# CROSS SECTIONS FOR COLLISION PROCESSES OF LI ATOMS INTERACTING WITH ELECTRONS, PROTONS, MULTIPLY CHARGED IONS, AND HYDROGEN MOLECULES

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The available experimental and theoretical cross section data for collision processes of Li atoms in the ground state and excited (up to n = 3) states with electrons, protons, and multiply charged ions have been collected and critically assessed. The electron-impact processes include excitation from the ground state, transitions between excited states with n = 2, 3, and ionization from all states considered. The heavy-particle-impact processes include excitation, ionization (for the proton case), and electron removal (the sum of ionization and electron capture). Well-established cross section scaling relationships have been used to generate the cross sections for processes for which no information was found in the literature. This approach was particularly extensively used for the collision processes involving excited Li states, and for collisions with protons and multiply charged ions. In addition, available data for collision processes of Li atoms and ions with neutral hydrogen molecules are shown. The "recommended" cross sections for the considered processes, generated either by critical assessment of available data or by a scaling procedure, have been fitted to simple analytic expressions which ensure correct asymptotic behavior of the cross sections. These recommended cross sections are presented by giving their analytic-fit expressions and tabulating the values of the parameters entering these analytic fits. For those reactions from the ground state for which there is a significant amount of cross section information, we also present the recommended cross sections in graphical form together with the cross section data used for their generation. The criteria for assessing the accuracy of the experimental data, theoretical calculations, and procedures used in determining the recommended cross sections are discussed. © 1997 Academic Press

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#### INTRODUCTION

#### **Database Scope**

The cross section information on inelastic processes of Li in its ground as well as in its excited states colliding with electrons, protons, and multiply charged ions is not only of fundamental interest but also of considerable importance for diagnostics of magnetically confined plasmas by means of Li-beam spectroscopy [1–4]. Injection of a beam of fast (1–10 keV/amu) neutral lithium atoms into the edge of a magnetically confined plasma delivers diagnostic information such as radial electron density profiles and concentrations and temperatures of impurity ions in a nonperturbing manner. The analysis of the emission lines of injected lithium

atoms, which provides information on the parameters of the plasma edge, requires knowledge of the populations of all excited atomic states, as well as of the Li-beam intensity attenuation. Evaluation of the diagnostic raw data relies on modeling the attenuation of the Li(n=2,3) state beam fractions [1]. The success of this diagnostic method is strongly dependent on the availability of reliable data for reaction cross sections of collisions of lithium atoms with plasma particles such as electrons, protons, and multiply charged impurity ions.

The scope of the present cross section database for collision processes of lithium atoms is therefore mainly determined by the above-described needs of Li-beam diagnostics

of fusion edge plasmas. The processes which will be considered in the present paper include electron-impact excitation and ionization, proton-impact excitation and electron removal (the inclusive process of ionization and electron capture), and excitation and electron removal by multicharged plasma impurity ions. These processes will be considered for both the ground and the excited lithium atom states with n = 2, 3. The excited states with  $n \ge 4$  can be considered as hydrogenic and if they need to be included, the cross sections can be estimated by scaling the corresponding n = 3 cross sections [5].

The energy range in which the cross sections for the above processes are considered extends from the threshold to several hundreds of keV for electron impact and from a few keV/amu up to several MeV/amu for heavy-particle impact. This energy range covers the needs of neutral Libeam diagnostics of both the fusion edge [1–4] and fusion core plasmas (or, more precisely, for the diagnostics of the velocity distribution of fusion-born alpha particles [6]).

Since Li-beam spectroscopy can also be used to determine the neutral pressure in the plasma chamber by analyzing the Li I emission lines along the injection beam line [7], available data for collision processes of Li I with neutral hydrogen molecules are also included.

### **Data Sources**

Cross section measurements of the collision processes considered usually involve lithium in its ground state. Electron-impact excitation of Li(2s) to its first excited state, Li(2p), has been measured by Leep and Gallagher [8], Hughes and Hendrickson [9], and Vuskovic et al. [10] from threshold up to 1400 eV. In the overlapping region of 10-200 eV, the results of these measurements mutually agree to within 15%. Within this accuracy they also agree with calculations [11, 12]. Electron-impact excitation cross section measurements exist also for the Li(2s)-Li(3s, 3d) transitions [13] in a wide energy range including the threshold region. In the energy region above 200 eV, these cross sections are in good (≤10%) agreement with the Born-approximation calculations of Ganas [11]. For the other transitions from Li(2s), as well as for the transitions between excited states, only theoretical cross sections [5, 12, 14] and approximate cross section formulas (such as those of van Regemorter [15] or Bates and Damgaard (see Ref. [5])) are available.

The experimental information for electron-impact ionization of Li(2s) has been reviewed and critically assessed by Lennon et al. [16]. These authors have also provided the recommended cross section for this process. For electron-impact ionization of excited states of Li only the semiempirical formula of Lotz [17, 18] is available.

Excitation cross sections of Li in its ground or excited state by proton impact are even less abundant than those by electron impact. The existing experimental cross section measurements for the Li(2s)-Li(2p) transition at low [19] and high [20] energies are supported by atomic-orbital close-coupling (AO–CC) calculations [21, 22]. For other proton-impact excitation transitions there is no direct cross section information at all. One way to estimate the cross sections for these transitions is to scale the electron-impact cross sections according to the prescription of Bates and Griffing [23] with a fitting parameter determined from the scaling of electron- and proton-impact experimental data for the Li(2s)-Li(2p) transition.

The proton-impact electron removal cross section can be obtained on the basis of electron capture data available at low energies and ionization data at higher energies. For proton-impact electron capture from Li(2s) there are experimental data at low and intermediate energy [24-28] supported by theoretical data [21, 22, 29-32]. Proton-impact electron capture cross sections from excited lithium states are available from multistate AO-CC calculations [22]. For ionization, experimental data are available in the low and intermediate energy range [27, 33] supported by the classicaltrajectory Monte Carlo calculations of Ref. [30]. In addition, scaled [34] proton-impact ionization cross sections for hydrogen [35-41] were used to establish the recommended curve. The ionization cross section for excited states can be determined by scaling the corresponding recommended protonimpact ionization cross section for Li(2s) [34].

Excitation cross sections of Li(2s) and Li(nl) by multiply charged ions are available from the AO-CC calculations of Ref. [42], but only for a limited number of transitions (n  $\leq$  3). For electron capture from Li(2s) by multiply charged ions (in charge states  $2 \le q \le 5$ ), experimental data which are supported by AO-CC calculations [33, 42] exist at low and intermediate energies [26-28, 33, 43, 44]. AO-CC calculations have been performed in Ref. [42] also for electron capture from the ground state and the 2p, 3s,p,d excited states of Li by ions in charge states  $2 \le q \le 6$ . Experimental cross sections for electron capture from Li(2p) by He<sup>2+</sup> ions are also available [45]. Although fragmentary, these cross section measurements and calculations are helpful in establishing a cross section scaling relationship for such processes. As demonstrated earlier [30, 42, 46, 47] the electron capture and the ionization cross sections show distinct scalings with respect to both the projectile charge [30, 46] and the electron binding energy in the initial state [42, 47, 48].

#### **Data Evaluation Criteria**

In determining the values of the recommended cross sections for a specific process, all the available cross section information for these processes as of December 1995 has been collected and critically assessed. For the cases where both experimental and theoretical data were available, preference was given to the experimental data of the highest accuracy, judged by the inherent potential of the applied experi-

mental method to generate accurate cross sections and by the care exercised to specify all the error sources in the measurement. The accuracy of the theoretical calculations was judged on the basis of their agreement with reliable experimental data, if such were available, or on the basis of the inherent potential of the applied method and the degree of sophistication in its implementation (e.g., number of states in the expansion basis, inclusion of all relevant couplings, etc).

The mutual consistency of the best available data sets, either experimental or theoretical, was taken as a guiding criterion for determination of the accuracy of recommended cross sections. For the processes where only theoretical data were available, the recommended cross section was determined on the basis of the assessed accuracy of individual data sets, judged by the inherent accuracy of the method, the physics included in its implementation, and the applicability of the method in a particular energy region. The accuracy of a method was judged both on general theoretical grounds and on the basis of the agreement of its results with reliable experimental or theoretical data in other cases. For reactions for which only one experimental or theoretical data set was available, usually that data set was taken as the basis for the recommended cross section, with an assigned accuracy equal to that claimed in the original source, or estimated on the basis of the accuracy of the applied method.

The accuracy of the cross sections generated by using certain scaling relationships was judged on the basis of general theoretical arguments and on demonstrated success of the scaling in other collision systems studied. In cases where there was reliable cross section information in a limited energy range only, the scaling relationships were used to extrapolate the cross section into a broader energy range.

#### **Data Presentation**

The recommended cross sections resulting from the critical data assessment or generated by a scaling relationship have been represented by relatively simple analytic fits, employing a limited number of fitting parameters. The fitting functions were chosen in such a way that they provide the asymptotically correct behavior of the cross section at both low and high collision energies. The fitting functions, therefore, provide fairly accurate extrapolations of the cross sections outside the energy range in which the critical assessment of the original data was performed. The expressions for the cross section fitting functions for the considered processes are given in the Data Sets, together with the values of fitting parameters in these functions and applicable scaling relations.

For reactions from the lithium ground state we present the recommended cross sections also in graphical form together with the data used for their derivation. These figures illustrate, at the same time, the uncertainties of the recommended cross sections for the considered reactions. References for Introduction and Data Sets

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#### EXPLANATION OF DATA SETS

- **DATA SET IA.** Electron-Impact Excitation Cross Sections of Li(nl); n,n'=2, 3; l < n; l' < n'
- **DATA SET IB.** Electron-Impact Ionization Cross Sections of Li(nl); n = 2, 3; l < n
- **DATA SET IIA.** Proton-Impact Excitation Cross Sections of Li(nl); n,n'=2, 3; l < n; l' < n'
- **DATA SET IIB.** Proton-Impact Electron Capture Cross Sections of Li (2s)
- **DATA SET IIC.** Proton-Impact Ionization Cross Sections of Li(nl); n = 2, 3; l < n
- **DATA SET IID.** Proton-Impact Electron Removal Cross Sections of Li(nl); n = 2, 3; l < n
- **DATA SET IIIA.** Excitation Cross Sections for Impact of  $A^{q+}$  ( $q \ge 2$ ) Ions on Li(nl); n,n' = 2, 3; l < n; l' < n'
- **DATA SET IIIB.** Single Electron Capture Cross Sections for Impact of  $A^{q+}$  ( $q \ge 2$ ) Ions on Li(nl); n = 2, 3; l < n
- **DATA SET IIIC.** Electron Removal Cross Sections for Impact of  $A^{q+}$  ( $q \ge 2$ ) Ions on Li(nl); n = 2, 3; l < n
- **DATA SET IVA.** Excitation Cross Sections for  $Li(2s) \rightarrow Li(2p)$  in Collisions with  $H_2$
- **DATA SET IVB.** Electron Capture Cross Sections for Li<sup>+</sup> into Li(2s) in Collisions with H<sub>2</sub>
- **DATA SET IVC.** Electron Removal Cross Sections for Li(2s) in Collisions with H<sub>2</sub>

#### Reaction

The reaction to which a particular data set pertains is written as

 $projectile + target \rightarrow reaction \ products \ observed$ 

Analytic Fit
Fit Parameters
Scaling Relations

The analytic fit, fit parameters, and/or scaling relations give the total cross section for the reaction considered. Symbols in the equations are defined as follows:

$\sigma$	Cross section in cm <sup>2</sup>
$\Delta E$	Threshold energy for excitation in eV
$E_{ m e}$	Electron impact energy in eV
$E_{ m p}$	Proton impact energy in keV/amu
$\vec{E}$	Impact energy in eV for electrons and in keV/amu for ions,
	used when the equation involves only one species
$E_{nl}$	Scaled impact energy in eV
$E_b(nl)$	Binding energy of the <i>nl</i> state in Li in eV
$I_{nl}$	Ionization energy of the $nl$ state in Li in eV (= $E_b(nl)$ )
$E_{ m red}$	Reduced collision energy
q	Projectile charge state
$n_{ m eff}$	Effective quantum number
Ry	Rydberg energy; 1 Ry = 13.606 eV
$A_j, B_j, P_j,$	Fit parameters; 1.0693 e-2 means $1.0693 \times 10^{-2}$
$a_j, b_j, c_j, q_j$	

#### **EXPLANATION OF DATA SETS continued**

Data Comparison and Recommended Fit

Each figure shows the total cross section versus energy for the reaction indicated at the top. The solid line shows the recommended fit. The symbols are keyed in the legend to the name of the first author, publication year, and reference number. E or T preceding the author's name indicates whether the work is experimental or theoretical.

Abscissa Projectile energy in eV for electrons and in keV/amu for ions and molecules.

Ordinate Cross section in cm<sup>2</sup> for the reaction.

Symbol key to data sources and recommended data as given by the Legend analytical fits; data sources are identified by first author and year of publication and reference number. E and T stand for experimental and theoretical data sources, respectively. The solid line (rec.) is the recommended cross section from the present assessment.

DATA SET IA. Electron-Impact Excitation Cross Sections of Li(nl); n, n' = 2, 3; l < n; l' < n' See page 160 for Explanation of Data Sets

Reaction

$$e + Li(nl) \rightarrow e + Li(n'l')$$

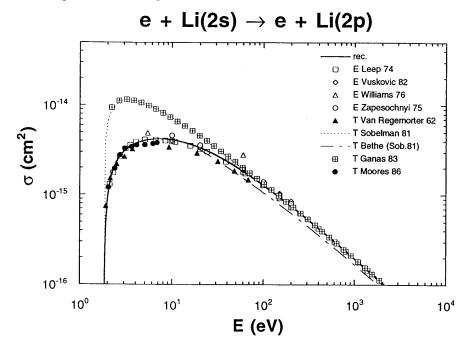
Analytic Fit

$$\sigma_{\rm e}^{\rm exc}(E) = \frac{5.984 \cdot 10^{-16}}{E} \left[ \frac{E - \Delta E}{E} \right]^{A_6} \left[ \sum_{j=1}^{4} \frac{A_j}{(E/\Delta E)^{j-1}} + A_5 \ln \left( \frac{E}{\Delta E} \right) \right]$$

## Fit Parameters

		- · · · · · · · · · · · · · · · · · · ·	<u></u>				
nl-n'l'	ΔE(eV)	$A_1$	$A_2$	$A_3$	$A_4$	$A_5$	$A_6$
		-	_		•	5	Ü
2s-2p	1.847	4.1818	-27.335	89.340	0	52.788	1.1971
2s-3s	3.372	4.7015	-4.6972	-3.0504	11.332	0	0.51449
2s-3p	3.833	1.4705	1.5511	0.94339	0	0.12721	0.53112
2s-3d	3.877	8.2190	18.868	-51.214	55.412	0	1.4119
		,					
2p-3s	1.525	1.0693e-2	-2.4093	5.7497	0	8.0951	0.55336
2p-3p	1.986	10.799	-7.9161	5.6946	0	0	0.60959
2p-3d	2.030	3.8735e-3	37.646	-5.2622	0	36.321	1.0935
3s-3p	0.461	8.4471e-2	225.8	0	0	322.51	1.0632
3s-3d	0.505	91.515	-48.338	127.34	0	0	1.0738
3p-3d	0.044	3.06044e-2	25.686	156.57	0	260.22	1.034

Fig. 1: Electron impact  $Li(2s) \rightarrow Li(2p)$  excitation cross sections; Refs. [5, 8, 10, 11, 14, 15, 49, 50].



DATA SET IA. Electron-Impact Excitation Cross Sections of Li(nl); n, n' = 2, 3; l < n; l' < n'See page 160 for Explanation of Data Sets

Fig. 2: Electron impact  $Li(2s) \rightarrow Li(3s)$  excitation cross sections; Refs. [5, 11, 13, 14, 51, 52].

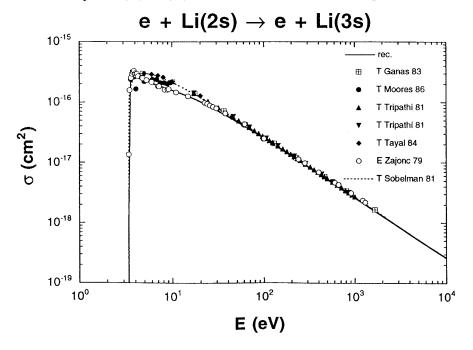
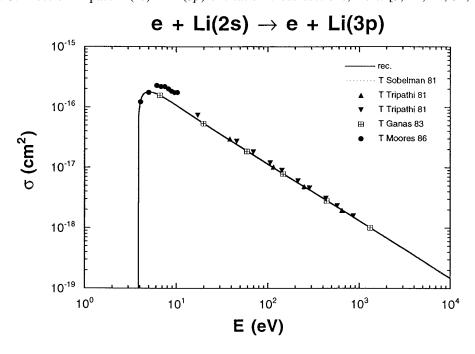
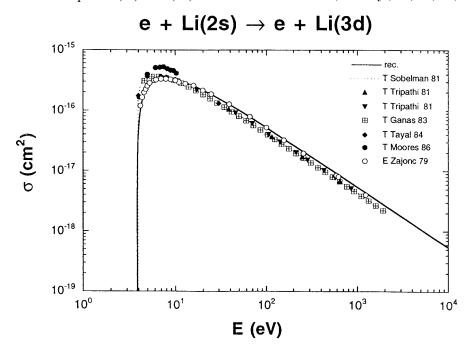


Fig. 3: Electron impact  $Li(2s) \rightarrow Li(3p)$  excitation cross sections; Refs. [5, 11, 14, 51, 52].



DATA SET IA. Electron-Impact Excitation Cross Sections of Li(nl); n, n' = 2, 3; l < n; l' < n' See page 160 for Explanation of Data Sets

Fig. 4: Electron impact  $Li(2s) \rightarrow Li(3d)$  excitation cross sections; Refs. [5, 11, 13, 14, 51, 52].



DATA SET IB. Electron-Impact Ionization Cross Sections of Li(nl); n=2, 3; l < nSee page 160 for Explanation of Data Sets

Reaction

$$e + Li(2s) \rightarrow Li^+ + 2e$$

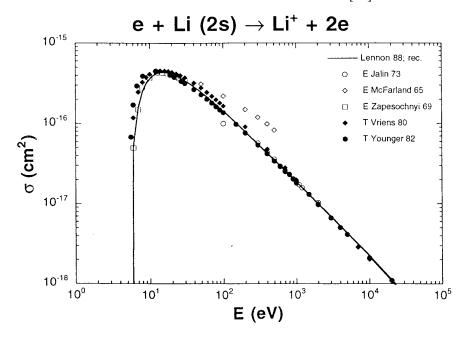
Analytic Fit

$$\sigma_{\rm e}^{\rm ion, Li(2s)}(E) = \frac{10^{-13}}{I_{2s}E} \left[ A \ln \left( \frac{E}{I_{2s}} \right) + \sum_{j=1}^{3} B_{j} \left( 1 - \frac{I_{2s}}{E} \right)^{j} \right]$$

Fit Parameters

I <sub>2s</sub>	A	В1	В2	В3
5.39	0.085	-0.004	0.757	-0.178

Fig. 5: Electron impact ionization cross sections of Li(2s); Refs. [16, 53–57]. The recommended curve is that of Lennon et al. [16].



DATA SET IB. Electron-Impact Ionization Cross Sections of Li(nl); n=2, 3; l < nSee page 160 for Explanation of Data Sets

Reaction

$$e + Li(nl) \rightarrow Li^+ + 2e$$

Analytic Fit

$$\sigma_{\rm e}^{\rm ion,Li(\it nl)}(E) = 10^{-14} \sum_{j=1}^{2} a_j q_j \frac{\ln\left(\frac{E}{P_j}\right)}{EP_j} \left\{ 1 - b_j \exp\left[-c_j\left(\frac{E}{P_j} - 1\right)\right] \right\}$$

$$P_1 = I_{nl}$$

P <sub>2</sub> (eV)	$q_1$	$q_2$	a <sub>l</sub>	a <sub>2</sub>	b <sub>1</sub>	b <sub>2</sub>	c <sub>1</sub>	c <sub>2</sub>
58	1	2	4	4.2	0.7	0.6	2.4	0.6
					=			
nl	2p	3s	3p	3d				
I <sub>nl</sub> (eV)	3.541	2.018	1.557	1.513	_			

DATA SET IIA. Proton-Impact Excitation Cross Sections of Li(nl); n, n' = 2, 3; l < n; l' < n' See page 160 for Explanation of Data Sets

Reaction

$$\mathrm{H}^+ + \mathrm{Li}(nl) \rightarrow \mathrm{H}^+ + \mathrm{Li}(n'l')$$

Analytic Fit

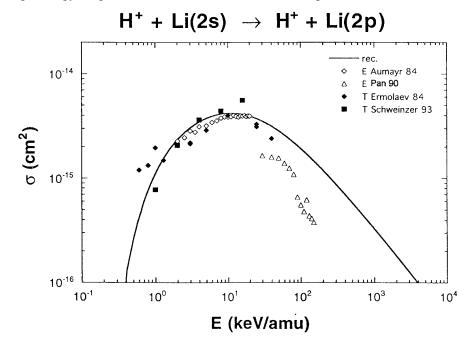
$$\sigma_{\rm p}^{\rm exc}(E_{\rm p}) = \sigma_{\rm e}^{\rm exc}(E_{\rm e})$$

$$E_{\rm p}({\rm keV/amu}) = 0.918 \ E_{\rm e}({\rm eV}) \left[ 1 - \frac{\Delta E({\rm eV})}{1.15 \ E_{\rm e}({\rm eV})} + \sqrt{1 - \frac{\Delta E({\rm eV})}{E_{\rm e}({\rm eV})}} \right]$$

See Data Set IA for  $\sigma_e^{\text{exc}}(E_e)$ .

Data Comparison and Recommended Fit

Fig. 6: Proton impact  $Li(2s) \rightarrow Li(2p)$  excitation cross sections; Refs. [19–22]. The recommended data for the high-energy range are based on the scaled electron impact excitation cross sections of Fig. 1.



# DATA SET IIB. Proton-Impact Electron Capture Cross Sections of Li(2s) See page 160 for Explanation of Data Sets

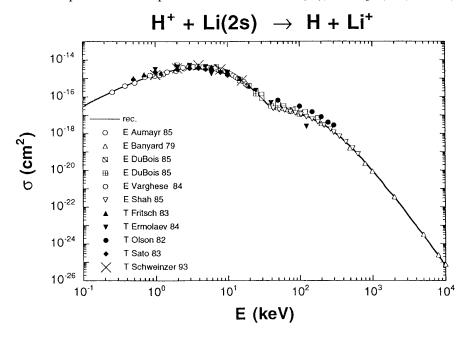
## Reaction

$$H^+ + Li(2s) \rightarrow H + Li^+$$

# Analytic Fit

No fit formula has been derived. The recommended data are given by the solid line drawn through the experimental data points in Fig. 7.

Fig. 7: Proton impact electron capture cross sections of Li(2s); Refs. [21, 22, 24-30, 32, 33].



DATA SET IIC. Proton-Impact Ionization Cross Sections of Li(nl);  $n=2,3;\ l< n$ See page 160 for Explanation of Data Sets

Reaction

$$H^+ + Li(nl) \rightarrow H^+ + Li^+ + e$$

Analytic Fit

$$\sigma_{\rm p}^{\rm ion,Li(2s)}(E) = 10^{-16} A_1 \left[ \frac{\exp(-A_2/E)\ln(1 + A_3E)}{E} + A_4 \frac{\exp(-A_5E)}{E^{A_6} + A_7E^{A_8}} \right]$$

## Fit Parameters

A <sub>1</sub>	17.401	A5	0.21151
A <sub>2</sub>	6.5623	A <sub>6</sub>	1.0551
A3	7.1943e6	A7	64.854
A4	67.115	A8	-1.4472

**Scaling Relations** 

$$\sigma_{\rm p}^{\rm ion,Li(2s)}(E_{2s}) = \left(\frac{E_b(H(1s))}{E_b({\rm Li}(2s))}\right)^2 \sigma_{\rm p}^{\rm ion,H(1s)}(E_{1s})$$

$$E_{2s} = \frac{E_b(\text{Li}(2s))}{E_b(H(1s))} E_{1s}$$

$$E_b(H(1s)) = 13.6 \text{ eV}, E_b(Li(2s)) = 5.39 \text{ eV}$$

 $\sigma_{\rm p}^{{\rm ion},{\rm H}(1s)}(E)$  is taken from Ref. [48].

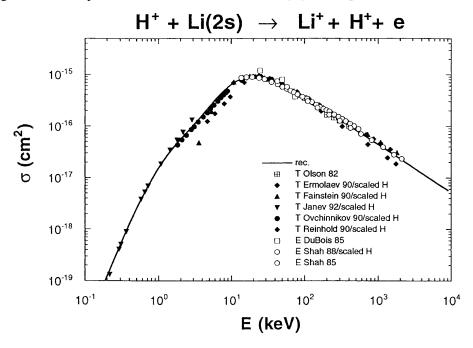
$$\sigma_{\mathrm{p}}^{\mathrm{ion,Li}(nl)}(E_{nl}) = \left(\frac{E_b(2s)}{E_b(nl)}\right)^2 \sigma_{\mathrm{p}}^{\mathrm{ion,Li}(2s)}(E_{2s})$$

$$E_{nl} = \frac{E_b(nl)}{E_b(2s)} E_{2s}$$

 $E_b(nl) = I_{nl}$  is given in Data Set IB.

DATA SET IIC. Proton-Impact Ionization Cross Sections of Li(nl);  $n=2,3;\ l< n$ See page 160 for Explanation of Data Sets

Fig. 8: Proton impact ionization cross sections of Li(2s); Refs. [27, 30, 33, 35–39, 41].



Reaction

$$H^+ + Li(2s) \rightarrow Li^+$$

Analytic Fit

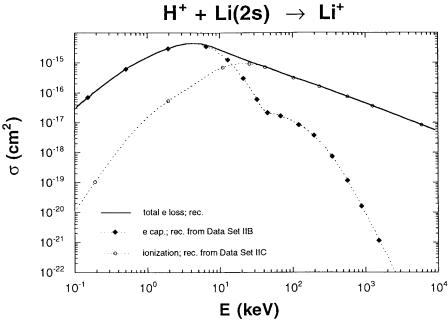
$$\sigma_{p}^{loss,Li(2s)}(E) = A_{1} \left[ \frac{\exp\left(-\frac{A_{2}}{E}\right) \ln\left(2.718 + \frac{A_{10}}{E}\right)}{1 + A_{3}E^{A_{4}} + A_{5}E^{A_{6}}} + A_{7} \frac{\exp\left(-\frac{A_{8}}{E}\right)(A_{9} + \ln E)}{E} \right]$$

$A_1$	5.7260e-18
$A_2$	0.2774610534
$A_3$	-0.9980483025
A <sub>4</sub>	0.005285640316
A <sub>5</sub>	0.002786487304
A <sub>6</sub>	0.6859035811
A <sub>7</sub>	553.7383722e2
A <sub>8</sub>	1.998895199
$A_9$	1.579992279
A <sub>10</sub>	7.521161583e-7
10	

DATA SET IID. Proton-Impact Electron Removal Cross Sections of Li(nl); n=2, 3; l < nSee page 160 for Explanation of Data Sets

Data Comparison and Recommended Fit

Fig. 9: Proton impact electron removal cross sections of Li(2s), based on the recommended electron capture and ionization cross sections from Figs. 7 and 8, respectively.



Reaction

$$H^+ + Li(nl) \rightarrow Li^+$$

Analytic Fit

$$\sigma_{\rm p}^{\rm loss,Li(nl)}(E) = 10^{-14} A_1 \left[ 1 - \exp\left(\frac{-A_2 \ln(2.718 + A_3 E)}{E}\right) \right]$$

nl	$A_1$	$A_2$	$A_3$
2p	0.94189	5.6482	0.0014910
3s	4.2572	2.2300	0.0014998
3p	3.2083	3.9346	0.0017891
3d	2.9719	4.6444	0.0012749

DATA SET IIIA. Excitation Cross Sections for Impact of  $A^{q+}$  ( $q \ge 2$ ) Ions on Li(nl); n, n' = 2, 3; l < n; l' < n'See page 160 for Explanation of Data Sets

Reaction

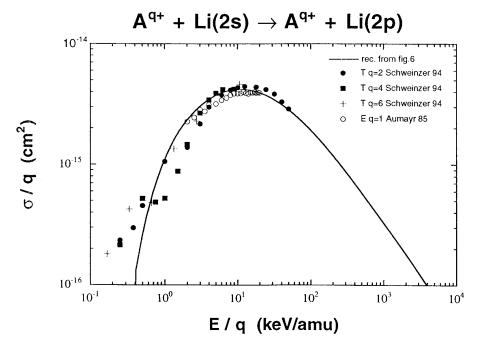
$$A^{q+}$$
 + Li( $nl$ )  $\rightarrow A^{q+}$  + Li( $n'l'$ )

Analytic Fit

$$\sigma_{A^{q^+}}^{\text{exc,Li}(nl)}(E) = q\sigma_{p}^{\text{exc,Li}(nl)}(E/q)$$

See Data Set IIA for  $\sigma_p^{\text{exc,Li}(nl)}(E)$ .

Fig. 10: Scaled Li(2s)  $\rightarrow$  Li(2p) excitation cross sections for impact of  $A^{q+}$  ( $q \ge 2$ ) ions; Refs. [24, 42].



DATA SET IIIB. Single Electron Capture Cross Sections for Impact of  $A^{q+}$  ( $q \ge 2$ ) Ions on Li(nl); n = 2, 3; l < nSee page 160 for Explanation of Data Sets

Reaction

$$A^{q+}$$
 + Li( $nl$ )  $\rightarrow A^{(q-l)+}$  + Li<sup>+</sup>

Analytic Fit

$$E_{\text{red}} = \frac{n_{\text{eff}}^2}{\sqrt{q}} E$$

$$n_{\text{eff}} = \sqrt{\frac{1}{2E_b(a.u.)}} = \sqrt{\frac{Ry}{E_b(eV)}}$$

$$\sigma_{A^{q+}}^{\text{cx,Li}(nl)}(E) = n_{\text{eff}}^4 q \sigma_{\text{red}}^{\text{cx}}(E_{\text{red}})$$

$$\left(1 - \exp\left(-\frac{E_{\text{red}}^{A_2}}{A_3}\right)\right)$$

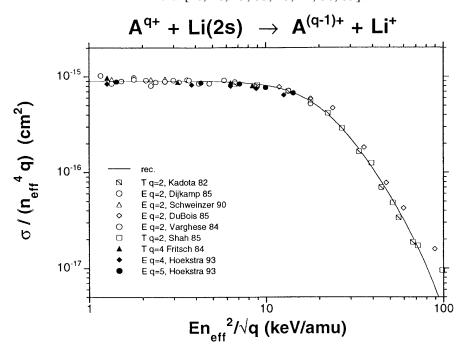
$$\sigma_{\text{red}}^{\text{cx}}(E) = A_1 \frac{E_{\text{red}}^{A_2} + A_4 E_{\text{red}}^{A_5}}{E_{\text{red}}^{A_2} + A_4 E_{\text{red}}^{A_5}}$$

The scaling relation for single electron capture is only valid for states with the same angular momentum l [42].

nl	A <sub>1</sub>	A <sub>2</sub>	A <sub>3</sub>	A <sub>4</sub>	A <sub>5</sub>
2s,3s	7.513e-10	3.14	8.307e5	1.41e-4	6.062
2p,3p	4.513e-10	3.204	6.738e5	6.828e-3	4.933
	,				

DATA SET IIIB. Single Electron Capture Cross Sections for Impact of  $A^{q+}$   $(q \ge 2)$  Ions on Li(nl); n = 2, 3; l < nSee page 160 for Explanation of Data Sets

Fig. 11: Scaled single electron capture cross sections for impact of  $A^{q+}$  ( $q \ge 2$ ) ions on Li(2s); Refs. [26, 28, 29, 33, 43, 44, 58, 59].



DATA SET IIIC. Electron Removal Cross Sections for Impact of  $A^{q+}$  ( $q \ge 2$ ) Ions on Li(nl); n = 2, 3; l < nSee page 160 for Explanation of Data Sets

Reaction

$$A^{q+}$$
 + Li( $nl$ )  $\rightarrow$  Li<sup>+</sup>

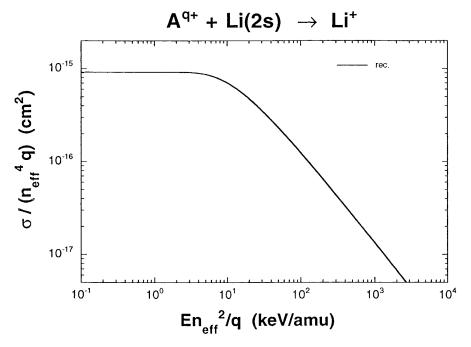
Analytic Fit

$$\begin{split} E_{\text{red}} &= \frac{n_{\text{eff}}^2}{q} E \\ n_{\text{eff}} &= \sqrt{\frac{1}{2E_b(a.u.)}} = \sqrt{\frac{Ry}{E_b(eV)}} \\ \sigma_{A_{\text{red}}}^{\text{loss,Li}(nl)}(E) &= n_{\text{eff}}^4 \cdot q \cdot \sigma_{\text{red}}^{\text{loss}}(E_{\text{red}}) \\ \sigma_{\text{red}}^{\text{loss}} &= 10^{-14} \cdot A_1 \cdot \{1 - \exp(-A_2 \cdot \ln(2.718 + A_3 E_{\text{red}})/E_{\text{red}})\} \end{split}$$

nl	A <sub>1</sub>	A <sub>2</sub>	A <sub>3</sub>
2s,3s	9.1752e-2	14.625	1.7989e-5
2p	6.3853e-2	21.693	3.8821e-4
3p	4.2051e-2	34.368	2.0483
3d	3.6782e-2	41.747	1.4183e-4

DATA SET IIIC. Electron Removal Cross Sections for Impact of  $A^{q+}$  ( $q \ge 2$ ) Ions on Li(nl); n = 2, 3; l < n See page 160 for Explanation of Data Sets

Fig. 12: Scaled electron removal cross sections for impact of  $A^{q+}$   $(q \ge 2)$  ions on Li(2s).



DATA SET IVA. Excitation Cross Sections for  $Li(2s) \rightarrow Li(2p)$  in Collisions with  $H_2$ See page 160 for Explanation of Data Sets

Reaction

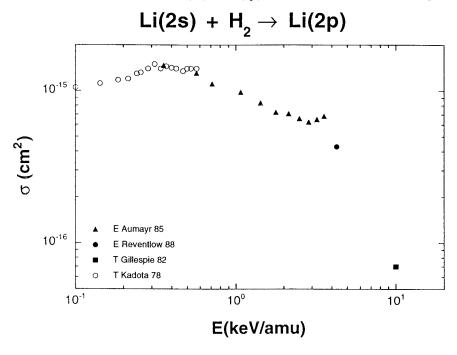
$$Li(2s) + H_2 \rightarrow Li(2p)$$

Analytic Fit

No fit formula has been derived.

Data Comparison

Fig. 13: Excitation cross sections for  $Li(2s) \rightarrow Li(2p)$  in collisions with  $H_2$ ; Refs. [58, 60–62].



DATA SET IVB. Electron Capture Cross Sections for  ${\rm Li}^+$  into  ${\rm Li}(2s)$  in Collisions with  ${\rm H}_2$  See page 160 for Explanation of Data Sets

Reaction

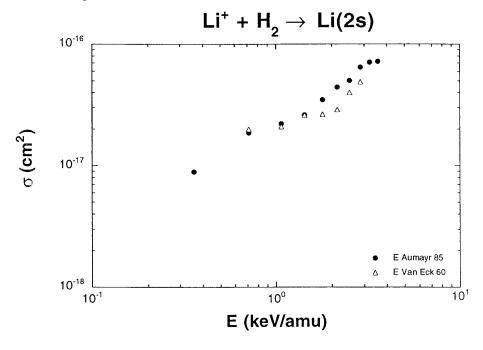
$$Li^+ + H_2 \rightarrow Li(2s)$$

Analytic Fit

No fit formula has been derived.

# Data Comparison

Fig. 14: Electron capture cross sections for Li<sup>+</sup> into Li(2s) in collisions with H<sub>2</sub>; Refs. [60, 63].



# DATA SET IVC. Electron Removal Cross Sections for Li(2s) in Collisions with H<sub>2</sub> See page 160 for Explanation of Data Sets

Reaction

$$Li(2s) + H_2 \rightarrow Li^+$$

Analytic Fit

No fit formula has been derived.

# Data Comparison

Fig. 15: Electron removal cross sections for Li(2s) in collisions with H<sub>2</sub>; Refs. [60, 63-66].

