections of collisions of Na(np) with  $\rm H^+$  and  $\rm He^{2+}$  ions resulting in Na electron loss. Eq.(9) was fitted to the reduced  $\rm He^{2+}$  cross section. For parameters see Tab 8

Ī	nl	$\mathbf{E_{low}}$	$\mathbf{A_1}$	$\mathbf{A_2}$	$A_3$	$\mathbf{A_4}$	$A_5$	$\mathbf{A}_{6}$
l	3s	0.2	3.70587	15.8977	$\text{-}6.4856 \!\cdot\! 10^{10}$	3.31056	0.04344	0.01715
l	3p	0.2	4.5237	23.7408	$-6.4855 \cdot 10^{10}$	1.2994	0.08556	-0.33615

Table H

Fit parameters for reduced cross sections of  $\mathrm{He}^{2+}$  impact of  $\mathrm{Na(nl)};\ n=3.$ 

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#### 5. Explanation of Tables

Table 1: Fit Parameters for Electron-Impact Target-Excitation Cross Sections

of Na(nl 
$$\rightarrow$$
 n'l'); n, n' = 3 - 5

 $nl \rightarrow n'l'$  Initial – final states of the Na atom

 $\Delta$  E Excitation energy of the EXC process in eV

 $A_1, \ldots, A_7$  Fit parameters as in Eq.(1)

Table 2: Fit Parameters for Electron-Impact Target-Ionization Cross Sections

of Na(nl); 
$$n = 3 - 5$$

nl Initial state of the Na atom

 $I_{nl}$  Ionization energy in eV

 $A_1, \ldots, A_6$  Fit parameters as in Eq.(2)

Tables 3 & 4: Fit Parameters for Proton-Impact Target-Excitation Cross Sections

of Na(nl 
$$\rightarrow$$
 n'l'); n, n' = 3 - 5

 $nl \rightarrow n'l'$  Initial – final states of the Na atom

 $A_1, \ldots, A_{12}$  Fit parameters as in Eq.(7)

Table 5: Fit Parameters for Proton-Impact Target-Electron-Loss Cross Sections

of Na(nl); 
$$n = 3 - 5$$

nl Initial state of the Na atom

 $A_1, \ldots, A_6$  Fit parameters as in Eq.(9)

### 6. Explanation of Graphs

Section 8.1: Electron-impact target-excitation cross sections of Na(nl  $\rightarrow$  n'l'); n, n' = 3 - 5

 $nl \rightarrow n'l'$ Initial – final states of the Na atom

Section 8.2: Electron-impact target-ionization cross sections from Na(nl); n = 3 - 5

nl Initial state of the Na atom

Section 8.3: Proton-impact target-excitation cross sections from Na(nl  $\rightarrow$  n'l'); n, n' = 3 - 5

 $nl \rightarrow n'l'$  Initial – final states of the Na atom

Section 8.4: Proton-impact target-electron-loss cross sections from Na(nl); n = 3 - 5

nl Initial state of the Na atom

## 7. Tables

$\mathbf{nl} \to \mathbf{n'l'}$	$\Delta \mathbf{E}$	$\mathbf{A_1}$	A <sub>2</sub>	A <sub>3</sub>	$\mathbf{A_4}$	$\mathbf{A_5}$	$\mathbf{A_6}$	$A_7$
$3s \rightarrow 3p$	2.09937	-23.3231	38.358	-5.70599	-3.4816	27.1453	0.453874	14.7003
$3s \rightarrow 3d$	3.61642	54.0317	-27.3057	-28.6423	35.1405	-0.288761	0.381653	1.04435
$3s \rightarrow 4s$	3.19192	2.51105	-10.8455	21.3071	-13.2455	0	0.58	11.3285
$3s \rightarrow 4p$	3.75248	10.5845	-44.94	74.7574	-40.3895	2.12788	$5.9750 \cdot 10^{-3}$	1.67677
$3s \rightarrow 4d$	4.28447	6.22968	10.1143	-34.6957	32.5314	0.13928	1.08379	2.04554
$3s \rightarrow 4f$	4.28855	0.753717	13.9336	-35.7825	31.9556	0.0297361	0.814152	1.67582
$3s \rightarrow 5s$	4.11711	18.3199	-52.2671	52.2258	4.31253	0.877115	0.504837	0.253928
$3p \rightarrow 3d$	1.51705	-274.892	380.104	-38.007	-51.4476	208.52	$3.6757 \cdot 10^{-3}$	2.21269
$3p \rightarrow 4s$	1.09255	-8.15967	19.8158	-29.2698	28.5195	5.47456	0.948679	24.7919
$3p \rightarrow 4p$	1.65311	4.87684	-11.1746	16.1142	-6.00012	0.100725	0.791831	14.9378
$3p \rightarrow 4d$	2.1851	-2.1686	-36.4101	86.9806	-38.8431	16.307	0.06977	2.2177
$3p \rightarrow 4f$	2.18918	2.3848	3.1897	-19.6921	21.5142	-0.0105359	0.839963	15.4706
$3p \rightarrow 5s$	2.01774	1.2911	-14.0441	29.5538	-16.5211	1.56757	0.02045	3.2114
$3d \rightarrow 4p$	0.13606	-4.17001	-10.1151	137.921	-59.7171	11.0426	3.96822	60.5028
$3d \rightarrow 4d$	0.668046	4.64022	15.006	-147.95	270.543	0.176582	2.6348	46.0857
$3d \rightarrow 4f$	0.672127	$-1.6638 \cdot 10^3$	$1.5201 \cdot 10^3$	334.707	$4.8787 \cdot 10^3$	$1.0803 \cdot 10^3$	2.38353	1.18888
$3d \rightarrow 5s$	0.50069	0.354729	11.0975	-38.9064	67.6696	0.0158897	2.77575	50.1735
$4s \to 3d$	0.4245	9.83953	-61.7689	180.035	-89.1436	0.208417	2.5022	49.9816
$4s \to 4p$	0.56056	-766.196	$1.45 \cdot 10^3$	0	0	539.17	3.36726	4.00164
$4s \to 4d$	1.09255	-1.05183	-73.0017	371.593	-654.485	-0.128653	4.49224	-47.2604
$4s \rightarrow 4f$	1.09663	-3.00114	-58.8159	333.103	-675.733	-0.11054	4.49224	-36.4141
$4s \rightarrow 5s$	0.92519	7.40763	-52.1312	116.889	-54.6344	1.06354	1.63344	10.6933
$4\mathrm{p} \to 4\mathrm{d}$	0.531986	$-2.1967 \cdot 10^3$	$3.4305 \cdot 10^5$	$-1.8810 \cdot 10^6$	$6.1742 \cdot 10^5$	$-2.2207 \cdot 10^4$	9.11098	-0.0493211
$4p \rightarrow 4f$	0.536067	411.469	$-2.3604 \cdot 10^3$	$4.932 \cdot 10^3$	$-2.3127 \cdot 10^3$	14.533	1.80954	1.5026
$4\mathrm{p} \to 5\mathrm{s}$	0.36463	-6.70865	-211.981	$1.3883 \cdot 10^3$	-522.46	16.0299	8.01689	36.2413
4d $\rightarrow$ 4f $^{\dagger}$	$4.08 \cdot 10^{-3}$	-335.85	$-1.7174 \cdot 10^3$	411.336	-2.99991	330.533	$3.3763 \cdot 10^{-5}$	11.1878
$5s \rightarrow 4d$	0.167356	4.25353	-45.5338	562.593	-151.995	$3.0812 \cdot 10^{-3}$	16.3001	560.193
$5s \rightarrow 4f$	0.171437	12.4203	-126.653	615.687	-306.243	-0.041334	4.36124	34.695

Table 1

Fit Parameters for Electron-Impact Target Excitation Cross Section of Na $(nl \rightarrow n'l')$ ; n, n' = 3 - 5 See page 16 for Explanation of Tables † The fit parameters for 4d  $\rightarrow$  4f are only valid above 0.2 eV.

nl	$I_{nl}$	$\mathbf{E_{low}}$	$\mathbf{A_1}$	$\mathbf{A_2}$	$\mathbf{A_3}$	$\mathbf{A_4}$	$A_5$	$\mathbf{A_6}$	A <sub>7</sub>
3s	5.13891	5.2	0	66.4483	24.5645	101.03	-5.0082	0	$4.37 \cdot 10^{-3}$
3р	3.03954	3.2	20.8332	-13.1449	-19.4089	33.258	0.542801	-56.3793	0.0379105
3d	1.52249	2.08	-105.202	-21.5898	485.919	-337.711	0.369663	331.13	0.0351848
4s	1.94699	2.5	-0.729955	-0.0916904	3.32036	-2.34172	$9.0515 \cdot 10^{-5}$	2.25425	3.72267
4p	1.38643	1.9	-28.9039	-6.49469	130.161	-92.2872	0.19249	91.127	0.176319
4d	0.850363	1.7	0.0711827	7.87424	-17.7004	8.79277	-0.0200515	-5.48488	-0.446075
4f	0.850363	1.3	1.8088	2.13387	-12.4468	8.35135	$-6.259 \cdot 10^{-3}$	-6.66904	-2.2193
5s	1.0218	1.5	-3.83331	-2.65103	21.742	-14.8678	$2.5528 \cdot 10^{-3}$	13.1159	1.28082

Table 2

Fit Parameters for Electron-Impact Target Ionization Cross Sections of the valence electron in Na(nl); n=3-5 See page 16 for Explanation of Tables.

Fits containing inner-shell ionization can be obtained using Eq.(4) & (3) together with Tab. D.

$\mathbf{nl}  o \mathbf{n'l'}$	$\mathbf{E_{low}}$	A <sub>1</sub>	$\mathbf{A_2}$	$A_3$	A <sub>4</sub>	$A_5$	$A_6$
$3s \rightarrow 3p$	0.2	899.91	0.813273	0.172984	0.171027	1.33781	-1.97329
$3s \rightarrow 3d$	0.2	2.35787	16.0799	$1.661 \cdot 10^8$	1.75626	1.88912	-3.32454
$3s \rightarrow 4s$	0.2	0.5291	11.1454	13.8	2.21	0.9258	-2.8909
$3s \rightarrow 4p$	0.3	12.287	1.00965	0.19894	-3.3202	4.7024	-6.149
$3s \rightarrow 4d$	1	0.09605	35.1151	0	6.5924	2.4005	-5.09985
$3s \rightarrow 4f$	1	0.4652	44.0372	0	1.51204	2.38218	-5.305
$3s \rightarrow 5s$	0.6	21.912	67.9026	2.72934	$3.5101 \cdot 10^{-3}$	0.941943	-3.9001
$3p \rightarrow 3d$	0.3	445.154	9.8646	0	0.0851	0.8208	-2.1403
$3p \rightarrow 4s$	0.2	875.942	0.0845244	3.2671	1.4616	0.12061	1.42592
$3p \rightarrow 4p$	0.3	13.2437	4.764	2.91617	1.44602	2.30177	-1.72801
$3p \rightarrow 4d$	0.2	795.051	4.7911	3.2671	$1.7546 \cdot 10^{-3}$	0.265715	-1.10414
$3p \rightarrow 4f$	0.5	17.6253	9.36216	0	0.892868	$7.8587 \cdot 10^{-3}$	0.782358
$3p \rightarrow 5s$	0.5	5.7944	6.98495	1.13626	107.387	6.9904	-7.1283
$3d \rightarrow 4p$	1	301.658	30.0346	0	35.9391	4.67224	-0.758748
$3d \rightarrow 4d$	0.2	30.3405	6.373	0	0.2148	0.2718	-1.382
$3d \rightarrow 4f$	0.2	8.8668	12.0228	1.26008	-1.73829	0.0960184	-1.04151
$3d \rightarrow 5s$	0.3	1.97042	2.82693	0	36.1299	8.32895	-0.842273
$4s \rightarrow 3d$	0.2	76.102	0.108	$1.4 \cdot 10^3$	4.79189	27.7	-45.7225
$4s \rightarrow 4p$	0.7	$3.0 \cdot 10^3$	0.181647	0.0152269	-1.00172	0.264541	0.553659
$4s \rightarrow 4d$	0.3	12.2821	7.48675	0	41.5655	2.9866	-2.8764
$4s \rightarrow 4f$	0.2	18.126	7.2308	0	0.3843	1.20817	-4.77267
$4s \rightarrow 5s$	1	4.57798	73.0856	11.2459	55.6678	3.64108	1.22198
$4p \to 4d$	0.2	$1.5105 \cdot 10^3$	41.0849	1.13114	5.48059	6.99795	-2.70534
$4\mathrm{p} \to 4\mathrm{f}$	0.2	98.1211	5.2274	0	0.1986	0.9862	-3.3092
$4\mathrm{p} \to 5\mathrm{s}$	0.2	695.167	0.379397	$1.2862 \cdot 10^{-3}$	-0.0266469	4.46338	-12.1889
$4d \rightarrow 4f$	0.4	$2.0 \cdot 10^3$	28.7819	0	35.9994	2.90774	-0.0355274
$5s \rightarrow 4d$	0.4	352.156	10.148	0	177.117	6.12077	-3.60091
$5s \rightarrow 4f$	0.4	50.441	12.0566	0	-2.32538	0.333314	-0.669005

Table 3 Fit parameters for proton-impact target excitation cross sections of  $Na(nl \rightarrow n'l')$ ; n, n' = 3 - 5 See page 16 for Explanation of Tables

$\boxed{\mathbf{nl} \rightarrow \mathbf{n'l'}}$	A <sub>7</sub>	A <sub>8</sub>	$\mathbf{A_9}$	A <sub>10</sub>	$\mathbf{A}_{11}$	A <sub>12</sub>
$3s \rightarrow 3p$	-9.90738	1.82931	20.1605	0.899862	0.934209	-0.012689
$3s \rightarrow 3d$	9.56875	14.1112	0.0318923	1.56873	1	9.13887
$3s \rightarrow 4s$	-6.0985	4.29572	$2.6 \cdot 10^{-3}$	2.1235	1.4632	93.1684
$3s \rightarrow 4p$	69.9622	30.4996	3.1234	1.48366	1.38235	-0.32704
$3s \rightarrow 4d$	21.6803	7.40333	$2.7 \cdot 10^{-3}$	1.91665	1	272.253
$3s \rightarrow 4f$	178.707	27.0857	0.0628	2.30125	$1.0 \cdot 10^{-10}$	29.7278
$3s \rightarrow 5s$	-43.6875	68.1887	1.82419	0.967314	6.44834	22.6012
$3p \rightarrow 3d$	-6.61	7.0552	0.2111	1.0887	1	26.1162
$3p \rightarrow 4s$	-95.267	-0.041652	13.4883	0.92967	0.126126	4.83299
$3p \rightarrow 4p$	34.7144	27.6903	0.19179	1.8542	0.525469	3.12512
$3p \rightarrow 4d$	-238.849	4.67249	6.89654	0.97723	-0.0730905	32.9442
$3p \rightarrow 4f$	-6.63413	-0.0354364	7.58916	1.01267	1	4.62623
$3p \rightarrow 5s$	8.6305	114.073	0.42788	1.3713	-1.70258	1.675
$3d \rightarrow 4p$	39.6619	1.22105	3.74937	0.881504	$2.8484 \cdot 10^{-7}$	24.8598
$3d \rightarrow 4d$	2.0156	0.4264	0.8904	2.6894	1	15.5586
$3d \rightarrow 4f$	7.83512	0.303191	0.0418302	0.788086	-1.89013	525.229
$3d \rightarrow 5s$	22.1788	0.981295	0.077633	1.8594	1	26.1051
$4s \rightarrow 3d$	74.7606	1.8727	7.4108	1.094	-41.05	-4.97677
$4s \rightarrow 4p$	67.7319	30.4687	17.8543	0.984028	1.78496	0.348832
$4s \rightarrow 4d$	47.503	67.1931	-0.91548	1.1443	0	100.0
$4s \rightarrow 4f$	1.0506	0.2524	$1.1 \cdot 10^{-3}$	2.35044	1	13.724
$4s \rightarrow 5s$	0.955863	0.0178534	$3.9414 \cdot 10^{-4}$	1.95208	-0.55916	61.0529
$4\mathrm{p} \to 4\mathrm{d}$	0.0721157	1.14453	$4.4491 \cdot 10^{-4}$	2.07563	3.00072	2.48347
$4\mathrm{p} \to 4\mathrm{f}$	0.5538	0.09157	0.0539	1.0939	1	9.278
$4\mathrm{p} \to 5\mathrm{s}$	0.276855	2.18819	0.0374898	0.954608	1.03331	$-1.3017 \cdot 10^{-3}$
$4d \rightarrow 4f$	39.7245	0.089685	1.96664	0.943349	$1.1334 \cdot 10^{-8}$	23.3783
$5s \rightarrow 4d$	283.157	4.75692	5.15505	2.46864	$8.1046 \cdot 10^{-4}$	20.1594
$5s \rightarrow 4f$	3.51249	-0.454977	0.0406219	1.83821	1.71289	14.6884

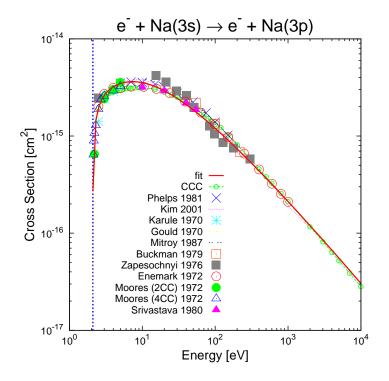
(cont.) Fit parameters for proton-impact target excitation cross sections of Na $(nl \rightarrow n'l')$ ; n, n' = 3 - 5See page 16 for Explanation of Tables

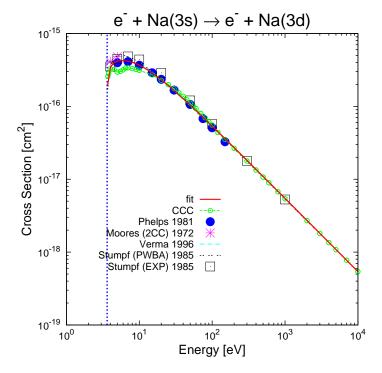
nl	$\mathbf{E_{low}}$	$\mathbf{A_1}$	$\mathbf{A_2}$	$A_3$	$\mathbf{A_4}$	$\mathbf{A}_{5}$	$\mathbf{A_6}$
3s	0.2	11.319	2.51212	$1.0 \cdot 10^5$	2.26648	0.172847	-0.73075
3р	0.2	27.8562	1.5103	$5.72 \cdot 10^4$	1.86786	0.0564	0.1081
3d	0.2	81.6464	1.4629	275.929	6.35454	0.372612	-0.0253238
4s	0.2	14.5812	1.0669	$5.16 \cdot 10^{13}$	27.661	0.249027	0.159263
4p	0.2	31.4476	1.3675	$3.1062 \cdot 10^9$	17.0752	0.665415	-0.369477
4d	0.2	66.0274	0.259161	$4.8614 \cdot 10^6$	942.831	8.1801	-12.8437
4f	0.2	76.1757	0.21478	131.206	20.4186	0.892532	-0.184057
5s	0.2	27.7031	0.135768	$2.0126 \!\cdot\! 10^{12}$	$1.260 \cdot 10^3$	4.14424	-3.75084

Table 5 Fit Parameters for Proton-Impact Target Electron Loss from Na(nl); n=3-5 See page 16 for Explanation of Tables

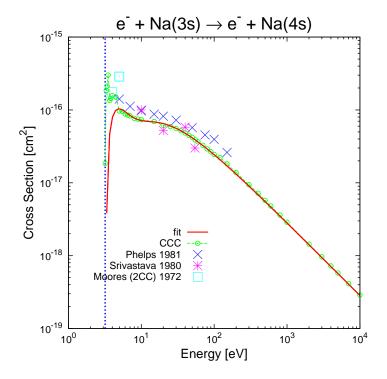
## 8. Graphs

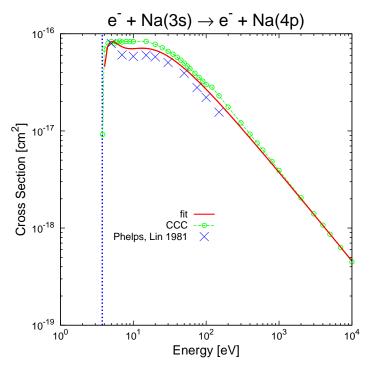
## 8.1. Electron-Impact Target Excitation Cross Sections

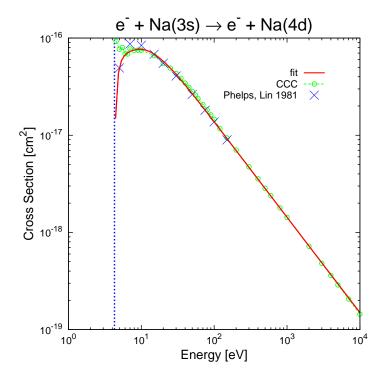


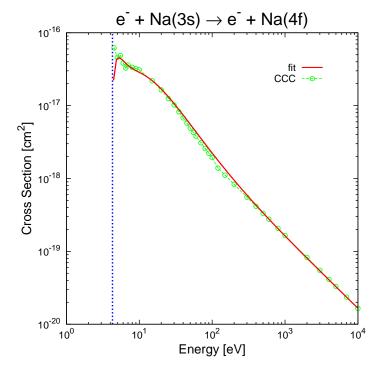


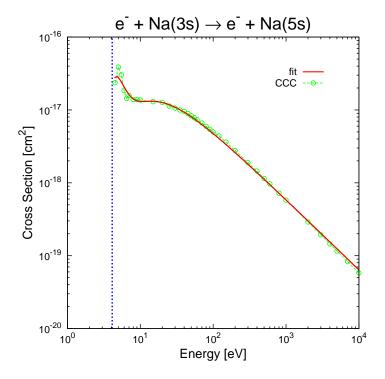
Graphs - 1

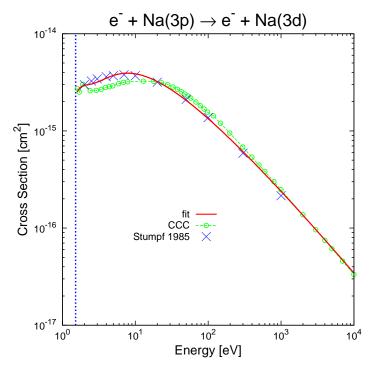


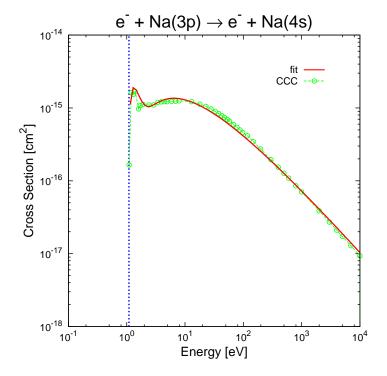


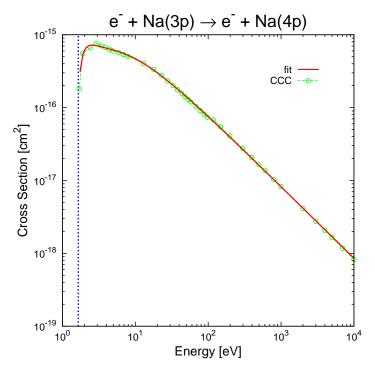


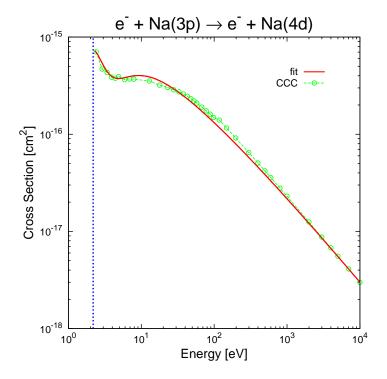


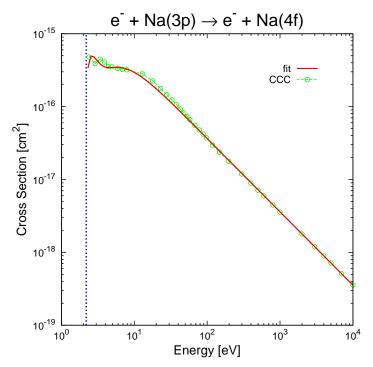


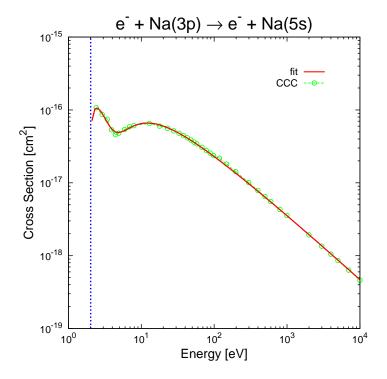


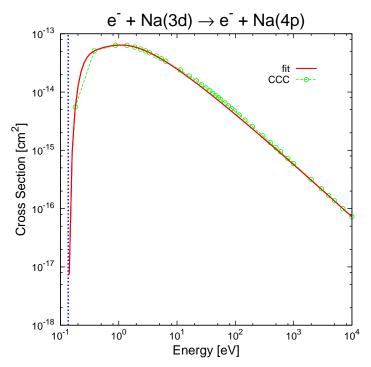


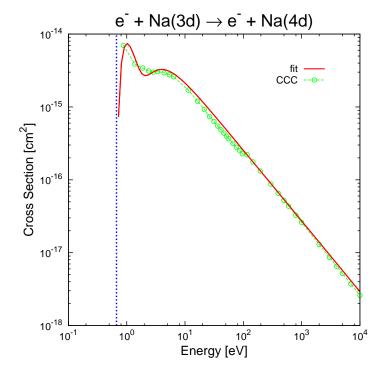


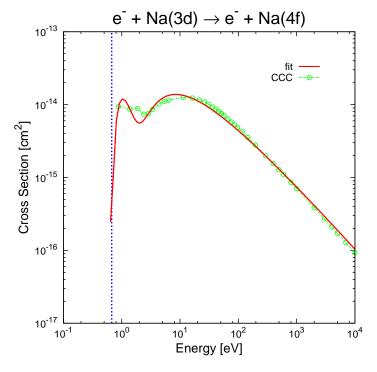


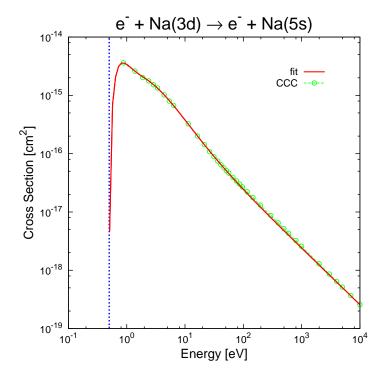


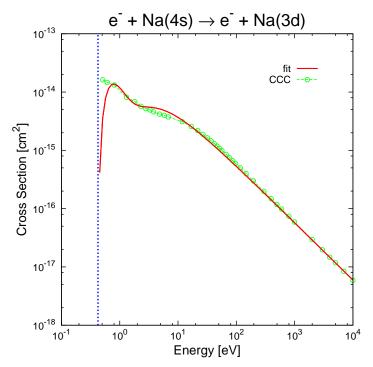


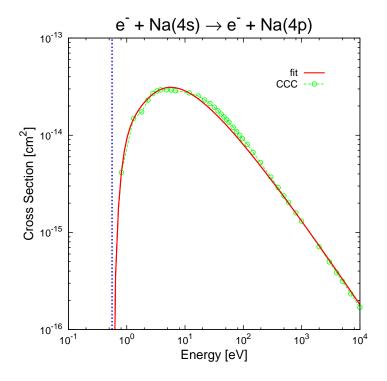


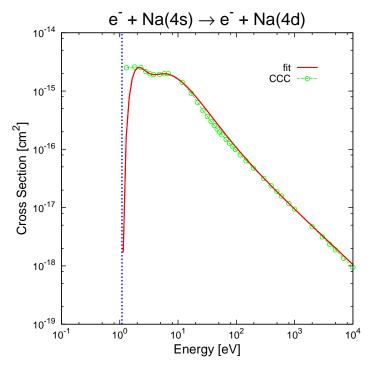


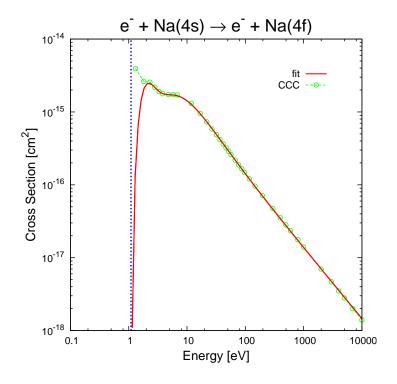


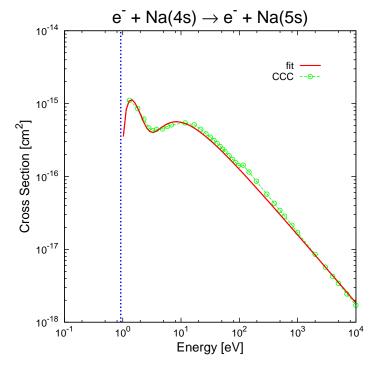




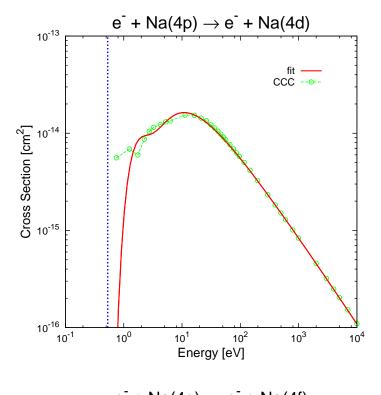


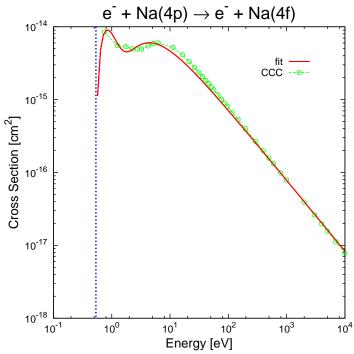




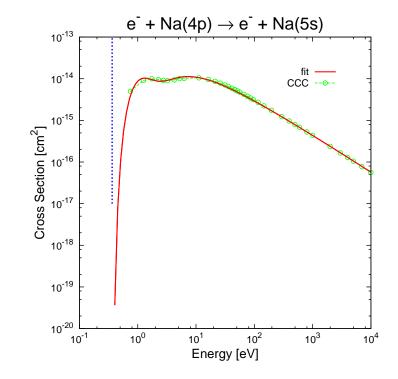


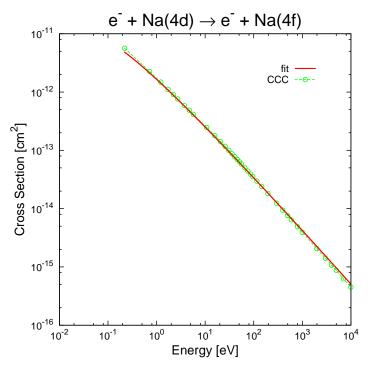
Graphs - 11

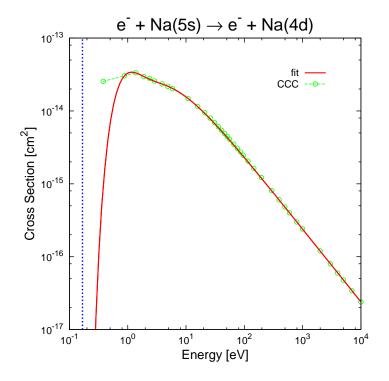


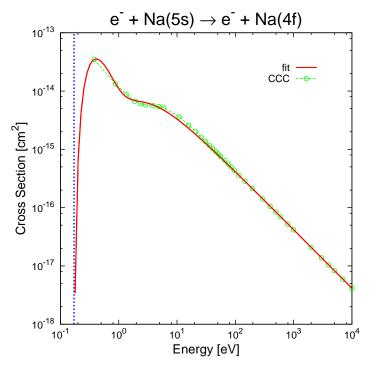


Graphs - 12

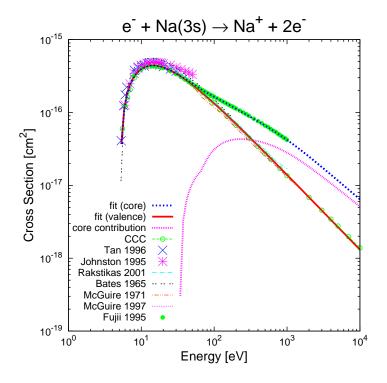


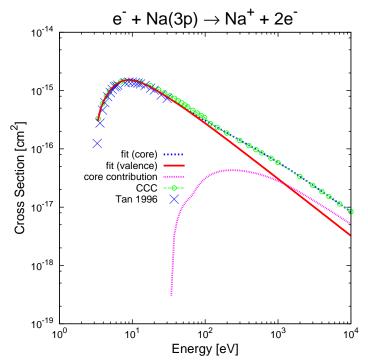




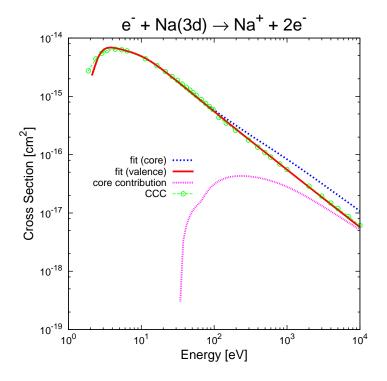


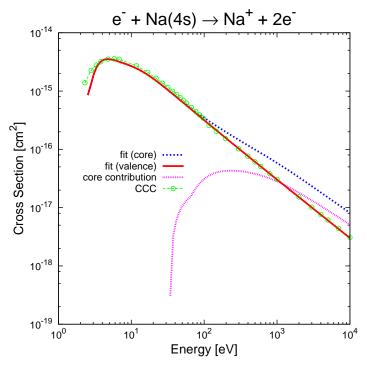
Graphs - 14

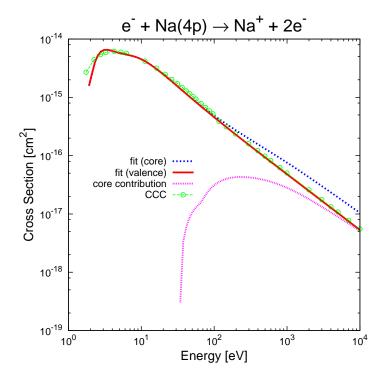


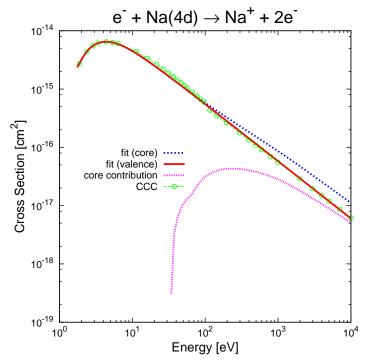


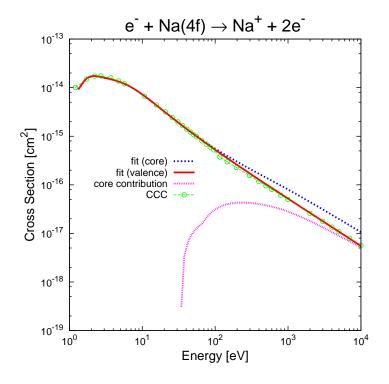
Graphs - 15

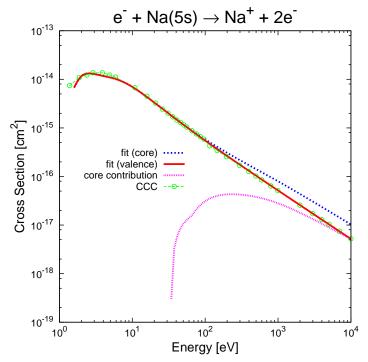


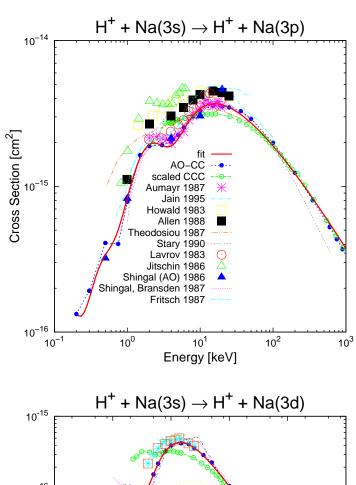


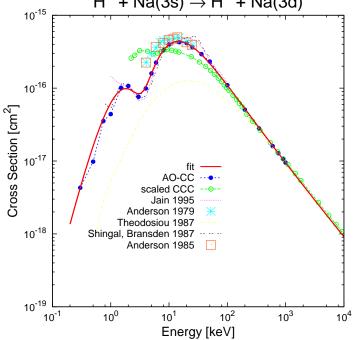




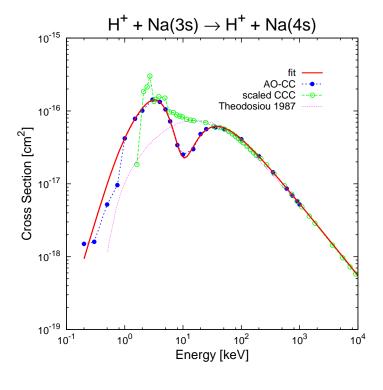


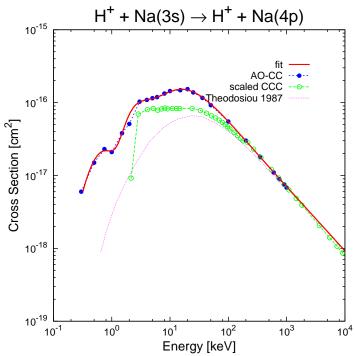


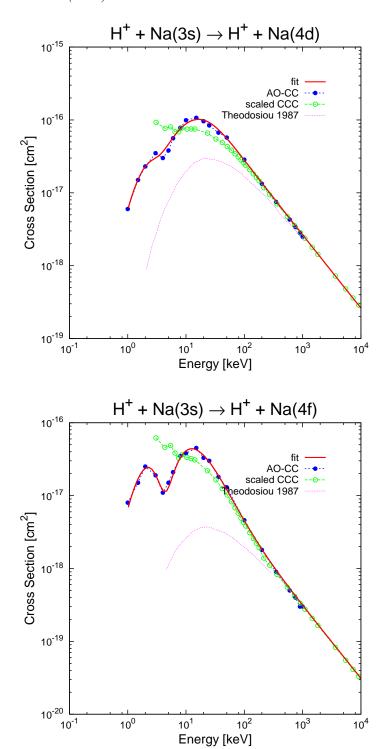


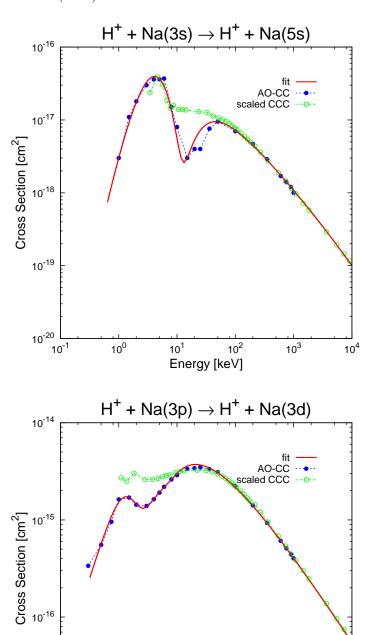


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10<sup>1</sup> 10<sup>2</sup> Energy [keV]

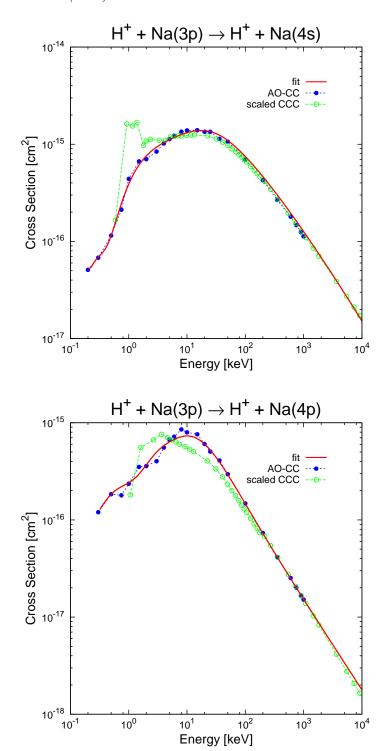
10<sup>3</sup>

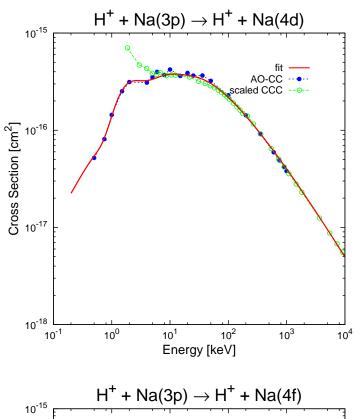
10<sup>4</sup>

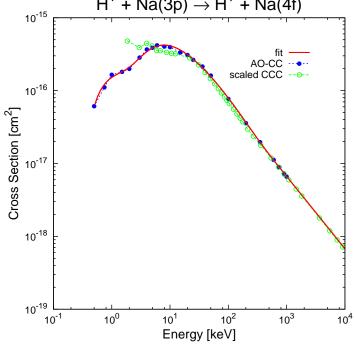
10<sup>-17</sup>

10<sup>-1</sup>

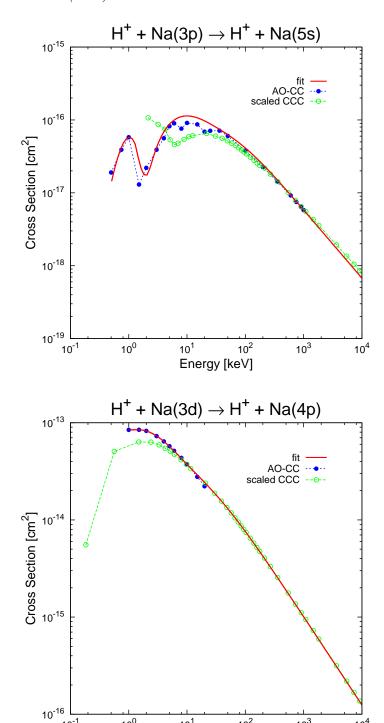
10<sup>0</sup>







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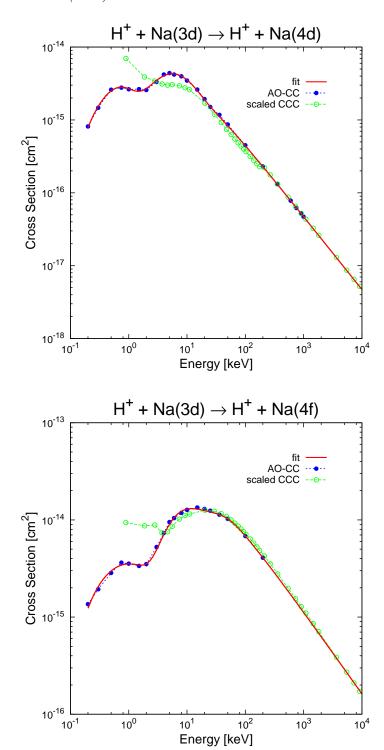
10<sup>1</sup> 10<sup>2</sup> Energy [keV]

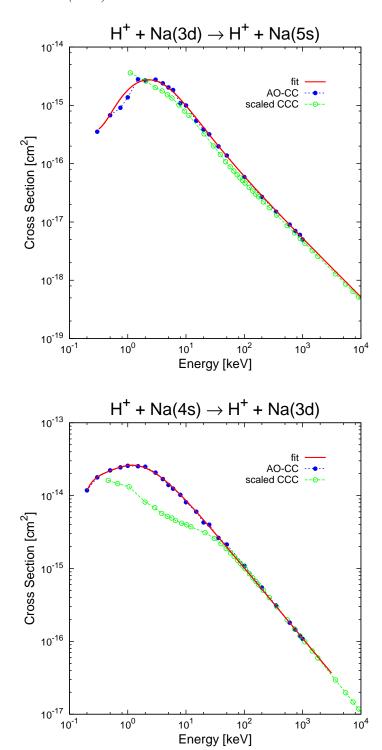
10<sup>3</sup>

10<sup>4</sup>

10<sup>0</sup>

10<sup>-1</sup>



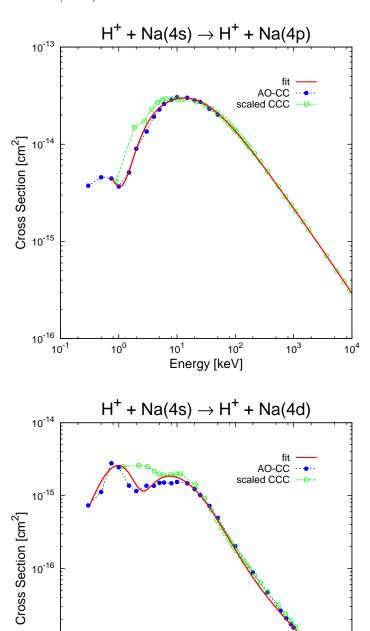


10<sup>-17</sup>

10<sup>-18</sup>

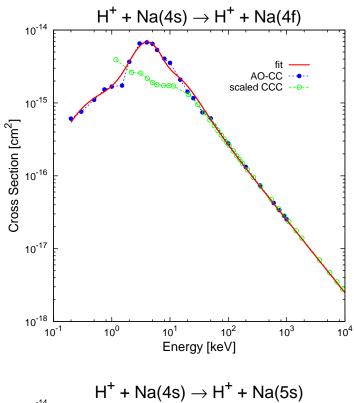
10<sup>-1</sup>

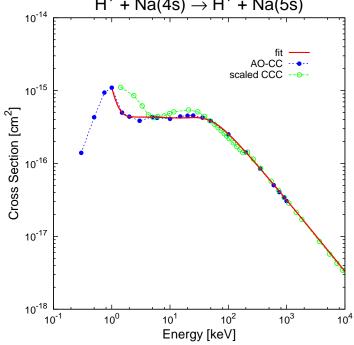
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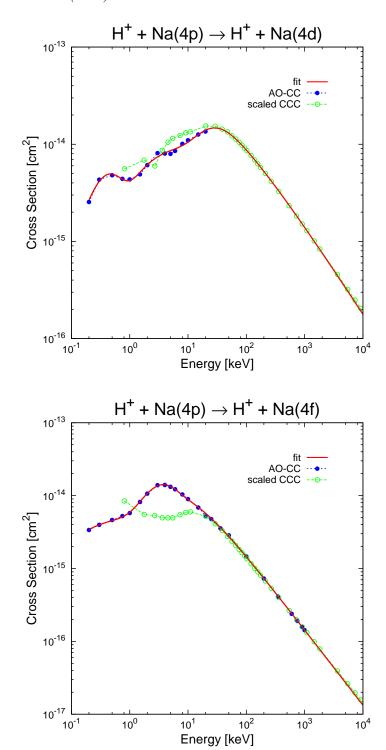


10<sup>1</sup> 10<sup>2</sup> Energy [keV] 10<sup>3</sup>

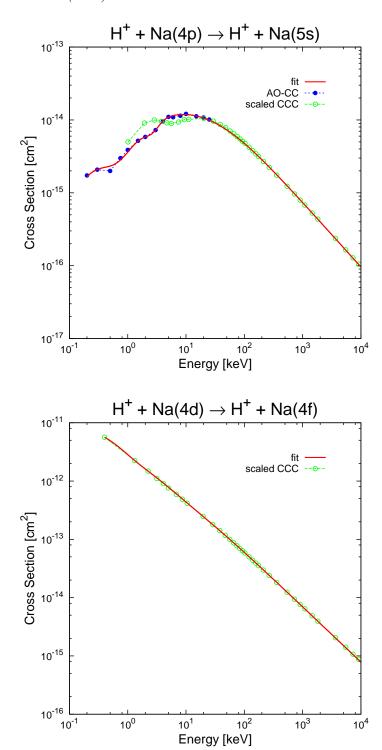
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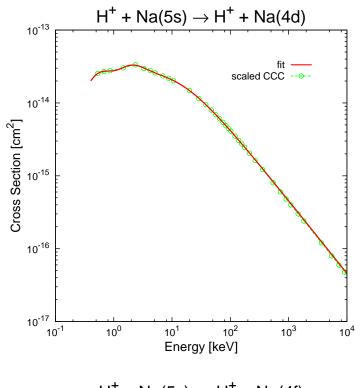


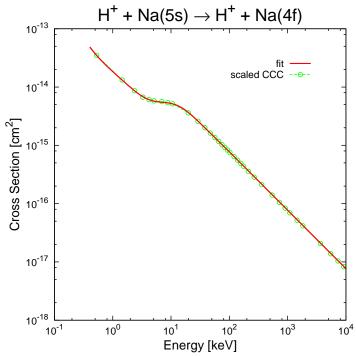


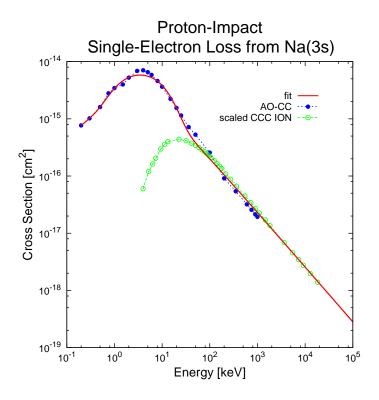


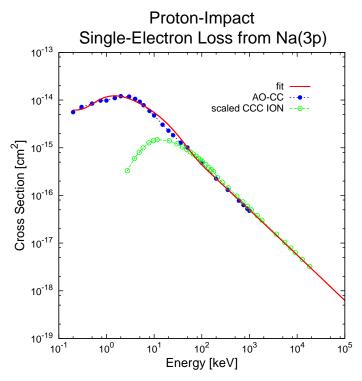
10<sup>-1</sup>



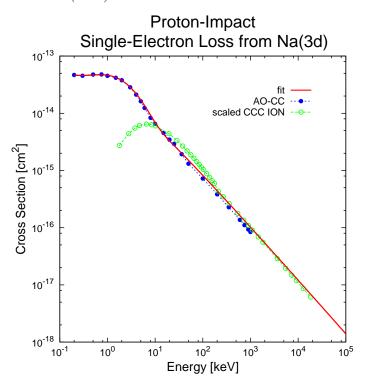


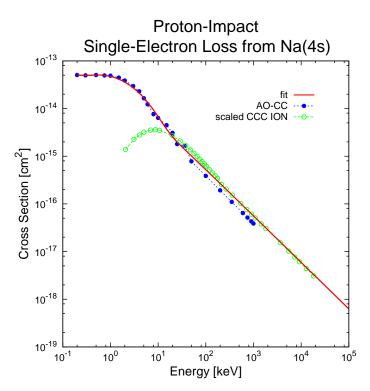




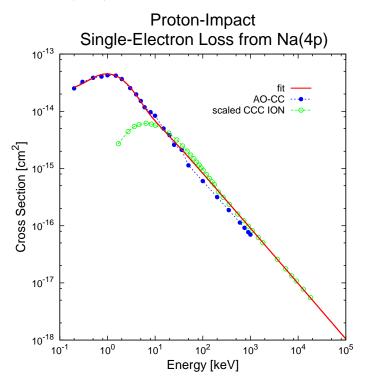


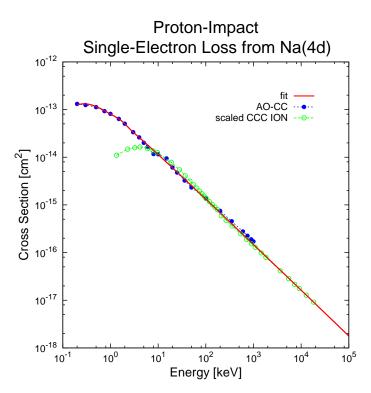
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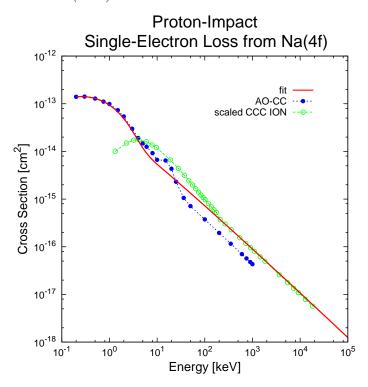


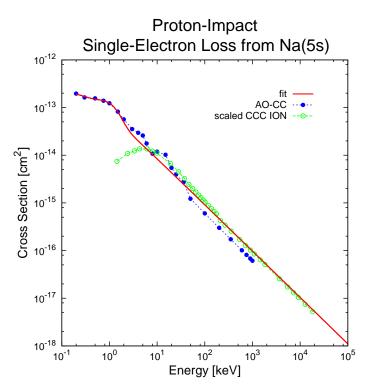
Graphs - 34





Graphs - 35





Graphs - 36