

INTERNATIONAL NUCLEAR DATA COMMITTEE

# ATOMIC COLLISION DATABASE FOR LI BEAM INTERACTION WITH FUSION PLASMAS

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## CONTENTS

Introd	luction	v
List o	of Reactions	vii
1.	Electron Impact Processes	1
1.1.	Excitation	1
1.2.	Ionization	45
2.	Proton Impact Processes	51
2.1.	Excitation	51
2.2.	Electron Removal	57
3.	Collision Processes with Multiply Charged Ions	75
3.1.	Excitation	75
3.2.	Electron Removal	79
Refer	rences	87

### **INTRODUCTION**

## 1. Purpose and Scope

The purpose of the present collisional data base for Li atoms is to provide a complete and self-consistent set of critically assessed cross section data required in the calculations of neutral Li-beam attenuation kinetics in a fusion plasma. These calculations also provide information about the stationary populations of excited states of Li-beam atoms which is used as basic input in the Li-beam emission spectroscopy of tokamak edge plasmas. Energetic neutral Li-beams (of several MeV) have also been proposed as a potential method for fusion alpha particle diagnostics. In view of these applications, the present collisional data base is constructed for Li-beam energies in the range from a few keV/amu up to several MeV/amu.

The considered collision processes between Li atoms and fusion plasma constituents include: electron impact excitation and ionization, proton impact excitation and electron removal, and excitation and electron removal by multiply charged impurity ions. These processes are considered for both the ground and excited lithium atom states up to 4d. The processes involving Li\* (4f) can be approximately constructed from those for nl  $\leq$  4d by using the scaling procedures discussed in the text. The excited states with  $n \geq 5$  can be considered as hydrogenic and if they need to be included in the attenuation kinetics, the cross sections for the relevant processes are considered in the energy range from threshold up to several hundreds keV (with a cross section extrapolation in the MeV region without relativistic corrections). The heavy particle collision processes are considered in the energy range extending from the adiabatic to the MeV/amu region.

## 2. Data Sources and Data Evaluation Criteria

The cross sections presented in the present collection are based on a critical assessment of the existing experimental and theoretical data, available mostly for the processes involving ground state Li atoms. The cross sections were taken from the journal literature as of December 1993 and no secondary sources were used. The cross sections for the processes involving excited states, or multiply charged ions, were obtained by using either theoretical cross section results (including semi-empirical analytic formulae and calculational procedures), or well established scaling relationships. In determining the recommended cross section values in cases where several sets of experimental or theoretical data (or both) were available, relative accuracy weights were given to the individual data sets on the basis of reliability of the experimental or theoretical method used and the degree of sophistication of performed measurement or calculation. 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 the recommended cross section. In the case of reactions with only one experimental (or theoretical) set available, the cross section was assigned an accuracy equal to that claimed in the original source (or on the basis of realibility of the method used). The accuracy of the scaling relationships, used to generate cross sections for which neither theoretical nor experimental data were available, was judged on the basis of general theoretical considerations and on the experience with their application to cases for which the comparison with experimental or theoretical results of known accuracy is possible.

## 3. Data Presentation

The evaluated or generated cross sections are presented in both tabular and graphical form. Each of the cross sections is documented with estimated accuracies for various energy ranges and with brief comments on the original data sources (where available), or on the procedure used for generating the cross section. The cross sections are additionally represented by analytic fit expressions, which reproduce the recommended cross section values with a specified rms deviation. For the majority of reactions, the analytic fit functions have correct asymptotic behaviour at both low and high collisional energies. Each of the analytic fit functions is supplemented with the values of its fitting parameters, and with an indication of its accuracy (rms and maximum deviation).

The analytic fit functions for the evaluated and generated cross sections are stored in the ALADDIN database system of the International Atomic Energy Agency The ALADDIN data file, containing the entire data information presented here, can be obtained from the IAEA Atomic and Molecular Data Unit on request.

# List of Reactions

# 1. Electron Impact Processes

# 1.1 Excitation

1.1.1	$e^{-} + Li(2s) \rightarrow e^{-} + Li^{*}(2p)$	2
1.1. <b>2</b>	$e^{-} + Li(2s) \rightarrow e^{-} + Li^{*}(3p)$	4
1.1.3	$e^{-} + Li(2s) \rightarrow e^{-} + Li^{*}(3s, 3d)$	6
1.1.4	$e^{-} + Li(2s) \rightarrow e^{-} + Li^{\bullet}(4p)$	8
1.1.5	$e^{-} + Li(2s) \rightarrow e^{-} + Li^{*}(4s, 4d)$	10
1.1.6	$e^{-} + Li^{*}(2p) \rightarrow e^{-} + Li^{*}(3s,3d)$	12
1.1.7	$e^{-} + Li^{*}(2p) \rightarrow e^{-} + Li^{*}(3p)$	14
1.1.8	$e^{-} + Li^{*}(2p) \rightarrow e^{-} + Li^{*}(4s, 4d)$	16
1.1.9	$e^{-} + Li^{*}(2p) \rightarrow e^{-} + Li^{*}(4p)$	18
1.1.10	$e^{-} + Li^{*}(3s) \rightarrow e^{-} + Li^{*}(3p) \dots$	20
1.1.11	$e^{-} + Li^{*}(3s) \rightarrow e^{-} + Li^{*}(3d) \dots$	22
1.1.12	$e^{-} + Li^{*}(3s) \rightarrow e^{-} + Li^{*}(4p) \dots \neg$	24
1.1 13	$e^{-} + Li^{*}(3s) \rightarrow e^{-} + Li^{*}(4s, 4d) \dots$	26
1.1.14	$e^{-} + Li^{*}(3p) \rightarrow e^{-} + Li^{*}(3d)$	28
1.1.15	$e^{-} + Li^{*}(3p) \rightarrow e^{-} + Li^{*}(4s, 4d)$	30
1 1.16	$e^{-} + Li^{*}(3p) \rightarrow e^{-} + Li^{*}(4p)$	32
1.1.17	$e^{-} + Li^{*}(3d) \rightarrow e^{-} + Li^{*}(4p)$	34
1.1.18	$e^{-} + Li^{*}(3d) \rightarrow e^{-} + Li^{*}(4s, 4d)$	36
1.1.19	$e^{-} + Li^{*}(4s) \rightarrow e^{-} + Li^{*}(4p) \dots$	38
1.1.20	$e^{-} + Li^{*}(4s) \rightarrow e^{-} + Li^{*}(4d) \dots$	40
1.1.21	$e^{-} + Li^{*}(4p) \rightarrow e^{-} + Li^{*}(4d)$	42

## 1.2 Ionization

1.2.1	$e^{-} + Li(2s) \rightarrow e^{-} + Li^{+} + e^{-} \dots$	46
121	$e^{-} + Li^{*}(nl) \rightarrow e^{-} + Li^{+} + e^{-}, n=2-4, l < n$	48

# 2. Proton Impact Processes

## 2.1 Excitation

2.1.1	$H^{+} + Li(2s) \rightarrow H^{+} + Li^{*}(2p) \dots \dots$	52
·2.1.2	$H^+ + Li^*(nl) \rightarrow H^+ + Li^*(n',l'), n,n'=2,3,4; l < n, l' < n \dots \dots \dots \dots \dots \dots \dots \dots$	54

## 2.2.1 Electron Removal

2.2.1	$H^+ + Li(2s) \rightarrow Li^+ + \dots$	58
2.2.2	$H^+ + Li^*(2p) \rightarrow Li^+ + \dots$	60
2.2.3	$H^{+} + Li^{*}(3s) \rightarrow Li^{+} + \dots$	62
2.2.4	$H^+ + Li^*(3p) \rightarrow Li^+ + \dots$	64
2.2.5	$H^+ + Li^*(3d) \rightarrow Li^+ + \dots$	66
2.2.6	$H^+ + Li^*(4s) \rightarrow Li^+ + \dots$	68
2.2.7	$H^+ + Li^*(4p) \rightarrow Li^+ + \dots$	70
2.2.8	$H^+ + Li^*(4d) \rightarrow Li^+ + \dots$	72

# 3. Collision Processes with Multiply Charged Ions

## 3.1. Excitation

3.1.1	$A^{q^+} + Li(nl) \rightarrow A^{q^+} + Li^{\prime}$	' (n'l'), n,n'=2,3,4; l <n; l'<n';="" q="">1</n;>	76
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# 3.2 Electron Removal

3.2.1	$A^{q^+} + Li(ns) \rightarrow Li^+ + \dots$	n=2,3,4; q>1	80
3.2.2	$A^{q^+} + Li^*(np) \rightarrow Li^+ + \dots$	n=2,3,4; q>1	82
3.2.3	$A^{q^+} + Li^*(nd) \rightarrow Li^+ + \dots$	n=3,4; q>1	84

# 1.1. Excitation

Energy	Velocity	Cross Section
(eV)	(cm/s)	(cm <sup>2</sup> )
2.00E+00	8.39E+07	9.13E-16
1.00E+00	1.19E+08	3.71E-15
5.00E+00	1.45E+08	4.16E-15
3.00E+00	1.68E+08	4.21E-15
.00E+01	1.88E+08	4.11E-15
2.00E+01	2.65E+08	3.37E-15
1.00E+01	3.75E+08	2.38E-15
5.00E+01	4.59E+08	1.83E-15
8.00E+01	5.30E+08	1.50E-15
1.00E+02	5.93E+08	1.28E-15
2.00E+02	8.39E+08	7.51E-16
4.00E+02	1.19E+09	4.26E-16
5.00E+02	1.45E+09	3.02E-16
8.00E+02	1.68E+09	2.36E-16
1.00E+03	1.88E+09	1.95E-16

Threshold Energy:  $E_{th} = \Delta E = 1.847 \text{ eV}$ 

Accuracy: E < 10 eV : 10 %, or better;  $10 \le E(eV) < 200 : 5 - 10 \%$ ;  $E \ge 200 \text{ eV} : 5 \%$ , or better

- Comments: (1) In the region above 200 eV the recommended cross section follows the experimental data of Leep and Gallagher [1] (including correction for cascading). The experimental data were normalized to the Born cross section at 1400 eV. In this energy region the data converge towards the theoretical cross section from Refs. [2 4].
  - (2) In the region 10 200 eV, experimental data of Leep and Galagher [1], Hughes [5] and Vuskovic et al [6] were used, which agree to within 15 %.
  - (3) The cross section from threshold to 10 eV have been experimentally determined by Leep and Gallagher [1] and is supported by the 5 states close coupling calculations of Moores [7] with a maximum discrepancy of 10 % at 5 eV.

Analytic expression

Cross section:

$$\sigma_{\rm exc} = \frac{5.984 \times 10^{-16}}{\Delta E X} \left[ \frac{E - \Delta E}{E} \right]^{A_6} \left[ \sum_{j=1}^{4} \frac{A_j}{X^{j-1}} + A_5 \ln X \right] \quad [\rm cm^2],$$

where  $X = E / \Delta E$ , and  $\Delta E$  and E are expressed in eV.

		Fitting coeffi	cients		
<b>A</b> <sub>1</sub>	A <sub>2</sub>	A <sub>3</sub>	A4	As	A <sub>6</sub>
4.1818	-27.335	89.340	0.0	52.788	1.1971

The rms deviation of the above fit to the recommended cross section is 2.1%. The maximum deviation is 7.8% at 2.04 eV.

ALADDIN evaluation function for cross section: NEEXH2

ALADDIN hierarchical labelling: EXC e Li [+0] (2s) e Li [+0] (2p)





----- Recommended Cross Section

– – Analytic Fit

Energy	Velocity	Cross Section
(eV)	(cm/s)	(cm <sup>2</sup> )
4.00E+00	1.19E+08	1.08E-16
6.00E+00	1.45E+08	1.67E-16
8.00E+00	1.68E+08	1.33E-16
1.00E+01	1.88E+08	·1.08E16
2.00E+01	2.65E+08	5.40E-17
4.00E+01	3.75E+08	2.74E-17
6.00E+01	4.59E+08	1.84E-17
8.00E+01	5. <b>30E+08</b>	1.40E-17
1.00E+02	5.93E+08	1.14E-17
2.00E+02	8.39E+08	5.95E-18
4.00E+02	1.19E+09	3.11E-18
6.00E+02	1.45E+09	2.12E-18
8.00E+02	1.68E+09	1.61E-18
1.00E+03	1.88E+09	1.30E-18

Threshold Energy:  $E_{th} = \Delta E = 3.833 \text{ eV}$ 

Accuracy: E < 100 eV: 30 %, or better;  $E \ge 100 \text{ eV}$ : 15 %, or better

<u>Comments</u>: There are no experimental data available for the  $2s \rightarrow 3p$  excitation cross section. The recommended cross section follows the theoretical cross section of Ganas [2].

Analytic expression

Cross section:

$$\sigma_{\rm exc} = \frac{5.984 \times 10^{-16}}{\Delta E X} \left[ \frac{E - \Delta E}{E} \right]^{A_6} \left[ \sum_{j=1}^{4} \frac{A_j}{X^{j-1}} + A_5 \ln X \right] \quad [\rm cm^2],$$

where  $X = E / \Delta E$ , and  $\Delta E$  and E are expressed in eV.

#### Fitting coefficients

A <sub>1</sub>	A <sub>2</sub>	A <sub>3</sub>	A4	A5	A6
1.4705	1.5511	0.94339	0.0	0.12721	0.53112

The rms deviation of the above fit to the recommended cross section is 1.1%. The maximum deviation is 6.5% at 3.94 eV.

ALADDIN evaluation function for cross section: NEEXH2

ALADDIN hierarchical labelling: EXC e Li [+0] (2s) e Li [+0] (3p)



----- Recommended Cross Section

- — Analytic Fit

 $e^{-} + Li(2s) \rightarrow e^{-} + Li^{*}(3s, 3d)$ 

Energy	y Velocity Cross Sections (cm <sup>2</sup> )		ions (cm <sup>2</sup> )
(eV)	(cm/s)	2s → 3s	2s → 3d
3.50E+00	1.11 <b>E+08</b>	2.34E - 16	-
4.00E+00	1.1 <b>9E+08</b>	3.08E - 16	4.55E-17
6.00E+00	1.45E+08	2.06E-16	3.14E-16
8.00E+00	1.68E+08	1.77E-16	3.54E-16
1.00E+01	1.88E+08	1.58E-16	3.33E-16
2.00E+01	2.65E+08	1.03E-16	2.22E-16
4.00E+01	3.75E+08	6.15E-17	1.25E-16
6.00E+01	4.59E+08	4.31E-17	8.52E-17
8.00E+01	5.30E+08	3.30E-17	6.44E-17
1.00E+02	5.93E+08	2.68E-17	5.16E-17
2.00E+02	8.39E+08	1.36E-17	2.53E-17
4.00E+02	1.19E+09	6.99E-18	1.25E-17
6.00TE+02	1.45E+09	4.69E18	8.21E-18
8.00E+02	1.68E+09	3.51E-18	6.09E-18
1.00E+03	1.88E+09	2.82E-18	4.86E-18

Threshold Energies :  $E_{th} = \Delta E$ ;  $E_{th}(2s \rightarrow 3s) = 3.372 \text{ eV}$ ;  $E_{th}(2s \rightarrow 3d) = 3.877 \text{ eV}$ 

Accuracy: E < 10 eV : 20 %, or better;  $10 \le E (eV) \le 100 : 20 \%$ , or better;

E > 100 eV : 15 %, or better

- Comments: (1) For energies above 100 eV the cross section for 2s → 3s, 3d transitions were derived on the basis of the experimental data of Zajonc and Gallagher [8] (which include corrections for cascading and polarisation). The data were normalized to the resonance line (2s → 2p transition) measured by Leep and Gallagher [1]. The recommended cross section in this region converges to the Bates-Damgaard approximation [4] and the Born approximation of Ganas [2].
  - (2) In the region 10 100 eV the cross sections follow the experimental data of Ref. [8]. The results of available calculations for 2s → 3s, 3d transitions (Refs. [4, 9]) in this energy range agree amongst themselves to within 5 20 %.
  - (3) The cross sections from threshold to 10 eV have been experimentally determined by Zajonc and Gallagher [8]. The five states close coupling calculations of Moores [7] are uncertain by as much as 40 % since higher states than n = 3 are not included in the basis set.

#### Analytic expression

Cross Section:

$$\sigma_{\rm exc} = \frac{5.984 \times 10^{-16}}{\Delta E X} \left[ \frac{E - \Delta E}{E} \right]^{A_6} \left[ \sum_{j=1}^{4} \frac{A_j}{X^{j-1}} + A_5 \ln X \right] \quad [\rm cm^2],$$

where  $X = E / \Delta E$ , and  $\Delta E$  and E are expressed in eV. Fitting coefficients

							Rms	Maxim	um Deviation
	A1	A <sub>2</sub>	A3	A4	A <sub>5</sub>	A <sub>6</sub>	Deviation (%)	%	at E (eV)
2s → 3s	4.7015	-4.6972	-3.0504	11.332	0.0	0.51449	16	5.7	3.46
2s → 3d	8.2190	1 <b>8.8</b> 68	-51.214	55.412	0.0	1.4119	1.9	4.8	5.41

ALADDIN evaluation function for cross section: NEEXH2

ALADDIN hierarchical labelling :



----- Recommended Cross Section

– – Analytic Fit

1.1.4.

Energy	Velocity	Cross Section
(eV)	(cm/s)	(cm <sup>2</sup> )
5.00E+00	1.33E+08	1.53E-17
6.00E+00	1.45E+08	2.16E-17
8.00E+00	1.68E+08	2.38E-17
1.00E+01	1.88E+08	2.22E-17
2.00E+01	2.65E+08	1.35E-17
4.00E+01	3.75E+08	7.53E-18
6.00E+01	4.59E+08	5.37E-18
8.00E+01	5.30E+08	4.21E-18
1.00E+02	5.93E+08	3.51E-18
2.00E+02	8.39E+08	1.98E-18
4.00E+02	1.19E+09	1.12E - 18
6.00E+02	1.45E+09	7.92E-19
8.00E+02 -	1.68E+09	6. <b>2</b> 1E-19
1.00E+03	1.88E+09	5.18E-19

Threshold Energy:  $E_{th} = \Delta E = 4.520 \text{ eV}$ 

Accuracy: E < 100 eV: 30 %, or better;  $E \ge 100 \text{ eV}$ : 15 %, or better

- <u>Comments</u>: (1) There are no experimental cross section data available for the 2s → 4p transition. For energies above 20 eV the recommended cross section lies between the Bates-Damgaard approximation [4] and the Born approximation of Ganas [2], which differ to within 50 - 30 % (up to 1 keV).
  - (2) In the energy region below 20 eV the recommended cross section was chosen about a factor of 2 smaller than the theoretical cross section of Ganas in accordance with the 2s → 4d transition where the theoretical data of Ganas overestimate the available data by a factor of 2.

Analytic expression

Cross section:

$$\sigma_{\text{exc}} = \frac{5.984 \times 10^{-16}}{\Delta E X} \left[ \frac{E - \Delta E}{E} \right]^{A_6} \left[ \sum_{j=1}^{4} \frac{A_j}{X^{j-1}} + A_5 \ln X \right] \quad [\text{cm}^2],$$

where  $X = E / \Delta E$ , and  $\Delta E$  and E are expressed in eV. Fitting coefficients

A1	A2	A3	A4	As	A <sub>6</sub>
0.17762	0.65765	-0.55430	0.0	0.12807	<b>0</b> .40125

The rms deviation of the above fit to the recommended cross section is 2.4%. The maximum deviation is 10.8% at  $4.60 \text{ eV}_{-}$ 

ALADDIN evaluation function for cross section: NEEXH2

ALADDIN hierarchical labelling: EXC e Li [+0] (2s) e Li [+0] (4p)



 $e^{-}$  + Li(2s)  $\rightarrow e^{-}$  + Li<sup>\*</sup>(4p)

– — Analytic Fit

 $e^- + Li(2s) \rightarrow e^- + Li^*(4s, 4d)$ 

Energy	nergy Velocity		Cross Sections (cm <sup>2</sup> )		
(eV)	(cm/s)	<u>2s → 4s</u>	2s → 4d		
4.50E+00	1.26E+08	6.23E-17	-		
5.00E+00	1.33E+08	5.48E-17	2.92E-17		
6.00E+00	1.45E+08	3.89E-17	4.45E-17		
8.00E+00	1.68E+08	2.66E-17	5.48E-17		
1.00E+01	1.88E+08	2.31E-17	5.56E-17		
2.00E+01	2.65E+08	1.60E-17	4.19E-17		
4.00E+01	3.75E+08	1.02E - 17	2.47E-17		
6.00E+01	4.59E+08	7.58E-18	1.73E-17		
8.00E+01	5.30E+08	6.08E-18	1.33E-17		
1.00E+02	5.93E+08	5.11E-18	1.07E-17		
2.00E+02	8.39E+08	2.89E-18	5.45E-18		
4.00E+02	1.19E+09	1.56E-18	2.77E-18		
6.00E+02	1.45E+09	1.05E-18	1.85E-18		
8.00E+02	1.68E+09	7.84E-19	1.38E-18		
1.00E+03	1.88E+09	6.31E-19	1.10E-18		

Threshold Energies :  $E_{th} = \Delta E$ ;  $E_{th}(2s \rightarrow 4s) = 4.340 \text{ eV}$ ;  $E_{th}(2s \rightarrow 4d) = 4.539 \text{ eV}$ 

Accuracy: E < 100 eV : 20 %, or better;  $E \ge 100 \text{ eV} : 15 \%$ , or better

Comments: For energies above 100 eV the cross sections for 2s → 4s, 4d transitions were derived on the basis of the experimental data of Zajonc and Gallagher [8] (which include corrections for cascading and polarisation). The data were normalized to the resonance line (2s → 2p transition) measured by Leep and Gallagher [1]. The recommended cross section in this region converges towards the results of the Bates-Damgaard approximation [4] and the Born approximation of Ganas [2].

#### Analytic expression

**Cross Section:** 

$$\sigma_{\rm exc} = \frac{5.984 \times 10^{-16}}{\Delta E \, \rm X} \left[ \frac{\rm E - \Delta E}{\rm E} \right]^{A_6} \left[ \sum_{j=1}^{4} \frac{A_j}{\rm X^{j-1}} + \rm A_5 \ln \rm X \right] \quad [\rm cm^2],$$

where $X =$	$E / \Delta E$ , and $\Delta E$ and $E$ are expressed in eV.
	Fitting coefficients

							Rms	Maxim	um Deviation
	A1	A2	A3	A <sub>4</sub>	A5	A <sub>6</sub>	Deviation (%)	%	at E (eV)
2s → 4s	1.0224	-3.1417	4.6479	-2.0315	0.0	1.7010E-02	3.8	7.76	54.68
2s → 4d	1.8676	-1.8193	0.26790	0.0	0.0	0.25478	1.7	6.7	4.79

ALADDIN evaluation function for cross section: NEEXH2

ALADDIN hierarchical labelling :

EXC e Li [+0] (2s) e Li [+0] (4s), for  $2s \rightarrow 4s$ EXC e Li [+0] (2s) e Li [+0] (4d), for  $2s \rightarrow 4d$ 





----- Recommended Cross Section

– — Analytic Fit

11

 $e^{-} + Li^{*}(2p) \rightarrow e^{-} + Li^{*}(3s, 3d)$ 

Energy	Velocity	Cross Sect	ions (cm <sup>2</sup> )
(eV)	(cm/s)	$2p \rightarrow 3s$	2p → 3d
2.00E+00	8.39E+07	4.98E-16	-
4.00E+00	1.19E+08	8.45E-16	2.90E-15
6.00E+00	1.45E+08	8.54E-16	3.28E-15
8.00E+00	1.68E+08	8.09E-16	3.18E-15
1.00E+01	1.88E+08	7.64E-16	3.04E-15
2.00E+01	2.65E+08	5.77E-16	2.30E-15
4.00E+01	3.75E+08	3.87E-16	1.55E-15
6.00E+01	4.59E+08	2.94E-16	1.19E-15
8.00E+01	5.30E+08	2.39E-16	9.77E-16
1.00E+02	5.93E+08	2.03E-16	8.34E-16
2.00E+02	8.39E+08	1.19E-16	4.96E-16
4.00E+02	1.19E+09	6.84E-17	2.87E-16
6.00E+02	1.45E+09	4.90E-17	2.07E-16
8.00E+02	1.68E+09	3.86E-17	1.63E-16
1.00E+03	1.88E+09	3.21E-17	1.35E-16

Threshold Energies :  $E_{th} = \Delta E$ ;  $E_{th}(2p \rightarrow 3s) = 1.525 \text{ eV}$ ;  $E_{th}(2p \rightarrow 3d) = 2.030 \text{ eV}$ 

Accuracy:  $E \le 20 \text{ eV}: 20 - 40\%$ ;  $20 < E(eV) \le 50: 10 - 20\%$ ; E > 50 eV: 10%

- <u>Comments</u>: (1) There is no experimental cross section information for these transitions. For energies above 20 eV the recommended cross sections for the 2p → 3s, 3d transitions are based on the Born results of Tripathi [9] (above 50 eV), and on the semi-empirical formula of Van Regermorter [4] and the Bates-Damgaard approximation [4] (below 50 eV). The results of the Bates-Damgaard approximation agree in this energy region to within 5 % with the Born calculations.
  - (2) In the energy region below 20 eV, the recommended cross sections for the 2p → 3s, 3d transitions are based on a weighted average of the results from the semi-empirical formula of Van Regemorter, Bates-Damgaard and Coulomb-Born approximations [4] and the 5-state close-coupling calculation of Moores [7].

Analytic expression Cross Section:

$$\sigma_{\rm exc} = \frac{5.984 \times 10^{-16}}{\Delta E X} \left[ \frac{E - \Delta E}{E} \right]^{A_6} \left[ \sum_{j=1}^{4} \frac{A_j}{X^{j-1}} + A_5 \ln X \right] \quad [\rm cm^2],$$

where  $X = E / \Delta E$ , and  $\Delta E$  and E are expressed in eV.

Fitting coefficients

							Rms	Maxim	um Deviation
	A1	A2	A3	A4	As	A <sub>6</sub>	Deviation (%)	%	at E (eV)
2p → 3s	1.0693E-02	-2.4093	5.7497	0.0	8.0951	0.55336	2.3	8.3	6.91
2p → 3d	3.8735E-03	37.646	-5.2622	0.0	36.321	1.0935	1.1	7.32	2.18

ALADDIN evaluation function for cross section: NEEXH2

ALADDIN hierarchical labelling :

EXC	с	Li	[+0]	(2p)	e	Li	[+0]	(3s),	for $2p \rightarrow 3s$
EXC	с	Li	{+0}	(2p)	c	Lı	[+0]	(3 <b>d</b> ),	for $2p \rightarrow 3d$

12



— Analytic Fit

Energy	Velocity	Cross Section
(eV)	(cm/s)	(cm <sup>2</sup> )
2.00E+00	8.39E+07	1.41E-16
1.00E+00	1.19E+08	8.46E-16
5.00E+00	1.45E+08	6.79E-16
3.00E+00	1.68E+08	5.57E-16
1.00E+01	1.88E+08	4.77E-16
2.00E+01	2.65E+08	2.76E-16
4.00E+01	3.75E+08	1.49E-16
5.00E+01	4.59E+08	1.03E-16
3.00E+01	5.30E+08	7.86E-17
1.00E+02	5.93E+08	6.37E-17
2.00E+02	8.39E+08	3.26E-17
4.00E+02	1.19E+09	1.62E-17
5.00E+02	1.45E+09	1.08E-17
8.00E+02	1.68E+09	8.09E-18
1.00E+03	1.88E+09	6.42E-18

Threshold Energy:  $E_{th} = \Delta E = 1.986 \text{ eV}$ 

Accuracy:  $E \le 20 \text{ eV}: 25 - 35\%$ ; E > 20 eV: 10 - 25%

<u>Comments</u>: There are no experimental data available for the  $2p \rightarrow 3p$  excitation cross section. The recommended cross section is based on the results of the Bates-Damgaard approximation [4], reduced by 10 - 30 % in the energy region below 30 eV.

#### Analytic expression

Cross section:

$$\sigma_{\rm exc} = \frac{5.984 \times 10^{-16}}{\Delta E X} \left[ \frac{E - \Delta E}{E} \right]^{A_6} \left[ \sum_{j=1}^{4} \frac{A_j}{X^{j-1}} + A_5 \ln X \right] \quad [\rm cm^2],$$

where  $X = E / \Delta E$ , and  $\Delta E$  and E are expressed in eV.

#### Fitting coefficients

A1	A <sub>2</sub>	A3	A4	As	A6
10.7 <b>9</b> 9	7.9161	5.6946	0.0	0.0	0.60959

The rms deviation of the above fit to the recommended cross section is 2.9%. The maximum deviation is 10.7% at 2.22 eV.

ALADDIN evaluation function for cross section: NEEXH2

ALADDIN hierarchical labelling: EXC e Li [+0] (2p) e Li [+0] (3p)

$$e^{-}$$
 + Li  $(2p) - e^{-}$  + Li  $(3p)$   
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----- Recommended Cross Section - --- Analytic Fit

 $e^{-} + Li^{*}(2p) \rightarrow e^{-} + Li^{*}(4s, 4d)$ 

Energy Velocity		Cross Sections (cm <sup>2</sup> )				
(eV)	(c <b>m/s</b> )	2p → 4s	2p → 4d			
3.00E+00	1.03E+08	1.61E-17	9.79E-17			
4.00E+00	1.19E+08	3.21E-17	2.36E-16			
6.00E+00	1.45E+08	4.31E-17	3.39E-16			
8.00E+00	1.68E+08	4.40E-17	3.55E-16			
1.00E+01	1.88E+08	<b>4.29E-</b> 17	3.51E-16			
2.00E+01	2.65E+08	3.41E-17	2.89E-16			
4.00E+01	3.75E+08	2.36E-17	2.03E-16			
6.00E+01	4.59E+08	1.84E-17	1.59E-16			
8.00E+01	5.30E+08	1.53E-17	1.31E-16			
1.00E+02	5.93E+08	1.32E-17	1.1 <b>1E-16</b>			
2.00E+02	8.39E+08	8.03E-18	6.60E-17			
4.00E+02	1.19E+09	4.70E-18	3.83E-17			
6.00E+02	1.45E+09	3.37E-18	2.76E-17			
8.00E+02	1.68E+09	<b>2.65E-1</b> 8	2.19E-17			
1.00E+03	1.88E+09	2.20E-18	1.83E-17			

Threshold Energies :  $E_{th} = \Delta E$ ;  $E_{th}(2p \rightarrow 4s) = 2.493 \text{ eV}$ ;  $E_{th}(2p \rightarrow 4d) = 2.692 \text{ eV}$ 

Accuracy: E < 20 eV : 30 - 50 %,  $E \ge 20 \text{ eV} : 10 - 30 \%$ 

- <u>Comments</u>: (1) There is no experimental cross section information for these transitions. In the energy range above 20 eV, the recommended cross sections for these transitions are based on the Bates-Damgaard aproximation [4], which agree with the semi-empirical formula of Van Regemorter [4] to within 5 15 %.
  - (2) In the region below 20 eV, the cross sections are based on a weighted average of the results from the Bates-Damgaard approximation and the Van Regemorter formula, with a larger weight given to the later.

Analytic expression

**Cross Section:** 

$$\sigma_{\text{exc}} = \frac{5.984 \times 10^{-16}}{\Delta E X} \left[ \frac{E - \Delta E}{E} \right]^{A_6} \left[ \sum_{j=1}^{4} \frac{A_j}{X^{j-1}} + A_5 \ln X \right] \quad [\text{cm}^2],$$

where $X =$	$E / \Delta E$ , and $\Delta E$ and $E$ are expressed in eV.				
Fitting coefficients					

							Rms	Maxim	um Deviation
	A1	A <sub>2</sub>	A <sub>3</sub>	A4	As	A <sub>6</sub>	Deviation (%)	%	at E (eV)
2p → 4s	2.5380E-05	0.21103	0.0	0.0	0.60611	0.67381	2.4	10.3	2.62
2p → 4d	0.26437	2.1252	0.0	0.0	5.1129	0.76764	1.1	2.1	<b>90.5</b> 1

ALADDIN evaluation function for cross section: NEEXH2

ALADDIN hierarchical labelling :

EXC	e	Li	[+0]	(2p)	e	Li	[+0]	(4s),	for $2p \rightarrow 4s$
EXC	е	Li	[+0]	(2p)	e	Li	[+0]	(4d),	for $2p \rightarrow 4d$



----- Recommended Cross Section

- Analytic Fit

Energy	Velocity	Cross Section
(eV)	(cm/s)	(cm <sup>2</sup> )
(01)	(011/3)	(cm)
3.00E+00	1.03E+08	5.93E-17
4.00E+00	1.19E+08	9.24E-17
6.00E+00	1.45E + 08	9.66E-17
8.00E+00	1.68E+08	8.79E-17
1.00E+01	1.88E+08	7.99E-17
2.00E+01	2.65E+08	5.27E-17
4.00E+01	3.75E+08	3.03E-17
6.00E+01	4.59E+08	2.10E-17
8.00E+01	5.30E+08	1.59E-17
1.00E + 02	5.93E+08	1.28E-17
2.00E+02	8.39E+08	6.38E-18
4.00E+02	1.19E+09	3.20E-18
6.00E+02	1.45E+09	2.13E-18
8.00E+02	1.68E+09	1.59E-18
1.00E+03	1.88E+09	1.28E-18

Threshold Energy:  $E_{th} = \Delta E = 2.673 \text{ eV}$ 

Accuracy: E < 20 eV : 20 - 40%,  $E \ge 20 \text{ eV} : 15 - 20\%$ 

<u>Comments</u>: There are no experimental data available for this transiton. The recommended cross section is based on the results of the Bates-Damgaard approximation [4], reduced by almost 100 % in the region of the cross section maximum.

#### Analytic expression

Cross section:

$$\sigma_{\text{exc}} = \frac{5.984 \times 10^{-16}}{\Delta E X} \left[ \frac{E - \Delta E}{E} \right]^{A_6} \left[ \sum_{j=1}^{4} \frac{A_j}{X^{j-1}} + A_5 \ln X \right] \quad [\text{cm}^2],$$

where  $X = E / \Delta E$ , and  $\Delta E$  and E are expressed in eV.

#### Fitting coefficients

A <sub>1</sub>	A <sub>2</sub>	A <sub>3</sub>	A4	A <sub>5</sub>	A6
2.1826	-2.3724	1.1869	0.0	0.0	0.54770

The rms deviation of the above fit to the recommended cross section is 1.9%. The maximum deviation is 3.8% at 8.46 eV.

ALADDIN evaluation function for cross section: NEEXH2

ALADDIN hierarchical labelling: EXC e Li [+0] (2p) e Li [+0] (4p)



----- Recommended Cross Section

— Analytic Fit

1.1.10.

Velocity	Cross Section
(cm/s)	(cm <sup>2</sup> )
4.59E+07	5.43E-14
5.30E+07	9.29E-14
5.93E+07	1.07E-13
8.39E+07	1.13E-13
1.19E+08	9.33E-14
1.45E+08	7.87E-14
1.68E+08	6.74E-14
1.88E+08	5.92E-14
2.65E+08	3.68E-14
3.75E+08	2.15E-14
4.59E+08	1.57E-14
5.30E+08	1.25E-14
5.93E+08	1.04E-14
8.39E+08	5.79E-15
1.19E+09	3.23E-15
1.45E+09	2.28E-15
1.68E+09	1.78E-15
1.88E+09	1.47E-15
	Velocity (cm/s) 4.59E+07 5.30E+07 5.93E+07 8.39E+07 1.19E+08 1.45E+08 1.45E+08 1.68E+08 2.65E+08 3.75E+08 4.59E+08 5.30E+08 5.30E+08 5.93E+08 8.39E+08 1.19E+09 1.45E+09 1.68E+09 1.88E+09

Threshold Energy:  $E_{th} = \Delta E = 0.461 \text{ eV}$ 

Accuracy: E < 5 eV : 20 - 40%;  $5 \le E(\text{eV}) < 20 : 10 - 20\%$ ; E > 20 eV : 10%

- <u>Comments</u>: (1) In the energy region above 20 eV, the recommended cross section follows the results of the first Born calculations of Tripathi [9]. In this energy region it practically coincides with the results of the Bates-Damgaard approximation [4].
  - (2) For energies below 20 eV, the recommended cross section is based on a weighted average of the Bates-Damgaard and Van Regemorter approximations [4], with a higher weight given to the later.
  - (3) The results of 5-state, close-coupling calculations of Moores [7] are generally consistent with the recommended cross section except in the threshold region.

#### Analytic expression

Cross section:

$$\sigma_{\rm exc} = \frac{5.984 \times 10^{-16}}{\Delta E X} \left[ \frac{E - \Delta E}{E} \right]^{A_6} \left[ \sum_{j=1}^{4} \frac{A_j}{X^{j-1}} + A_5 \ln X \right] \quad [\rm cm^2],$$

where  $X = E / \Delta E$ , and  $\Delta E$  and E are expressed in eV.

Fitting coefficients

A1	A <sub>2</sub>	A <sub>3</sub>	A4	A <sub>5</sub>	A <sub>6</sub>
8.4471E-02	225.80	0.0	0.0	322.51	1.0632

The rms deviation of the above fit to the recommended cross section is 2.1%. The maximum deviation is 7.2% at 2.29 eV.

ALADDIN evaluation function for cross section: NEEXH2

ALADDIN hierarchical labelling: EXC e Li [+0] (3s) e Li [+0] (3p)





----- Recommended Cross Section - -- Analytic Fit

21

Energy Velocity		Cross Section
(eV)	(cm/s)	(cm <sup>2</sup> )
2.00E+00	8.39E+07	1.41E-16
6.00E-01	4.59E+07	1.96E-14
8.00E-01	5.30E+07	2.91E-14
1.00E+00	5.93E+07	2.88E-14
2.00E+00	8.39E+07	1.98E-14
4.00E+00	1.19E+08	1.15E-14
6.00E+00	1.45E+08	8.06E-15
8.00E+00	1.68E+08	6.23E-15
1.00E+01	1.88E+08	5.13E-15
2.00E+01	2.65E+08	2.71E-15
4.00E+01	3.75E+08	1.38E-15
6.00E+01	4.59E+08	9.21E-16
8.00E+01	5.30E+08	6.90E-16
1.00E+02	5.93E+08	5.54E-16
2.00E+02	8.39E+08	2.78E-16
4.00E+02	1.19E+09	1.41E-16
6.00E+02	1.45E+09	9.35E-17
8.00E+02	1.68E+09	7.01E-17
1.00E+03	1.88E+09	5.62E-17

Threshold Energy:  $E_{th} = \Delta E = 0.505 \text{ eV}$ 

Accuracy:  $E \le 5 \text{ eV}: 30 - 50\%$ ;  $5 < E(eV) \le 20: 20 - 30\%$ ; E > 20 eV: 15 - 20%

Comments :The recommended cross section for this reaction has been constructed by using the<br/>Bates-Damgaard approximation [4]. The results of this approximation in the energy region<br/>around the cross section maximum have been reduced by almost a factor of two, in<br/>accordance with the similar reduction factor for the Bates-Damgaard results in the case of the<br/> $2s \rightarrow 3p$  transition.

Analytic expression

Cross section:

$$\sigma_{\rm exc} = \frac{5.984 \times 10^{-16}}{\Delta E X} \left[ \frac{E - \Delta E}{E} \right]^{A_6} \left[ \sum_{j=1}^{4} \frac{A_j}{X^{j-1}} + A_5 \ln X \right] \quad [\rm cm^2],$$

where  $X = E / \Delta E$ , and  $\Delta E$  and E are expressed in eV.

Fitting coefficients						
A1	A <sub>2</sub>	A <sub>3</sub>	A4	As	A <sub>6</sub>	
93.515	-48.338	127.34	0.0	0.0	1.0738	

The rms deviation of the above fit to the recommended cross section is 1.0%. The maximum deviation is 2.85% at 0.53 eV.

ALADDIN evaluation function for cross section: NEEXH2

ALADDIN hierarchical labelling: EXC e Li [+0] (3s) e Li [+0] (3d)



----- Recommended Cross Section

- — Analytic Fit

Energy	Velocity	Cross Section
(eV)	(cm/s)	(cm <sup>2</sup> )
1.20E+00	6.50E+07	1.83E-15
1.50E+00	7.26E+07	3.83E-15
2.00E+00	8.39E+07	3.48E-15
4.00E+00	1.19E+08	1. <b>75</b> E15
6.00E+00	1.45E+08	1.14E-15
8.00E+00	1.68E+08	<b>8.67E-1</b> 6
1.00E+01	1.88E+08	7.04E-16
2.00E+01	2.65E+08	3.79E-16
4.00E+01	3.75E+08	<b>2.10E-1</b> 6
6.00E+01	4.59E+08	1.50E-16
8.00E+01	5.30E+08	1.19E-16
1.00E+02	5.93E+08	9.87E-17
2.00E+02	8.39E+08	5.60E-17
4.00E+02	1.19E+09	<b>3.17E-17</b>
6.00E+02	1.45E+09	<b>2.25E</b> -17
8.00E+02	1.68E+09	1.76E-17
1.00E+03	1.88E+09	1.46 <b>E</b> -17

Threshold Energy:  $E_{th} = \Delta E = 1.148 \text{ eV}$ 

Accuracy: E < 30 eV : 100 %, or higher;  $E \ge 30 \text{ eV} : 20 - 50 \%$ 

<u>Comments</u>: The cross section for this reaction has been generated from the Bates-Damgaard approximation [4]. We note that the use of the semi-empirical formula of Van Regemorter gives values which are about 2 orders of magnitude lower (for a value of the oscillator strength about  $10^{-5}$ ).

Analytic expression

Cross section:

$$\sigma_{\text{exc}} = \frac{5.984 \times 10^{-16}}{\Delta E X} \left[ \frac{E - \Delta E}{E} \right]^{A_6} \left[ \sum_{j=1}^{4} \frac{A_j}{X^{j-1}} + A_5 \ln X \right] \quad [\text{cm}^2],$$

where  $X = E / \Delta E$ , and  $\Delta E$  and E are expressed in eV.

#### Fitting coefficients

A1	A <sub>2</sub>	A <sub>3</sub>	A4	As	A6
2.2416	28.938	0.0	0.0	3.2109	0.65586

The rms deviation of the above fit to the recommended cross section is 1.3%. The maximum deviation is 4.7% at 1.2 eV.

ALADDIN evaluation function for cross section: NEEXH2

ALADDIN hierarchical labelling: EXC e Li [+0] (3s) e Li [+0] (4p)



----- Recommended Cross Section

— Analytic Fit

 $e^{-} + Li^{*}(3s) \rightarrow e^{-} + Li^{*}(4s, 4d)$ 

1	1	12
т.	L.	13.

Velocity	Cross Sections (cm <sup>2</sup> )		
(cm/s)	3s → 4s	3s → 4d	
5.93E+07	3.74E-16	_	
6.50E+07	1.91E-15	1.09E - 16	
7.26E+07	2.44E-15	4.29E-16	
8.39E+07	2.60E-15	5.93E-16	
1.19E+08	2.16E-15	6.03E-16	
1.45E+08	1.71E-15	5.24E-16	
1.68E+08	1.41E-15	4.63E-16	
1.88E+08	1.20E-15	4.10E-16	
2.65E+08	6.78E-16	2. <b>59E</b> -16	
3.75E+08	3.66E-16	1. <b>49E</b> -16	
4.59E+08	2.51E-16	1.04E-16	
5.30E+08	1.93E-16	7.96E-17	
5.93E+08	1.57E-16	6.46E-17	
8.39E+08	8.03E-17	3.30E-17	
1.19E+09	4.04E-17	1.66E-17	
1.45E+09	2.67E-17	1.11 <b>E-17</b>	
1.68E+09	1.99E-17	8.33E-18	
1.88E+09	1.60E-17	6.65E-18	
	Velocity (cm/s) 5.93E+07 6.50E+07 7.26E+07 8.39E+07 1.19E+08 1.45E+08 1.68E+08 1.68E+08 2.65E+08 3.75E+08 4.59E+08 5.30E+08 5.93E+08 8.39E+08 1.19E+09 1.45E+09 1.68E+09 1.88E+09	VelocityCross Section(cm/s) $3s \rightarrow 4s$ $5.93E+07$ $3.74E-16$ $6.50E+07$ $1.91E-15$ $7.26E+07$ $2.44E-15$ $8.39E+07$ $2.60E-15$ $1.19E+08$ $2.16E-15$ $1.45E+08$ $1.71E-15$ $1.68E+08$ $1.41E-15$ $1.88E+08$ $1.20E-15$ $2.65E+08$ $6.78E-16$ $3.75E+08$ $3.66E-16$ $4.59E+08$ $2.51E-16$ $5.30E+08$ $1.57E-16$ $8.39E+08$ $8.03E-17$ $1.19E+09$ $4.04E-17$ $1.45E+09$ $2.67E-17$ $1.68E+09$ $1.99E-17$ $1.88E+09$ $1.60E-17$	

Threshold Energies :  $E_{th} = \Delta E$ ;  $E_{th}(3s \rightarrow 4s) = 0.968 \text{ eV}$ ;  $E_{th}(3s \rightarrow 4d) = 1.167 \text{ eV}$ 

Accuracy: E < 20 eV : 25 - 40% E > = 20 eV : 15 - 25%

Comments: The cross sections for these reactions are based on the Bates-Damgaard approximation [4]. The cross section values in the region around the cross section maximum have been reduced by a factor close to two, to account for the cross section overestimates of this approximation observed in the case of the 3s → 3p and over transitions.

#### Analytic expression

Cross Section:

$$\sigma_{\rm exc} = \frac{5.984 \times 10^{-16}}{\Delta E X} \left[ \frac{E - \Delta E}{E} \right]^{A_6} \left[ \sum_{j=1}^{4} \frac{A_j}{X^{j-1}} + A_5 \ln X \right] \quad [\rm cm^2],$$

				Fitting	coefficien	its				
							Rms	Maximum Deviation		
	A1	A2	A3	A <sub>4</sub>	As	A <sub>6</sub>	Deviation (%)	%	at E (eV)	
3s → 4s	26.504	-39.124	43.298	0.0	0.0	1.1070	2.7	12.1	0.98	
3s → 4d	11.143	-31.172	49.954	-25.011	0.0	1.0462	2.2	6.7	1.17	

ALADDIN evaluation function for cross section: NEEXH2

ALADDIN hierarchical labelling :

EXC e Li [+0] (3s) e Li [+0] (4s), for  $3s \rightarrow 4s$ EXC e Li [+0] (3s) e Li [+0] (4d), for  $3s \rightarrow 4d$


 $e^{-} + Li^{*}(3s) \rightarrow e^{-} + Li^{*}(4s, 4d)$ 

----- Recommended Cross Section

— Analytic Fit

27

Energy	Velocity	Cross Section
(eV)	<b>(cm</b> /s)	$(cm^2)$
6.00E-02	1.45E+07	4.56E-13
8.00E-02	1 <b>.68</b> E+07	7.33E-13
1.00E-01	1.88E+07	8.36E-13
2.00E-01	2.65E+07	8.90E-13
4.00E-01	3.75E+07	7.32E-13
6.00E-01	4.59E+07	6.09E-13
8.00E-01	5.30E+07	5.21E-13
1.00E+00	5.93E+07	4.55E-13
2.00E+00	8.39E+07	2.85E-13
4.00E+00	1.19E+08	1.74E-13
6.00E+00	1.45E+08	1.29E-13
8.00E+00	1.68E+08	1.03E-13
1.00E+01	1.88E+08	8.64E-14
2.00E+01	<b>2.65E+08</b>	4.93E-14
4.00E+01	3.75E+08	2.76E-14
6.00E+01	4.59E+08	1.92E-14
8.00E+01	5.30E+08	1.48E-14
1.00E+02	5.93E+08	1.22E-14
2.00E+02	8.39E+08	6.55E-15
4.00E+02	1. <b>19</b> E+09	3.50E-15
6.00E+02	1.45E+09	2.40E-15
8.00E+02	1.68E+09	1.84E-15
1.00E+03	1.88E+09	1.50E-15

Threshold Energy:  $E_{th} = \Delta E = 0.044 \text{ eV}$ 

Accuracy:  $E \le 2 \text{ eV}: 20 - 40\%$ ;  $2 \le E(\text{eV}) \le 10: 10 - 20\%$ ; E > 10 eV: 10 - 15%

<u>Comments</u>: (1) In the energy region above 10 eV, the recommended cross section follows the results of the first Born calculations of Tripathi [9], which to within 5 - 10 % agree with the results of the Bates-Damgaard approximation [4].

(2) For energies below 10 eV, the recommended cross section is a weighted average of the Bates-Damgaard and Van Regemorter approximations [4]. The results of 5-state close-coupling calculations [7] are consistent with the recommended cross section above 6 eV.

### Analytic expression

Cross section:

$$\sigma_{\rm exc} = \frac{5.984 \times 10^{-16}}{\Delta E X} \left[ \frac{E - \Delta E}{E} \right]^{A_6} \left[ \sum_{j=1}^4 \frac{A_j}{X^{j-1}} + A_5 \ln X \right] \quad [\rm cm^2],$$

where  $X = E / \Delta E$ , and  $\Delta E$  and E are expressed in eV.

#### Fitting coefficients

A1	A <sub>2</sub>	A <sub>3</sub>	A4	A <sub>5</sub>	A6
3.0644E-02	25.686	156.57	0.0	260.22	1.0340

The rms deviation of the above fit to the recommended cross section is 2.5%. The maximum deviation is 6 1% at 25.92 eV.

ALADDIN evaluation	function for	cross section:	NEEXH2

ALADDIN hierarchical labelling: EXC e Li [+0] (3p) e Li [+0] (3d)



Legend:

----- Recommended Cross Section

 $e^{-} + Li^{*}(3p) \rightarrow e^{-} + Li^{*}(4s, 4d)$ 

Energy	Velocity	Cross Sect	ions (cm <sup>2</sup> )
(eV)	(cm/s)	3p → 4s	3p → 4d
6.00E-01	4.59E+07	6.35E-15	_
8.00E-01	5.30E+07	1.10E-14	6.04E-15
1.00E + 00	5.93E+07	1.34E-14	1.08E - 14
2.00E+00	8.39E+07	1.63E-14	1.88E-14
4.00E+00	1.19E+08	1.36E-14	1.80E-14
6.00E+00	1.45E+08	1.12E-14	1.55 <b>E</b> -14
8.00E+00	1.68E+08	9.51E-15	1.35E-14
1.00E+01	1.88E+08	8.32E-15	1.20E - 14
2.00E+01	2.65E+08	5.24E-15	7.75E-15
4.00E+01	3.75E+08	3.14E-15	4.78E-15
6.00E+01	4.59E+08	2.29E-15	3.55E-15
8.00E+01	5.30E+08	1.83E-15	2.85E-15
1.00E+02	5.93E+08	1.54E-15	2.39E-15
2.00E+02	8.39E+08	8.71 <b>E</b> -16	1.37E-15
4.00E+02	1.19E+09	4.86E-16	7.73E-16
6.00E+02	1.45E+09	3.43E-16	5.50E-16
8.00E+02	1.68E+09	2.68E-16	4.30E-16
1.00E+03	1.88E+09	<b>2.21E-16</b>	3.53E-16

Threshold Energies :  $E_{th} = \Delta E$ ;  $E_{th}(3p \rightarrow 4s) = 0.507 \text{ eV}$ ;  $E_{th}(3p \rightarrow 4d) = 0.706 \text{ eV}$ 

Accuracy:  $E \le 5 \text{ eV} : 30 - 50 \%$ ;  $5 < E(\text{eV}) \le 20 : 20 - 30 \%$ ; E > 20 eV : 15 - 20 %

<u>Comments</u>: The recommended cross sections are based on a weighted average of the results generated by the Bates-Damgaard approximation and the semi-empirical formula of Van Regemorter [4], with a large relative weight given to the formula of Van Regemorter (except in the threshold region).

Analytic expression

Cross Section:

$$\sigma_{\rm exc} = \frac{5.984 \times 10^{-16}}{\Delta E \,\mathrm{X}} \left[ \frac{\mathrm{E} - \Delta \mathrm{E}}{\mathrm{E}} \right]^{\mathrm{A}_{6}} \left[ \sum_{j=1}^{4} \frac{\mathrm{A}_{j}}{\mathrm{X}^{j-1}} + \mathrm{A}_{5} \ln \mathrm{X} \right] \quad [\mathrm{cm}^{2}],$$

where X =	$E / \Delta E$ , and $\Delta E$ and $E$ are expressed in eV.
	Fitting coefficients

							Rms	Maxim	um Deviation
	A <sub>1</sub>	A <sub>2</sub>	A3	A4	A5	A <sub>6</sub>	Deviation (%)	%	at E (eV)
3p → 4s	0.63837	-7.7593	31.415	0.0	48.437	0.72376	06	2.8	0.53
3p → 4d	9.0728E-03	35.528	26.256	0.0	81.124	1.0 <b>792</b>	0.7	1.8	1.01

ALADDIN evaluation function for cross section: NEEXH2

ALADDIN hierarchical labelling :

EXC	с	Li	[+0]	(3p)	e	Li	[+0]	(4s),	for $3p \rightarrow 4s$
EXC	e	Lı	[+0]	(3p)	с	Li	[+0]	(4d),	for $3p \rightarrow 4d$



 $e^{-} + Li^{*}(3p) \rightarrow e^{-} + Li^{*}(4s, 4d)$ 

Legend:

----- Recommended Cross Section

– Analytic Fit

31

Energy	Velocity	Cross Section
(eV)	(cm/s)	(cm <sup>2</sup> )
8.00E-01	5.30E+07	4.57E-15
1.00E+00	5.93E+07	6.25E-15
2.00E+00	8.39E+07	6.20E-15
4.00E+00	1.19E+08	4.40E-15
6.00E+00	1.45 <b>E+08</b>	3.39E-15
8.00E+00	1.68E+08	2.77E-15
1.00E+01	1.88E+08	2.36E-15
2.00E+01	2.65E+08	1.37E-15
4.00E+01	3.75 <b>E+08</b>	7.52E-16
6.00E+01	4.59E+08	5.12E-16
8.00E+01	5.30E+08	3.87E-16
1.00E+02	5.9 <b>3E+08</b>	3.12E-16
2.00E+02	8.39E+08	1.56E-16
4.00E+02	1.19 <b>E+09</b>	7.82E-17
6.00E+02	1.45E+ <b>09</b>	5.18E-17
8.00E+02	1.68E+09	3.85E-17
1.00E+03	1.88E+09	3.08E-17

### Threshold Energy: $E_{th} = \Delta E = 0.687 \text{ eV}$

Accuracy: 
$$E \le 5 \text{ eV} : 30 - 50 \%$$
;  $5 < E (eV) \le 20 : 20 - 30 \%$ ;  $E > 20 \text{ eV} : 15 - 20 \%$ 

 $\frac{\text{Comments}:}{\text{Bates-Damgaard approximation [4], which have been reduced by almost a factor of 2, in accordance with the case of the 3p <math>\rightarrow$  4s, 4d transitions.

Analytic expression

Cross section:

$$\sigma_{\rm exc} = \frac{5.984 \times 10^{-16}}{\Delta E X} \left[ \frac{E - \Delta E}{E} \right]^{A_6} \left[ \sum_{j=1}^{4} \frac{A_j}{X^{j-1}} + A_5 \ln X \right] \quad [\rm cm^2],$$

where  $X = E / \Delta E$ , and  $\Delta E$  and E are expressed in eV.

# Fitting coefficients

A <sub>1</sub>	A <sub>2</sub>	A <sub>3</sub>	A4	As	A6
51.569	-135.44	179.55	-89.337	0.0	0.28319

The rms deviation of the above fit to the recommended cross section is 4.3%. The maximum deviation is 10.1% at 0.69 eV.

ALADDIN evaluation function for cross section: NEEXH2

ALADDIN hierarchical labelling: EXC e Li [+0] (3p) e Li [+0] (4p)





Legend:

—— Recommended Cross Section

– – Analytic Fit

33

Energy	Velocity	Cross Section
(eV)	(cm/s)	(cm <sup>2</sup> )
7.00E-01	4.96E+07	1.95E-16
8.00E-01	5.30E+07	3.50E-16
1.00E+00	5.93E+07	5.36E-16
2.00E+00	8.39E+07	8.11E-16
4.00E+00	1.19E+08	7.46E-16
6.00E+00	1.45E+08	6.37E-16
8.00E+00	1.68E+08	5.52E-16
1.00E+01	1.88E+08	4.86E-16
2.00E+01	2.65E+08	3.02E16
4.00E+01	3.75E+08	1.75E-16
6.00E+01	4.59E+08	1.26E-16
8.00E+01	5.30E+08	1.01E-16
1.00E+02	5.93E+08	8.41E-17
2.00E+02	8.39E+08	4.72E-17
4.00E+02	1.19E+09	2.63E-17
6.00E+02	1.45E+09	1.85E-17
8.00E+02	1.68E+09	1.44E-17
1.00E+03	1.88E+09	1.19E-17

Threshold Energy:  $E_{th} = \Delta E = 0.643 \text{ eV}$ 

Accuracy: E < 3 eV : 30 - 50%;  $3 \le E(eV) \le 20 : 20 - 30\%$ ; E > 20 eV : 10 - 20%

<u>Comments</u>: The recommended cross section for this reaction is based on the semi-empirical formula of Van Regemorter [4] up to 25 eV, and on the results of the Bethe-Born approximation [4] for energies above 25 eV. The Bates-Damgaard approximation gives results which for energies above 10 eV agree to within 10 % with the recommended cross section, but with decreasing energy they become increasingly larger (about a factor of two in the region above the cross section maximum).

Analytic expression

Cross section:

$$\sigma_{\rm exc} = \frac{5.984 \times 10^{-16}}{\Delta E X} \left[ \frac{E - \Delta E}{E} \right]^{A_6} \left[ \sum_{j=1}^{4} \frac{A_j}{X^{j-1}} + A_5 \ln X \right] \quad [\rm cm^2],$$

where  $X = E / \Delta E$ , and  $\Delta E$  and E are expressed in eV.

		Fitting coeffi	Fitting coefficients				
A <sub>1</sub>	A <sub>2</sub>	A <sub>3</sub>	A4	As	A <sub>6</sub>		
2.0954	-4.3576	4.5639	0.0	2.4089	0.90076		

The rms deviation of the above fit to the recommended cross section is 1.7%. The maximum deviation is 9.75% at 0.65 eV.

ALADDIN evaluation function for cross section: NEEXH2

ALADDIN hierarchical labelling: EXC e Li [+0] (3d) e Li [+0] (4p)

$$e^{-} + Li(3d) - e^{-} + Li(4p)$$

Legend:

----- Recommended Cross Section

- — Analytic Fit

 $e^- + Li^*(3d) \rightarrow e^- + Li^*(4s, 4d)$ 

Energy	Velocity	Cross Sections $(cm^2)$	
(eV)	(cm/s)	3d → 4s	3d → 4d
6.00E-01	4 59E+07	9.13E-16	_
8.00E-01	5.30E+07	1.09E-15	2.77E-15
1.00E+00	5.93E+07	1.07E-15	3.56E-15
2.00E+00	8.39E+07	8.24E-16	2.94E-15
4.00E+00	1.19E+08	5.50E-16	1.94E-15
6.00E+00	1.45E+08	4.13E-16	1.47E-15
8.00E+00	1.68E+08	3.31E-16	1.17E-15
1.00E+01	1.88E+08	2.78E-16	9.87E-16
2.00E+01	2.65E+08	1.53E-16	5.55E-16
4.00E+01	3.75E+08	7.98E-17	3.10E-16
6.00E+01	4.59E+08	5.37E-17	2.20E-16
8.00E+01	5.30E+08	4.05E-17	1.72E-16
1.00E+02	5.93E+08	3.25E-17	1.41E-16
2.00E+02	8.39E+08	1. <b>61E-</b> 17	7.45E-17
4.00E+02	1.19E+09	7.99E-18	3.81E-17
6.00E+02	1.45E+09	5.31E-18	2.56E-17
8.00E+02	1.68E+09	4.01E-18	1.93E-17
1.00E+03	1.88E+09	3.21E-18	1.54E-17

Threshold Energies :  $E_{th} = \Delta E$ ;  $E_{th}(3d \rightarrow 4s) = 0.463 \text{ eV}$ ;  $E_{th}(3d \rightarrow 4d) = 0.662 \text{ eV}$ 

Accuracy: E < 3 eV: 50 - 120 %;  $3 < E(eV) \le 20: 30 - 50 \%$ ; E > 20 eV: 10 - 20 %

<u>Comments</u>: The recommended cross sections for the  $3d \rightarrow 4s$ , 4d transitions are based on the results of the Bates-Damgaard approximation [4], which in the region below 20 eV are appropriately reduced in accordance with the overestimation of the cross section for the  $3d \rightarrow 4p$  transition.

# Analytic expression

**Cross Section:** 

$$\sigma_{\text{exc}} = \frac{5.984 \times 10^{-16}}{\Delta E X} \left[ \frac{E - \Delta E}{E} \right]^{A_6} \left[ \sum_{j=1}^{4} \frac{A_j}{X^{j-1}} + A_5 \ln X \right] \quad [\text{cm}^2],$$

where X =	$E / \Delta E$ , and $\Delta E$ and $E$ are expressed in eV.
	Fitting coefficients

							Rms	Maxim	um Deviation
	A1	A <sub>2</sub>	<b>A</b> 3	A4	As.	A <sub>6</sub>	Deviation (%)	%	at E (eV)
3d → 4s	5.3737	-9.6628	10.042	0.0	0.0	0.95506	3.1	8.9	0.47
3d → 4d	23.821	-74.423	144.03	-83.310	0.0	0.72786	7.2	12.7	15.4

ALADDIN evaluation function for cross section: NEEXH2

ALADDIN hierarchical labelling :

EXC	с	Li	[+0]	(3d)	c	Li	[+0]	(4s),	for $3d \rightarrow 4s$
EXC	e	Lı	[+0]	(3d)	с	Li	[+0]	(4d),	for $3d \rightarrow 4d$



 $e^{-} + Li^{*}(3d) \rightarrow e^{-} + Li^{*}(4s, 4d)$ 

---- Recommended Cross Section

— Analytic Fit

37

Energy	Velocity	Cross Section
(eV)	(cm/s)	(cm <sup>2</sup> )
2.00E-01	2.65E+07	2.53E-13
4.00E-01	3.75E+07	8.23E-13
6.00E-01	4.59E+07	9.31E-13
8.00E-01	5.30E+07	9.15E-13
1.00E+00	5.93E+07	8.69E-13
2.00E+00	8.39E+07	6.62E-13
4.00E+00	1.19E+08	4.44E-13
6.00E+00	1.45E+08	3.39E-13
8.00E+00	1.68E+08	2.78E-13
1.00E+01	1.88E+08	2.36E-13
2.00E+01	2.65 <b>E+08</b>	1.40E-13
4.00E+01	3.75E+08	8.06E-14
6.00E+01	4.59E+08	5.77E-14
8.00E+01	5.30E+08	4.55E-14
1.00E+02	5.93E+08	3.78E-14
2.00E+02	8.39E+08	2.09E-14
4.00E+02	1.19E+09	1.15E-14
6.00E+02	1.45E+09	8.04E-15
8.00E+02	1.68E+09	6.22E-15
1.00E+03	1.88E+09	5.11E-15

#### Threshold Energy: $E_{th} = \Delta E = 0.180 \text{ eV}$

Accuracy: E < 2 eV : 30 - 50 %;  $2 \le E (eV) \le 5 : 20 - 30 \%$ ; E > 5 eV : 15 - 20 %

<u>Comments</u>: The recommended cross section for this reaction is based on a weighted average of the results of the Bates-Damgaard and Van Regemorter approximations [4], with a large weight given to the later. The results of these approximations differ by a factor of two in the region of the cross section maximum, but rapidly converge to each other for energies above 2 eV.

#### Analytic expression

Cross section:

$$\sigma_{\rm exc} = \frac{5.984 \times 10^{-16}}{\Delta E X} \left[ \frac{E - \Delta E}{E} \right]^{A_6} \left[ \sum_{j=1}^{4} \frac{A_j}{X^{j-1}} + A_5 \ln X \right] \quad [\rm cm^2],$$

where  $X = E / \Delta E$ , and  $\Delta E$  and E are expressed in eV.

Fitting coefficients							
A1	A <sub>2</sub>	A <sub>3</sub>	A4	A5	A <sub>6</sub>		
7.2489E-02	816.84	0.0	0.0	992.70	1.1539		

The rms deviation of the above fit to the recommended cross section is 2.6%. The maximum deviation is 13.5% at 0.24 eV.

ALADDIN evaluation function for cross section: NEEXH2

ALADDIN hierarchical labelling: EXC e Li [+0] (4s) e Li [+0] (4p)

$$(0)$$
  $(0)$ 

 $e^{-} + Li^{*}(4s) \rightarrow e^{-} + Li^{*}(4p)$ 

Legend:

----- Recommended Cross Section

- — Analytic Fit

Energy	Velocity	Cross Section
(eV)	(cm/s)	$(cm^2)$
·		·
2.10E-01	2.72E+07	1.72E-13
4.00E-01	3.75E+07	2.55E-13
6.00E-01	4.59E+07	2.14E-13
8.00E-01	5.30E+07	1.81E-13
1.00E+00	5.93E+07	1.57E-13
2.00E+00	8.39E+07	9.49E-14
4.00E+00	1.19E+08	5.37E-14
6.00E+00	1.45E+08	3.73E-14
8.00E+00	1.68E+08	2.84E-14
1.00E+01	1.88E+08	2.29E-14
2.00E+01	2.65E+08	1.15E-14
4.00E+01	3.75E+08	5.72E-15
6.00E+01	4.59E+08	3.79E-15
8.00E+01	5.30E+08	2.83E-15
1.00E+02	5.93E+08	2.26E-15
2.00E+02	8.39E+08	1.13E-15
4.00E+02	1.19E+09	5.75E-16
6.00E+02	1.45E+09	3.83E-16
8.00E+02	1.68E+09	2.88E-16
1.00E+03	1.88E+09	2.30E-16

Threshold Energy:  $E_{th} = \Delta E = 0.199 \text{ eV}$ 

Accuracy: 
$$E < 2 eV: 40 - 100\%; 2 \le E(eV) \le 5: 20 - 40\%; E > 5 eV: 15 - 20\%$$

<u>Comments</u>: The recommended cross section for this reaction is based on the results of the Bates-Damgaard approximation [4], which has been reduced by a varying factor in the energy region around the cross section maximum, in accordance with the reduction of corresponding results in the 4s  $\rightarrow$  4p case. At the energy of the cross section maximum (0.3 - 0.4 eV) this factor amounts to about two, and at 10 eV it becomes 1.03.

# Analytic expression

Cross section:

$$\sigma_{\rm exc} = \frac{5.984 \times 10^{-16}}{\Delta E X} \left[ \frac{E - \Delta E}{E} \right]^{A_6} \left[ \sum_{j=1}^{4} \frac{A_j}{X^{j-1}} + A_5 \ln X \right] \quad [\rm cm^2],$$

where  $X = E / \Delta E$ , and  $\Delta E$  and E are expressed in eV. Fitting coefficients

The rms deviation of the above fit to the recommended cross section is 2.0%. The maximum deviation is 4.9% at 1.16 eV.

ALADDIN evaluation function for cross section NEEXH2

ALADDIN hierarchical labelling  $\cdot$  EXC e Li [+0] (4s)  $\_$ c Li [+0] (4d)

$$(1)$$
  $(1)$ 

 $e^{-} + Li^{*}(4s) \rightarrow e^{-} + Li^{*}(4d)$ 

Legend:

----- Recommended Cross Section

- — Analytic Fit

1.1.21.

 $e^{-} + Li^{*}(4p) \rightarrow e^{-} + Li^{*}(4d)$ 

Energy	Velocity	Cross Section
(eV)	<b>(cm</b> /s)	$(\mathrm{cm}^2)$
<b></b>		
2.00E-02	8.45E+06	1.02E-12
4.00E-02	1.19E+07	6.00E-12
6.00E - 02	1.45E+07	6.84E-12
8.00E-02	1.68E+07	6.84E-12
1.00E-01	1 <b>.88E+07</b>	6.56E-12
2.00E - 01	2.65E+07	5.03E-12
4.00E-01	3.75E+07	3.39E-12
6.00E-01	4.59E+07	2.60E-12
8.00E-01	5.30E+07	2.13E-12
1.00E+00	5.93E+07	1.81E-12
2.00E+00	8.39E+07	1.08E-12
4.00E+00	1.19E+08	6.19E-13
6.00E+00	1.45E+08	4.4 <b>3</b> E-13
8.00E+00	1.68E+08	3.50E-13
1.00E+01	1.88E+08	2.91E-13
2.00E+01	2.65E+08	1.63E-13
4.00E+01	3.75E+08	9.00E-14
6.00E+01	4.59E+08	6.26E-14
8.00E+01	5.30E+08	4.85E-14
1.00E+02	5.93E+08	4.02E-14
2.00E+02	8.39E+08	2.19 <b>E</b> 14
4.00E+02	1.19E+09	1.16E-14
6.00E+02	1.45E+09	8.03E-15
8.00E+02	1.68E+09	6.20E-15
1.00E+03	1.88E+09	5.05E-15

Threshold Energy:  $E_{th} = \Delta E = 0.019 \text{ eV}$ 

Accuracy: E < 0.5 eV : 30 - 40%;  $0.5 \le E(eV) \le 2 : 20 - 30\%$ ; E > 2 eV : 10 - 20%

<u>Comments</u>: (1) The recommended cross section for this transition is based on the Bethe-Born and Van Regemorter approximations [4]. The reults of the two approximations coincide above 0.3 eV.

(2) In the energy region below 0.04 eV, the recommended cross sections follows the results of the semi-empirical formula of Van Regemorter.

### Analytic expression

Cross section:

$$\sigma_{\text{exc}} = \frac{5.984 \times 10^{-16}}{\Delta E X} \left[ \frac{E - \Delta E}{E} \right]^{A_6} \left[ \sum_{j=1}^{4} \frac{A_j}{X^{j-1}} + A_5 \ln X \right] \quad [\text{cm}^2],$$

where  $X = E / \Delta E$ , and  $\Delta E$  and E are expressed in eV.

Fitting coefficients

$A_1$	A <sub>2</sub>	A3	A4	As	A <sub>6</sub>
0.11 <b>050</b>	126.57	382.62	0 0	778.86	0. <b>92</b> 249

The rms deviation of the above fit to the recommended cross section is 0.6%. The maximum deviation is 2.11% at 0.98 eV

ALADDIN hierarchical labelling: EXC c  $L_1$  [+0] (4p) c  $L_1$  [+0] (4d)

$$10^{-11}$$
  $10^{-10}$ 

 $e^{-} + Li^{*}(4p) \rightarrow e^{-} + Li^{*}(4d)$ 

----- Recommended Cross Section

- — Analytic Fit

43

# 1.2. Ionization

Energy	Velocity	Cross section
(eV)	(cm/s)	(cm <sup>2</sup> )
5.50E+00	1.39E+08	6.54E-18
6.00E+00	1.45E+08	<b>4.92E</b> -17
8.00E+00	1.68E+08	<b>2.45E-16</b>
1.00E+01	1.88E+08	<b>3.58E-16</b>
2.00E+01	2.65E+08	<b>4.10E-16</b>
4.00E+01	3.75E+08	<b>2.86</b> E-16
6.00E+01	4.59E+08	2.14E-16
8.00E+01	5.30E+08	1.71E-16
1.00E+02	5.93E+08	1.43E-16
2.00E+02	8.39E+08	7.92E-17
4.00E+02	1.19E+09	4.30E-17
6.00E+02	1.45E+09	2.98E-17
8.00E+02	1.68E+09	<b>2.30E-17</b>
1.00E+03	1.88E+09	1.88E-17
2.00E+03	2.65E+09	9.95E-18
4.00E+03	3.75E+09	5.26E-18
6.00E+03	4.59E+09	3.61E-18
8.00E+03	5.30E+09	2.77E-18
1.00E+04	5.93E + 09	2.25E-18

Threshold energy:  $E_{th} = I = 5.39 \text{ eV}$ 

Accuracy:  $E \le 30 \text{ eV} : 15\%$ ; E > 30 eV : 10%

<u>Comments</u>: The cross section for this reaction is taken from the analytic fit to the recommended data of Lennon et al [10].

# Analytic fitting function

Cross section:

$$\sigma_{\text{ion}} = \frac{10^{-13}}{\text{I E}} \left[ A \ln \left( \frac{\text{E}}{\text{I}} \right) + \sum_{J=1}^{5} B_{J} \left( 1 - \frac{\text{I}}{\text{E}} \right)^{J} \right] \quad [\text{cm}^{2}]$$

where the parameter A is a Bethe coefficient, determined from fitting the high energy cross section with the expression

$$\sigma_{\rm ton} = \frac{10^{-13}}{\rm I E} \left[ A \ln (E) + B \right] [cm^2] ,$$

where I and E are expressed in eV.

#### Fitting parameters

Α	<b>B</b> 1	B <sub>2</sub>	<b>B</b> 3	<b>B</b> 4	B5
0.085	-0.004	0.757	-0.178	0.0	0.0

ALADDIN evaluation function for cross section: BELI

ALADDIN hierarchical labelling: ION e Li [+0] (2s) e H [+1] e



----- Recommended Cross Section

 $e^{-} + Li^{*}(nl) \rightarrow e^{-} + Li^{+} + e^{-}, n=2-4, l < n$ 

Energy	Velocity		Cross sections (cm <sup>2</sup> )	
(eV)	(cm/s)	nl=2p	nl=3p	nl = 4p
1.00E+00	5.93E+07	_	_	3.75E-15
2.00E+00	8.39E+07		2.51E-15	1.87E-14
4.00E+00	1.19E+08	2.15E-16	6.01E-15	1.76E-14
6.00E+00	1.45E+08	8.77E-16	5.79E-15	1.48E-14
8.00E+00	1.68E+08	1.11E-15	5.26E-15	1.28E-14
1.00E+01	1.88E+08	1.16E-15	4.77E-15	1.12E-14
2.00E+01	2.65E+08	9.69E-16	3.27E-15	7.20E-15
4.00E+01	3.75E+08	6.81E-16	2.08E-15	4.40E-15
6.00E+01	4.59E+08	5.33E-16	1.56E-15	3.24E-15
8.00E+01	5.30E+08	4.43E-16	1.27E-15	2.60E-15
1.00E + 02	5.93E+08	3.82E-16	1.07E-15	2.19E-15
2.00E+02	8.39E+08	2.36E-16	6.31E-16	1.26E-15
4.00E+02	1.19E+09	1.40E - 16	3.63E-16	7.12E-16
6.00E+02	1.45E+09	1.02E - 16	2.61E-16	5.06E-16
8.00E+02	1.68E+09	8.13E-17	2.05E-16	3.97E-16
1.00E+03	1.88E+09	6.79E-17	1.70E-16	3.28E-16
2.00E+03	2.65E+09	3.84E-17	9.45E-17	1.80E-16
4.00E+03	3.75E+09	2.14E-17	5.20E-17	9.85E-17
6.00E+03	4.59E+09	1.51E-17	3.65E-17	6.88E-17
8.00E+03	5.30E+09	1.18E-17	2.83E-17	5.33E-17
1.00E+04	5.93E+09	9.72E-18	2.33E-17	<b>4.37E</b> -17

Threshold energies:  $I_{n1}$  (eV), 2p = 3.541, 3s = 2.018, 3p = 1.557, 3d = 1.513, 4s = 1.050, 4p = 0.870, 4d = 0.851, 4f = 0.850

Accuracy: Unspecified within 20 - 80 %

Comments: In the absence of a consistent set of data for the cross sections of these reactions, the use of the semi-impirical formulae of Lotz [11,12] is suggested :

$$\sigma_{nl}(E) = 10^{-14} \sum_{i=1}^{2} a_{i} q_{i} \frac{\ln(E/P_{i})}{E P_{i}} \left\{ 1 - b_{i} \exp\left[ -c_{i} \left( \frac{E}{P_{i}} - 1 \right) \right] \right\} \quad [cm^{2}],$$

where E is expressed in units of eV,  $P_i$  is the binding energy of the electron in the i-th subshell, q<sub>i</sub> is the number of equivalent electrons in the i-th subshell, and  $a_i$ ,  $b_i$  and  $c_i$  are numerical coefficients given in the table below

P <sub>1</sub> (eV)	$P_2(eV)$	<b>q</b> 1	<b>q</b> 2	a1	a2	b1	<b>b</b> <sub>2</sub>	c1	c2
I <sub>nl</sub> (eV)	58	1	2	4.0	4.2	0.7	0.6	2.4	0.6

ALADDIN evaluation function for cross section: EIONLT

ALADDIN hierarchical labelling: ION e Li [+0] (nl) e H [+1] e

$$e^{-} + Li^{*}(nl) \rightarrow e^{-} + Li^{+} + e^{-}$$
, n=2-4, l





— Recommended Cross Section

# 2.1. Excitation

Energy	Velocity	Cross Section
(eV/amu)	(cm/s)	(cm <sup>2</sup> )
2.00E+03	6.21E+07	7.04E-16
5.00E+03	9.82E+07	3.81E-15
1.00E+04	1.39E+08	4.36E-15
2.00E+04	1.96E+08	3.60E-15
5.00E+04	3.11E+08	2.12E-15
1.00E+05	4.39E+08	1.28E-15
2.00E+05	6.21E+08	7.43E-16
5.00E+05	9.82E+08	3.48E-16
1.00E+06	1.39E+09	1.93E-16
2.00E+06	1.96E+09	1.07E - 16

Threshold Energy:  $E_{th} = \Delta E = 1.847 \text{ eV}$ 

 $E_p < 2 \text{ keV/amu}$ : Indeterminate;  $2 \le E_p (\text{keV/amu}) \le 20$ : 10-20 %; Accuracy:  $E_p > 20$  (keV/amu) : 10-15 % ( $E_p$  is the proton energy)

Comments: (1) The recommended cross section for this transition is obtained by scaling the corresponding recommended electron impact excitation cross section according to the relations (see e.g. Bates and Griffing [13])

$$\sigma_{\rm p}({\rm E}_{\rm p}) = \sigma_{\rm e}({\rm E}_{\rm e}), \tag{a}$$

$$E_{p}(keV/amu) = 0.918 E_{e}(eV) \left[ 1 - \frac{\Delta E(eV)}{\lambda E_{e}(eV)} + \left(\frac{\Delta E(eV)}{E_{e}(eV)}\right)^{1/2} \right]$$
(b)

1

where  $\lambda = 1.15$  and the subscripts e and p indicate that the corresponding quantity is related to the electron and proton case, respectively.

(2) The value  $\lambda = 1.15$  in Eq. (b) has been chosen to adjust the scaled cross section to the experimental data of Aumayr et al [14] and to the results of atomic orbital close-coupling calculations of Ermolaev [15] and Schweinzer et al [20], both available at intermediate and low energies.

NEEXH2 for the cross section as a function of  $E_e(eV)$ ALADDIN evaluation function for cross section: ALADDIN hierarchical labelling: EXC H [+1] Li [+0] (2s) H [+1] Li [+0] (2p)

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



Legend:

---- Recommended Cross Section

Energy	Velocity	Cross sections (cm <sup>2</sup> )	
(eV/amu)	(cm/s)	<u>2s</u> → 3p	2s → 4p
5.00E+03	9.82E+07	1.76E-16	1.44E-17
1.00E+04	1.39E+08	1.22E-16	2.32E-17
2.00E+04	1.96E+08	6.28E-17	1. <b>49E</b> -17
5.00E+04	3.11E+08	2.45E-17	6.87E-18
1.00E+05	4.39E+08	1.22E-17	3.71E-18
2.00E+05	6.21E+08	6.11E-18	2.07E-18
5.00E+05	9.82E+08	2.49E-18	9.36E-19
1.00 <b>E+0</b> 6	1.39E+09	1.27E-18	5.10E-19
2.00E+06	1.96E+09	6.50E-19	2.77E-19

# 2.1.2. $H^+ + Li(nl) \rightarrow H^+ + Li^*(n'l'); n,n' = 2,3,4; l < n; l' < n'$

<u>Threshold Energy</u>:  $E_{th} = \Delta E = |E_{nl} - E_{n'l'}|$  (see reactions in Section 1.1)

<u>Accuracy</u>: The accuracy of scaled cross sections  $\sigma_p(E_p)$  is believed to be within 20 - 50 % in the region below the energy of the cross section maximum, and about 15 - 20 % in the energy region above the cross section maximum.

<u>Comments</u>: In the absence of any cross section information for these reactions, their cross sections can be estimated by scaling the corresponding electron impact excitation cross sections according to the relations (see e.g. [13])

$$\sigma_{p}(E_{p}) = \sigma_{e}(E_{e}), \tag{a}$$

$$E_{p}(keV/amu) = 0.918 E_{e} (eV) \left[ 1 - \frac{\Delta E(eV)}{1.15 E_{e}(eV)} + \left( \frac{\Delta E(eV)}{E_{e}(eV)} \right)^{1/2} \right]$$
(b)

where  $\sigma_e(E_e)$  is the electron impact cross section at an electron energy  $E_e$  (expressed in eV) and  $\sigma_p(E_p)$  is the proton impact cross section at an energy  $E_p$  (expressed in keV/amu). The range of validity of relations (a),(b) is  $E_p$  (keV/amu) > 0.46  $\Delta E$  (eV).

ALADDIN evaluation function for cross section: NEEXH2 for the cross section as a function of Ee (eV)

ALADDIN hierarchical labelling: EXC H [+1] Li [+0] (nl) H [+1] Li [+0] (n'l')

$$H^{+} + Li(nl) \rightarrow H^{+} + Li^{*}(n'l'); n,n'=2,3,4; l< n; l< n; l'< n'$$



Legend:

—— Recommended Cross Section

# 2.2. Electron Removal

Energy	Velocity	Cross Section
(eV/amu)	(cm/s)	(cm <sup>2</sup> )
5.00E+02	3.11E+07	590E-16
1.00E+03	4.39E+07	1.52E-15
2.00E+03	6.21E+07	3.40E-15
5.00E+03	9.82E+07	5.18E-15
1.00E+04	1.39E+08	2.68E-15
2.00E+04	1.96E+08	1.26E-15
5.00E+04	3.11E+08	6.23E-16
1.00E+05	4.39E+08	3.31E-16
2.00E+05	6.21E+08	1.76E-16

Accuracy: E < 0.1 keV/amu: Indeterminate;  $0.1 \le E (\text{keV/amu}) < 2:15-30\%$ ;  $2 \le E (\text{keV/amu}) < 20:10-15\%$ ;  $E \ge 20 \text{ keV/amu}: 10\%$ 

- Comments: (1) For energies below 2 keV/amu the recommended electron loss cross section is based on the experimental electron capture data of Varghese et al [16]. In the energy range 2 - 20 keV/amu, where the electron loss cross section is still dominated by the electron capture channel, the recommended cross section is based on the experimental data of Aumayr and Winter [17], Shah et al [18] and Varghese et al [16], which agree to within 10 % in the overlapping energy region. The AO-based close-coupling calculations of Fritsch and Lin [19], Ermolaev [15] and Schweinzer et al [20] are also consistent with the recommended cross section values.
  - (2) For energies above 20 keV/amu, the recommended cross section is based on the experimental data of DuBois and Toburen [21], DuBois [22] and Shah et al [18], which in the overlapping region agree to within 10 %.

# Analytic expression

Cross section:

$$\sigma_{\rm exc} = 10^{-16} \,A_1 \left[ \frac{\exp\left(-A_2 \,/\, E\right) \,\ln\left(1 + A_3 E\right)}{E} + \frac{A_4 \,\exp\left(-A_5 E\right)}{E^{A_6} + A_7 E^{A_8}} \right] \qquad [\rm cm^2]$$

where E is expressed in keV/amu.

Fitting parameters					
A1 - A4	17.401	6.5623	7.1943E+06	67.115	
A5 - A8	0.21151	1.0551	64.854	-1.4472	

The rms deviation of the above fit to the recommended cross section is 1.9%. The maximum deviation is 4.1% at 1.2 keV/amu.

ALADDIN evaluation function for cross section: HEXC3

ALADDIN hierarchical labelling: ELREM H [+1] Li [+0] (2s) Li [+1]

$$10^{-14}$$
  $10^{-14}$   $10^{-16}$ 

 $H^{+} + Li(2s) \rightarrow Li^{+} + ...$ 

Legend:

----- Recommended Cross Section

- — Analytic Fit

Energy	Velocity	Cross Section
(eV/amu)	(cm/s)	(cm <sup>2</sup> )
1.00E+01	4.39E+06	1.09E-14
2 00E+01	6.21E+06	1.08E-14
5 00E+01	9.82E+06	1.06E-14
1.00E+02	1.39E+07	1.05E-14
2.00E+02	1.96E+07	1.04E-14
5.00E+02	3.11E+07	1.00E-14
1.00E+03	4.39E+07	9.58E-15
2.00E+03	6.21E+07	8.08E-15
5.00E+03	9.82E+07	5.76E-15
1.00E+04	1. <b>39</b> E+08	3.95E-15
2.00E+04	1.96E+08	2.34E-15
5.00E+04	3.11E+08	1.04E-15
1.00E+05	4.39E+08	5.62E-15
2.00E+05	6.21E+08	2.99E-16
5.00E+05	9.82E+08	1.31E-16
1.00E+06	1.39E+09	7.75E-17

Accuracy:  $E < 0.04 \text{ keV/amu}: 30-40\%; \quad 0.04 \le E (\text{keV/amu}) < 1:30\%;$  $1 \le E (\text{keV/amu}) < 20: 15-20\%; \quad E \ge 20 \text{ keV/amu}: 10-15\%$ 

- Comments: (1) In the intermediate energy range 1 20 keV/amu, the recommended electron loss cross section follows the multi-state AO close-coupling calculations of Schweinzer et al [20].
  - (2) In the energy region below 1 keV/amu, the electron loss cross section coincides with the electron capture cross section, and has been constructed by using the scaled cross section of Ref. [20] for A<sup>q+</sup> + Li (np) collisions.
  - (3) In the energy region above 30 keV/amu, the electron loss cross section coincides with the ionization cross section and been obtained by scaling, with respect to the electron binding energy, the proton impact ionization cross section from Ref. [23].

Analytic expression

Cross section:

$$\sigma_{\text{loss}} = 10^{-14} \text{ A}_1 \left[ 1 - \exp \left\{ \frac{-A_2 \ln (e + A_3 E)}{E} \right\} \right] \quad [\text{cm}^2]$$
where E is expressed in keV/amu.
  
Fitting coefficients
  
A\_1 A\_2 A\_3

.

0.94189 5.6482 1.4910E-03

The rms deviation of the above fit to the recommended cross section is 5.2%. The maximum deviation is 13.4% at 10 eV/amu.

ALADDIN evaluation function for cross section: HLOSS2

ALADDIN hierarchical labelling: ELREM H [+1] Li [+0] (2p) Li [+1]

2.2.2.

$$(10^{-14})_{10^{-17}}$$
  $(10^{-17})_{10^{-17}}$   $(10^$ 

 $H^{+} + Li^{*}(2p) \rightarrow Li^{+} + ...$ 

---- Recommended Cross Section - - - Analytic Fit

Energy	Velocity	Cross Section
(eV/amu)	(cm/s)	(cm <sup>2</sup> )
1.00E+01	4.39E+06	4.34E-14
2.00E+01	6.21E+06	<b>4.22E-1</b> 4
5.00E+01	9.82E+06	4.12E-14
1.00E+02	1.39E+07	4.06E-14
2.00E+02	1 <b>.96E+07</b>	4.01E-14
5.00E+02	3.11E+07	3.90E-14
1.00E+03	4.39E+07	3.82E-14
2.00E+03	6.21E+07	3.21E-14
5.00E+03	9.82E+07	1.53E-14
1.00E+04	1.39E+08	8.22E-15
2.00E+04	1.96E+08	4.34E-15
5.00E+04	3.11E+08	<b>1.90E-15</b>
1.00E+05	4.39E+08	1.01E-15
2.00E+05	6.21E+08	5.39E-16
5.00E+05	9.82E+08	2.37E-16
1.00E+06	1.39E+09	1. <b>29E-1</b> 6

Accuracy: E < 0.5 keV/amu : 20-40%;  $0.5 \le E (\text{keV/amu}) < 25 : 15-20\%$ ;  $E \ge 25 \text{ keV/amu} : 10-15\%$ 

- <u>Comments</u>: (1) There exists theoretical information on the electron loss cross section for this collision system only for the energy range 0.4 - 2.2 keV/amu [20]. The cross section was calculated by using the close-coupling method with a large AO basis. These data were extended towards lower energies (where ionization is negligible) by using the classical cross section scaling for electron capture [24].
  - (2) For energies above 25 keV/amu, the electron loss cross section coincides with the ionization cross section, and was constructed by scaling the recommended proton-impact ionization cross section of hydrogen atoms from Ref. [23].

(3) The form of the analytic expression for  $\sigma_{\text{loss}}$  given below follows the idea of Ref. [25]. Analytic expression

Cross section:

$\sigma_{\rm loss} = 10^{-14} \rm A_1$	$\left[1 - \exp\left\{\frac{-A_2\ln\left(e + A_3\right)}{E}\right\}\right]$	$\left[ \frac{E}{2} \right] \left[ cm^2 \right]$
where E is expres	sed in keV/amu.	
	Fitting coefficients	
A1	A <sub>2</sub>	A3
4.2572	2.2300	1.4998E-03

The rms deviation of the above fit to the recommended cross section is 4.1%. The maximum deviation is 10.9% at 2.41 keV/amu.

ALADDIN evaluation function for cross section: HLOSS2

ALADDIN hierarchical labelling: ELREM H [+1] LI [+0] (3s) Li [+1]
$$(10^{-14})$$
  $(10^{-14})$   $(10^{-14})$   $(10^{-14})$   $(10^{-14})$   $(10^{-14})$   $(10^{-14})$   $(10^{-14})$   $(10^{-14})$   $(10^{-14})$   $(10^{-14})$   $(10^{-16})$   $(10$ 

 $H^{+} + Li^{*}(3s) \rightarrow Li^{+} + ...$ 

Legend:

----- Recommended Cross Section

--- Analytic Fit

Energy	Velocity	Cross Section
(eV/amu)	(cm/s)	(cm <sup>2</sup> )
1.00E+01	4.39E+06	3.60E-14
2.00E+01	6.21E+06	3.55E-14
5.00E+01	9.82E+06	3.45E-14
1.00E+02	1.39E+07	3.41E-14
2.00E+02	1:96E+07	3.36E-14
5.00E+02	3.11E+07	3.12E-14
1.00E+03	4.39E+07	2.82E-14
2.00E+03	6.21E+07	2.41E-14
5.00E+03	9.82E+07	1.74E-14
1.00E+04	1.39E+08	1.04E-14
2.00E+04	1.96E+08	5.63E-15
5.00E+04	3.11E+08	2.51E-15
1.00E+05	4.39E+08	1.36E-15
2.00E+05	6.21E+08	7.34E-16
5.00E+05	9.82E+08	3.25E-16
1.00E+06	1.39E+09	1.75E-16

E < 0.5 keV/amu : 20-40%;  $0.5 \le E (\text{keV/amu}) < 25 : 15-20\%$ ; Accuracy:  $E \ge 25 \text{ keV/amu} : 10-15\%$ 

- Comments: (1) In the energy range 1 20 keV/amu extensive AO-based close-coupling calculations for this cross section are available [20]. The electron loss cross section for energies below 1 keV/amu coincides with that for electron capture and has been constructed by extending the data of Schweinzer et al [20] from the region around 1 keV/amu using the classical scaling relationship [24].
  - (2) For energies above 30 keV/amu, the electron loss cross section is identical with that for ionization, and was constructed by scaling the recommended proton-impact ionization cross section for hydrogen from Ref. [23].

•

(3) The form of the analytic expression for  $\sigma_{\text{loss}}$  given below follows the idea of Ref. [25]. Analytic expression

Cross section:

$$\sigma_{\text{loss}} = 10^{-14} \text{ A}_1 \left[ 1 - \exp\left\{\frac{-A_2 \ln (e + A_3 E)}{E}\right\} \right] \text{ [cm}^2\text{]}$$
where E is expressed in keV/amu.
  
Fitting coefficients
  
A\_1 A\_2 A\_3
  
3.2083 3.9346 1.7891E-03

The rms deviation of the above fit to the recommended cross section is 4.9%. The maximum deviation is 15.1% at 1.00 eV/amu.

ALADDIN evaluation function for cross section: HLOSS2

ALADDIN hierarchical labelling: ELREM H [+1] Li [+0] (3p) Li [+1]

$$(10^{-14})_{10^{-16}}$$

 $H^+ + Li^*(3p) \rightarrow Li^+ + \dots$ 

Legend:

----- Recommended Cross Section

- – – Analytic Fit

Energy	Velocity	Cross Section
(eV/amu)	(cm/s)	(cm <sup>2</sup> )
1.00E+01	4 <b>39E+0</b> 6	3.05E-14
2.00E+01	6.21E+06	3.03E-14
5.00E+01	9.82E+06	2.96E-14
1.00E+02	1.39E+07	2.92E-14
2.00E+02	1.96E+07	2.87E-14
5.00E+02	3.11E+07	2.84E-14
1.00E+03	4.39E+07	2.79E-14
2.00E+03	6.21E+07	2.70E-14
5.00E+03	9.82E+07	1.98E-14
1.00E+04	1.39E+08	1.12E-14
2.00E+04	1.96E+08	5.93E-15
5.00E+04	3.11E+08	2.61E-15
1.00E+05	4.39E+08	1.43E-15
2.00E+05	6.21E+08	7.70E-16
5.00E+05	9.82E+08	3.36E-16
1.00E+06	1.39E+09	1.78E-16

Accuracy: E < 0.5 keV/amu : 20-40%;  $0.5 \le E (\text{keV/amu}) < 20 : 15-20\%$ ;  $E \ge 20 \text{ keV/amu} : 10-15\%$ 

- Comments: (1) In the energy range 1 20 keV/amu, the recommended cross section represents the data of the elaborate AO-based close-coupling calculations of Schweinzer [20]. For energies below 1 keV/amu, the cross section was constructed by using the classical cross section scaling relationships for electron capture [24].
  - (2) For energies above 30 keV/amu, the electron loss cross section coincides with that for ionization and has been obtained by scaling the recommended proton-impact hydrogen ionization cross section from Ref. [23].

Analytic expression

Cross section:

$$\sigma_{\text{loss}} = 10^{-14} A_1 \left[ 1 - \exp\left\{ \frac{-A_2 \ln(e + A_3 E)}{E} \right\} \right] [cm^2]$$

where E is expressed in keV/amu.

Fitting coefficients

<b>A</b> <sub>1</sub>	A2	A <sub>3</sub>
<b>2.97</b> 19	4.6444	1.2749E-03

The rms deviation of the above fit to the recommended cross section is 3.9%. The maximum deviation is 9.07% at 4.51 keV/amu.

ALADDIN evaluation function for cross section: HLOSS2

ALADDIN hierarchical labelling: ELREM H [+1] Li [+0] (3d) Li [+1]



 $H^+ + Li^*(3d) \rightarrow Li^+ + \dots$ 



Energy	Velocity	Cross Section
(eV/amu)	(cm/s)	(cm <sup>2</sup> )
1.00E+01	4.39E+06	1 52E-13
2.00E+01	6.21E+06	1.52E-13
5.00E+01	9.82E+06	1.50E-13
1.00E+02	1.39E+07	1.49E-13
2.00E+02	1.96E+07	1.48E-13
5.00E+02	3.11E+07	1.45E-13
1.00E+03	4.39E+07	1.28E-13
2.00E+03	6.21E+07	7.73E-14
5.00E+03	9.82E+07	3.30E-14
1.00E+04	1.39E+08	1.74E-14
2.00E+04	1.96E+08	9.22E-15
5.00E+04	3.11E+08	4.04E-15
1.00E+05	4.39E+08	2.13E-15
2.00E+05	6.21E+08	1.14E-15
5.00E+05	9.82E+08	4.88E-16
1.00E+06	1.39E+09	2.64E-16

Accuracy: E < 0.5 keV/amu: 30-40 %; 0.5 ≤ E (keV/amu) < 30: 20-30  $c_c$ ; E ≥ 30 keV/amu: 15-20 %

<u>Comments</u>: No experimental or theoretical data is available for this reaction. The recommended cross section has been constructed from that for electron loss from the 3s state (reaction 2.2.3) by applying the classical scaling relations  $\sigma \sim n_*^4 \sigma_0$ ,  $E \sim n_*^2 E_0$ , where  $n_*$  is the effective principal quantum number, and  $\sigma_0$  and  $E_0$  are constants (see [25]).

Analytic expression

Cross section:

$$\sigma_{\text{loss}} = 10^{-14} \text{ A}_1 \left[ 1 - \exp\left\{ \frac{-A_2 \ln (e + A_3 E)}{E} \right\} \right] \text{ [cm}^2 \text{]}$$
where E is expressed in keV/amu.  
Fitting coefficients  
A\_1 A\_2 A\_3  
16.240 1.1957 1 6519E-03

The rms deviation of the above fit to the recommended cross section is 4.9%. The maximum deviation is 12.6% at 1.27 keV/amu.

ALADDIN	evaluation	function fo	or cross secti	on: H	LOSS2

ALADDIN hierarchical labelling: ELREM H [+1] Li [+0] (4s) Li [+1]

$$H^+ + Li^*(4s) \rightarrow Li^+ + \dots$$



- – – Analytic Fit

Energy	Velocity	Cross Section
(eV/amu)	(cm/s)	(cm <sup>2</sup> )
1.00E+01	4.39E+06	1.13E-13
2.00E+01	6.21E+06	1.12E-13
5.00E+01	9.82E+06	1.11E-13
1.00E+02	1.39E+07	1.11E-13
2.00E+02	1 <b>:96E+07</b>	1.10E-13
5.00E+02	3.11E+07	1.06E-13
1.00E+03	4.39E+07	9.58E-14
2.00E+03	6.21E+07	7.37E-14
5.00E+03	9.82E+07	3.68E-14
1.00E+04	1.39E+08	1. <b>98E-1</b> 4
2.00E+04	1.96E+08	1.05E-14
5.00E+04	3.11E+08	4.65E-15
1.00E+05	4.39E+Ö8	2.50E-15
2.00E+05	6.21E+08	1.33E-15
5.00E+05	9.82E+08	5.80E-16
1.00E+06	1.39E+09	3.05E-16

Accuracy: E < 0.5 keV/amu : 30-40 %;  $0.5 \le E (\text{keV/amu}) < 10 : 20-30 \%$ ;  $E \ge 10 \text{ keV/amu} : 15-20 \%$ 

<u>Comments</u>: No experimental or theoretical data is available for this reaction. The recommended cross section has been constructed from that for electron loss from the 3p state (reaction 2.2.4) by applying the classical scaling relations  $\sigma \sim n_*^4 \sigma_0$ ,  $E \sim n_*^2 E_0$ , where  $n_*$  is the effective principal quantum number, and  $\sigma_0$  and  $E_0$  are constants (see [25]).

Analytic expression

Cross section:

$$\sigma_{\text{loss}} = 10^{-14} \text{ A}_1 \left[ 1 - \exp\left\{ \frac{-A_2 \ln (e + A_3 E)}{E} \right\} \right] \quad [\text{cm}^2]$$
where E is expressed in keV/amu.
$$\frac{\text{Fitting coefficients}}{A_2} \qquad A_3$$

A<sub>1</sub> A<sub>2</sub> A<sub>3</sub> 11.041 2.0596 1.7696E-03

The rms deviation of the above fit to the recommended cross section is 3.6%. The maximum deviation is 11.1% at 1.0 MeV/amu.

ALADDIN evaluation function for cross section: HLOSS2

ALADDIN hierarchical labelling: ELREM H [+1] Li [+0] (4p) Li [+1]

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 $H^{+} + Li^{*}(4p) \rightarrow Li^{+} + \dots$ 

---- Recommended Cross Section --- Analytic Fit

Energy	Velocity	Cross Section
(eV/amu)	(cm/s)	(cm <sup>2</sup> )
1.00E+01	4.39E+06	1.01E-13
2.00E+01	6.21E+06	9.99E-14
5.00E+01	9.82E+06	9.82E-14
1.00E+02	1.39E+07	9.79E-14
2.00E+02	1.96E+07	9.69E-14
5.00E+02	3.11E+07	9.40E-14
1.00E+03	4.39E+07	8.79E-14
2.00E+03	6.21E+07	8.05E-14
5.00E+03	9.82E+07	4.28E-14
1.00E+04	1.39E+08	2.28E-14
2.00E+04	1.96E+08	1.20E-14
5.00E+04	3.11E+08	5.22E-15
1.00E+05	4.39E+08	2.77E-15
2.00E+05	6.21E+08	1.48E-15
5.00E+05	9.82E+08	6.31E-16
1.00E+06	1.39E+09	3.33E-16

Accuracy: E < 0.5 keV/amu : 30-40 %; 0.5 ≤ E (keV/amu) < 10 : 20-30 %; E ≥ 10 keV/amu : 15-20 %

<u>Comments</u>: No experimental or theoretical data are available for this cross section. The recommended cross section has been constructed from that for electron loss from the 3d state (reaction 2.2.5) by applying the classical scaling relations  $\sigma \sim \mathbf{n}_{\bullet}^4 \sigma_0$ ,  $E \sim \mathbf{n}_{\bullet}^2 E_0$ }, where  $\mathbf{n}_{\bullet}$  is the effective principal quantum number, and  $\sigma_0$  and E<sub>0</sub> are constants (see [25]).

Analytic expression

Cross section:

$\sigma_{\rm loss} = 10^{-14} \rm A_1$	$\left[1-\exp{i\theta}\right]$	$\frac{-A_2 \ln (e + A_2)}{E}$	$\left. \frac{A_3E}{B_3E} \right\}$	[cm <sup>2</sup> ]
where E is expres	ssed in keV.	amu.	,	
	<b>Fitting</b>	coefficients		
A <sub>1</sub>		A2		A <sub>3</sub>
10.191		2.6200	1.	0166E-03

The rms deviation of the above fit to the recommended cross section is 4.5%. The maximum deviation is 11.8% at 2.23 keV/amu.

ALADDIN evalu	ation function	for cross section:	HLOSS2

ALADDIN hierarchical labelling: ELREM H [+1] Li [+0] (4d) Li [+1]

$$(1)$$
  $(1)$ 

 $H^+ + Li^*(4d) \rightarrow Li^+ + \dots$ 

----- Recommended Cross Section

--- Analytic Fit

## 3.1. Excitation

_					
	Energy / q	Velocity / $\sqrt{q}$	Cross sections $/ q (cm^2)$		)
	(eV/amu)	(cm/s)	<u>2s</u> → 2p	2s → 3p	2s → 4p
	2.00E+03	6.21E+07	7.04E-16	_	_
	5.00E+03	9.82E+07	3.81E-15	1.76E-16	1.44E-17
	1.00E+04	1.39E+08	4.36E-15	1.22E-16	2.32E-17
	2.00E+04	1.96E+08	3.60E-15	6.28E-17	1. <b>49E-1</b> 7
	5.00E+04	3.11E+08	2.12E-15	2.45E-17	6.87E-18
	1.00E+05	4.39E+08	1.28E-15	1.22E-17	3.71E-18
	2.00E+05	6.21E+08	7.43E-16	6.11E-18	2.07E-18
	5.00E+05	9.82E+08	3.48E-16	2.49E-18	9.36E-19
	1.00E+06	1.39E+09	1.93E-16	1.27E-18	5.10E-19
	2.00E+06	1.96E+09	1.07E-16	6.50E-19	2.77E-19

.1.	A <sup>q+</sup>	+ Li(nl) -	► A <sup>q+</sup>	+ Li <sup>*</sup> (n'l')	); n,n'=2,3,4; l <n; l'<n';="" q="">1</n;>
-----	-----------------	------------	-------------------	--------------------------	--

Threshold Energies : See reactions in section 1.1.

- <u>Accuracy</u>: The accuracy of the reduced cross sections  $\tilde{\sigma}(\tilde{E})$  is believed to be within a factor of two for reduced energies  $\tilde{E}$  below the cross section maximum, about 40 60 % in the region of the maximum of  $\sigma$ , and within 20 30 % for higher reduced energies.
- Comments: (1) For excitation from ground state Li (2s) to Li (2p) there exist extensive atomic orbital close-coupling calculations [20] which support the scaling given below in the reduced energy range 2 50 keV/amu.
  - (2) In the absence of any systematic cross section information for all other excitation processes, their cross sections can be estimated by using the corresponding proton impact excitation cross sections  $\sigma_p$  (E<sub>p</sub>) of section 2 and the scaling relationships

$$\sigma_{q}(E) = q \sigma_{p}(E/q), \qquad (a)$$

or, in the reduced form,

$$\widetilde{\sigma} = \sigma_q(E)/q = \sigma_p(E/q) = \sigma_p(E)$$
 (b)

where E is the collision energy in keV/amu.





----- Recommended Cross Section

# 3.2. Electron Removal

Energy x $n_*^2/q$	Vel. x $n_*/\sqrt{q}$	Cross section / n <sup>4</sup> q
(eV/amu)	(cm/s)	(cm <sup>2</sup> )
1.00E + 01	4.39E+06	8.91E-16
2.00E+01	6.21E+06	8.91E-16
5.00E+01	9.82E+06	8.91E-16
1.00E+02	1.39E+07	8.91E-16
2.00E+02	1.96E+07	8.91E-16
5.00E+02	3.11E+07	8.91E-16
1.00E+03	4.39E+07	8.91E-16
2.00E+03	6.21E+07	8.90E-16
5.00E+03	9.82E+07	8.58E-16
1.00E+04	1.39E+08	7.01E-16
2.00E+04	1.96E+08	4.82E-16
5.00E+04	3.11E+08	2.33E-16
1.00E+05	4.39E+08	1.25E-16
2.00E+05	6.21E+08	6.48E-17
5.00E+05	9.82E+08	2.63E-17
1.00E+00	1.39E+06	9.18E-16
2.00E+00	1.96E+06	9.18E-16

- Accuracy:  $En_*^2/q < 10 \text{ keV/amu} : 20-30 \%$ ;  $10 \le En_*^2/q \ge 30 \text{ keV/amu} : 15 \%$  or better. where  $n_*$  is the effective principal quantum number ( $n_*^{-2} = 2E_b$ ,  $E_b$  being the reduced energy in atomic units).
- <u>Comments</u>: (1) In the reduced energy region E  $n^2/q < 10$  keV/amu there exist experimental cross section data for electron capture from Li (2s) by He<sup>2+</sup> impact (Dijkamp et al [26], Varghese et al [16]) and by impact of q=4 and q=5 ions (Hoekstra et al [27]). Extensive AO-close coupling electron capture calculations in this reduced energy region are available for Li (2s) + Be<sup>4+</sup> ions by Fritsch and Lin [28] and Li (2s, 3s) + A<sup>(2-6)+</sup> ions [20], with A<sup>q+</sup> being a fully stripped ion. All these cross sections, when represented in a reduced form  $\sigma = \sigma/n^4$ , q, agree with each other to within 15%.
  - (2) In the reduced energy range  $E n_{*}^{2}/q > 30 \text{ keV/amu}$ , where electron removal is dominated by the ionization process, the cross section can be optained by scaling the proton-impact cross section according to :

$$\tilde{\sigma} = \sigma/n_{\star}^4 q$$
,  $\tilde{E} = E n_{\star}^2/q$ 

(3) The form of the analytic expression for  $\sigma_{loss}$  given follows the idea of Ref. [25]. Analytic expression

Reduced Cross section:

$$\widetilde{\sigma_{\text{loss}}} = 40^{-14} \text{ A}_1 \left[ 1 - \exp\left\{ -A_2 \ln\left(e + A_3 \widetilde{E}\right) / \widetilde{E} \right\} \right] \quad [\text{cm}^2]$$

#### Fitting coefficients

A1	A2	A <sub>3</sub>		
9.1752E-02	14.625	1.7989E-05		

The rms deviation of the above fit to the recommended cross section is 1.3% The maximum deviation is 4.1% at 42.1 keV/amu

ALADDIN evaluation function for cross section HLOSS2  
ALADDIN hierarchical labelling : ELREM A 
$$[+q>1]$$
 Li  $[+0]$  (ns) Li  $[+1]$ 





Energy x n <sup>2</sup> /q	Vel. x $n_*/\sqrt{q}$	Cross sections / $n_*^4 q$ (cm <sup>2</sup> )	
(eV/amu)	(cm/s)	2p	3p and 4p
1.00E+01	4.39E+06	6.39E-16	4.21E-16
2.00E+01	6.21E+06	6.39E-16	4.21E-16
5.00E+01	9.82E+06	6.39E-16	4.21E-16
1.00E+02	1.39E+07	6.39E-16	4.21E-16
2.00E+02	1.96E+07	6.39E-16	4.21E-16
5.00E+02	3.11E+07	6.39E-16	4.21E-16
1.00E+03	4.39E+07	6.39E-16	4.21E-16
2.00E+03	6.21E+07	6.39E-16	4.21E-16
5.00E+03	9.82E+07	6.30E-16	4.20E-16
1.00E+04	1.39E+08	5.66E-16	4.07E-16
2.00E+04	1.96E+08	4.23E-16	3.45E-16
5.00E+04	3.11E+08	2.26E-16	2.10E-16
1.00E+05	4.39E+08	1.26E-16	1.23E-16
2.00E+05	6.21E+08	6.74E-17	6.73E-17
5.00E+05	9.82E+08	2.89E-17	2.89E-17
1.00E+06	1.39E+09	1.55E-17	1.52E-17

 $\begin{array}{ll} \underline{\text{Accuracy:}} & \text{En}_*^2/q < 10 \text{ keV/amu: } 30\text{-}40 \ \%; & 10 \leq \text{En}_*^2/q \ (\text{keV/amu}) < 30: 20 - 30 \ \%; \\ & \text{En}_*^2/q \geq 30 \ \text{keV/amu: } 20 \ \% \ \text{or better}, \\ & \text{where } n_* \text{ is the effective principal quantum number } ( \ n_*^{-2} = 2E_b \ , E_b \ \text{being the reduced} \\ & \text{energy in atomic units}). \end{array}$ 

<u>Comments</u>: (1) In the reduced energy region below 10 keV/amu, there exist extensive atomic-orbital close-coupling electron capture cross section calculations [20] for the Li\* (2p) +  $A^{q+}$  (q=2, 4, 6) systems where  $A^{q+}$  is a fully stripped ion. In a reduced form  $\tilde{\sigma} = \sigma/n_*^4 q$ , these cross sections agree with each other to within 10% but are higher than the experimental data of Gieler et al [29] by 20 - 40%. For n  $\geq$  3 and q  $\geq$  2 there are neither experimental or theoretical data available for these reactions and the n<sup>4</sup>-scaling has to be used.

(2) In the reduced energy region above 30 keV/amu, the cross section for these reactions can be obtained by q-scaling the proton impact cross section for Li<sup>\*</sup> (np) according to :

$$\tilde{\sigma} = \sigma/n_*^4 q$$
,  $\tilde{E} = E n_*^2/q$ 

#### Analytic expression

**Reduced Cross section:** 

$$\widetilde{\sigma}_{\text{loss}} = 10^{-14} \text{ A}_1 \left[ 1 - \exp\left[ -A_2 \ln\left(e + A_3 \widetilde{E}\right) / \widetilde{E} \right] \right] \quad [\text{cm}^2]$$

#### where $A_1$ , $A_2$ , $A_3$ for 2p, 3p, and 4p are Fitting coefficients

	A1			A <sub>2</sub>			А	3	
2p	6.3853E-02			21.693			3.8821	E-0	4
3p and 4p	4.2051E-02			34.368			2.0483	E-0	14
ALADDIN evalu	ation function for	cross section	<u>n:</u>	HLOSS2					
ALADDIN hiera	rchical labelling.	ELREM	Α	[+q>1]	Li	[+0]	(np)	Lı	[+1]



- Recommended Cross Section

Energy x $n_*^2/q$	Vel. x $n_*/\sqrt{q}$	Cross section / n <sup>4</sup> q
(eV/amu)	(cm/s)	(cm <sup>2</sup> )
1.00E+01	4.39E+06	3.68E-16
2.00E+01	6.21E+06	3.68E-16
5.00E+01	9.82E+06	3.68E-16
1.00E+02	1.39E+07	3.68E16
2.00E+02	1.96E+07	3.68E-16
5.00E+02	3.11E+07	3.68E-16
1.00E+03	4.39E+07	3.68E-16
2.00E+03	6.21E+07	3.68E-16
5.00E+03	9.82E+07	3.68E-16
1.00E+04	1.39E+08	3.62E-16
2.00E+04	1.96E+08	3.22E-16
5.00E+04	3.11E+08	2.09E-16
1.00E+05	4.39E+08	1.26E-16
2.00E+05	6.21E+08	6.99E-17
5.00E+05	9.82E+08	3.02E-17
1.00E+06	1.39E+09	1.58E-17

 $\begin{array}{ll} \underline{\text{Accuracy:}} & En_{\star}^2/q < 10 \ \text{keV/amu: } 30\text{-}40 \ \%; & 10 \leq En_{\star}^2/q \ (\text{keV/amu}) < 30: 20 - 30 \ \%; \\ & En_{\star}^2/q \geq 30 \ \text{keV/amu: } 20 \ \% \ \text{or better }, \\ & \text{where } n_{\star} \ \text{is the effective principal quantum number } (n_{\star}^{-2} = 2E_b, E_b \ \text{being the reduced energy in atomic units}). \end{array}$ 

<u>Comments</u>: There are no experimental or theoretical data for these reactions. The electron removal cross section can be estimated (within the above specified accuracies) by using the q- and n-scaling of the corresponding proton-impact cross section for Li<sup>\*</sup>(3d), according to :

$$\widetilde{\sigma} = \sigma/n_*^4 q$$
,  $\widetilde{E} = E n_*^2/q$ 

Analytic expression

**Reduced** Cross section:

$$\widetilde{\sigma_{\text{loss}}} = 10^{-14} \text{ A}_1 \left[ 1 - \exp\left\{ -A_2 \ln\left(e + A_3 \widetilde{E}\right) / \widetilde{E} \right\} \right] \quad [\text{cm}^2]$$

Fitting coefficients

ALADDIN evaluation function for cross section: HLOSS2 ALADDIN hierarchical labelling: ELREM A [+q>1] Li [+0] (nd) Li [+1]

$$A^{q+} + Li^{*}(nd) \rightarrow Li^{+} + ...; n=3,4; q>1$$



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