Multichannel K-matrix method

$$|\gamma\,\mu\rangle = \begin{cases} |\gamma_0\,\mu\rangle & \text{(open channel)} \\ |\gamma_c\,\mu\rangle & \text{(closed channel)} \end{cases}$$

where γ: channel intex, μ: configuration series

$$\langle\gamma'\,\mu'\,|\,\gamma\,\mu\rangle = \delta_{\gamma'\gamma}\,\delta_{\mu'\mu} \quad \text{(orthogonality)}$$

$$\langle\gamma'_0\,\mu'\,|\,H\,|\,\gamma_0\,\mu\rangle = \delta_{\gamma'_0\gamma_0}\,\delta_{\mu'\mu}\,\varepsilon_{\gamma_0\mu} \quad \text{(Prediagonalization)}$$

Define

$$|\Phi_{\gamma_0 E}\rangle = |\gamma_0 E\rangle + \Sigma'_{\gamma}\, d\varepsilon\ \mathcal{P}\,|\gamma\varepsilon\rangle\ \frac{\langle\gamma\varepsilon|K(E)|\gamma_0 E\rangle}{E-\varepsilon}$$

where $\Sigma' = (\Sigma + \int)$, $\mathcal{P}$ denotes the principal integral

$\Longrightarrow$ $$\langle\gamma'\varepsilon|H-E|\Phi_{\gamma_0 E}\rangle = 0$$

$\Longrightarrow$ $$\langle\gamma'\varepsilon'|K(E)|\gamma_0 E\rangle = \langle\gamma'\varepsilon'|V(E)|\gamma_0 E\rangle + \Sigma'_{\gamma}\, d\varepsilon\ \mathcal{P}\,\langle\gamma'\varepsilon'|V(E)|\gamma\varepsilon\rangle \times \frac{\langle\gamma\varepsilon|K(E)|\gamma_0 E\rangle}{E-\varepsilon}$$

The energy-dependent ***V*** matrix is given by

$$\langle \gamma' \varepsilon' | V(E) | \gamma \varepsilon \rangle = \langle \gamma' \varepsilon' | H - E | \gamma \varepsilon \rangle - (\varepsilon - E)\, \delta_{\gamma' \gamma}\, \delta(\varepsilon - \varepsilon')$$

Orthogonality:

$$\langle \Phi_{\gamma_0' E'} | \Phi_{\gamma_0 E} \rangle = \delta(E' - E)$$
$$\times \left[\delta_{\gamma_0' \gamma_0} + \pi^2 \Sigma_{\gamma''_0} \langle \gamma_0'' E | K(E) | \gamma_0' E \rangle \right.$$
$$\left. \times \langle \gamma_0'' E | K(E) | \gamma_0 E \rangle \right]$$

Eigenchannels

$$|\Gamma E\rangle = \Sigma_{\gamma_0} |\Phi_{\gamma_0 E}\rangle U_{\gamma_0\Gamma}(E) \cos \eta_\Gamma(E)$$ (normalized)

where the transformation matrix $U_{\gamma_0\Gamma}(E)$ and the eigenphase shift η_Γ are obtained by diagonalizing the *on the energy shell* **K** *matrix, i.e.*

$$\Sigma_{\gamma_0'} \langle \gamma_0 E | K(E) | \gamma_0' E \rangle U_{\gamma_0'\Gamma}(E) = -\pi^{-1} \tan \eta_\Gamma U_{\gamma_0\Gamma}(E)$$

Total eigenphase shift:

$$\eta_{tot} = \Sigma_\Gamma \eta_\Gamma$$

$$= \eta_0 + \tan^{-1}[(\Gamma_w / 2) / (E_{res} - E)],$$ η_0: background

Channel wave function

$$|\gamma_0 E^-\rangle = \Sigma_\Gamma \, |\Gamma E\rangle \, C_{\Gamma\gamma_0}, \quad \text{(normalized)}$$

where $C_{\Gamma\gamma} = e^{-i\,\eta_\Gamma} \tilde{U}_{\Gamma\gamma} \, e^{-i\,\delta_\gamma}$, and δ_γ is the scattering phase shift of the outgoing electron in the open channel γ, i.e.,

$$\xi_{\varepsilon l}(r) \xrightarrow[\text{at large } r]{} [2/(\pi k)]^{1/2} \sin[k - (\pi l/2) + (q/k)\ln(2kr) + \sigma_l^C + \delta_\gamma],$$

where q is the effective nuclear charge, $k = \varepsilon^{1/2}$ is the momentum, and σ_l^C is the Coulomb phase shift.

Photoionization cross sections

Total and partial cross sections:

$$\sigma_{tot} = \sum_{\gamma_0} \sigma_{\gamma_0}, \qquad \sigma_{\gamma_0} = 4\pi^2 \alpha f_{\gamma_0 I} \quad (\text{in unit of } a_0^2)$$

Where

$$f^{(L)}_{\gamma_0 I}(E) = \frac{\Delta E}{3 g_I} \sum_{\text{all M's}} \left| \langle \Psi_I | \Sigma \vec{\mathbf{r}}_i | \gamma_0 E^- \rangle \right|^2$$

$$f^{(V)}_{\gamma_0 I}(E) = \frac{4}{3 g_I (\Delta E)} \sum_{\text{all M's}} \left| \langle \Psi_I | \Sigma \vec{\nabla}_i | \gamma_0 E^- \rangle \right|^2$$

$\Delta E = E - E_I$ is the excitation energy in Ry,

$g_I = (2S_I+1)(2L_I+1)$, and Ψ_I is the initial state.

Discretized K matrix

If γ represents a closed channel,

$$K^{(1)} \equiv \sum_{\gamma} \sum_{\nu_\gamma} \langle \gamma' \varepsilon' | V(E) | \gamma \varepsilon_{\nu_\gamma} \rangle \frac{\langle \gamma \varepsilon_{\nu_\gamma} | K(E) | \gamma_0 E \rangle}{E - \varepsilon_{\nu_\gamma}}$$

$$= \langle \gamma' \varepsilon' | V(E) \, X(E) \, | K(E) | \gamma_0 E \rangle$$

where

$$\langle \gamma' \varepsilon_{\nu'} | X(E) | \gamma \varepsilon_{\nu} \rangle = \delta_{\gamma' \gamma} \, \delta_{\nu' \nu} \frac{1}{E - \varepsilon_{\nu}}$$

Discretized K matrix (Conti.)

If γ represents an open channel,

$$K^{(2)} \equiv \sum_{\gamma} \sum_{i} \mathcal{P} \int_{\varepsilon_i}^{\varepsilon_{i+1}} \mathrm{d}\varepsilon \, \langle \gamma' \varepsilon' | V(E) | \gamma \varepsilon \rangle \, \frac{\langle \gamma \varepsilon | K(E) | \gamma_0 E \rangle}{E - \varepsilon}$$

Use *N*-point Lagrange interpolation:

$$f(x) = \sum_{m'} \sum_{m} \alpha_{mm'} f(x_m) \, x^{m'-1}, \quad m, m' = 1,\ldots, N$$

$$\langle \gamma' \varepsilon' | V(E) | \gamma \varepsilon \rangle \sim \sum_{m'} \sum_{m} \alpha_{mm'} \langle \gamma' \varepsilon' | V(E) | \gamma \varepsilon_m \rangle \, \varepsilon^{m'-1}$$

$$\langle \gamma \varepsilon | K(E) | \gamma_0 E \rangle \sim \sum_{n'} \sum_{n} \alpha_{nn'} \langle \gamma \varepsilon_n | K(E) | \gamma_0 E \rangle \, \varepsilon^{n'-1}$$

Discretized K matrix (Conti.)

$$K^{(2)} = \langle \gamma' \varepsilon' | V(E) Y(E) K(E) | \gamma_0 E \rangle$$

where

$$\langle \gamma' \varepsilon_m | Y(E) | \gamma \varepsilon_n \rangle = \delta_{\gamma' \gamma} \sum_i Y_{mn}^{(i)}$$

and

$$Y_{mn}^{(i)} = \sum_{m'} \sum_{n'} \alpha_{mm'} \alpha_{nn'} \int_{\varepsilon_i}^{\varepsilon_{i+1}} d\varepsilon \, \mathcal{P} \, \frac{\varepsilon^{m'+n'-2}}{E - \varepsilon}$$

Discretized K matrix (Conti.)

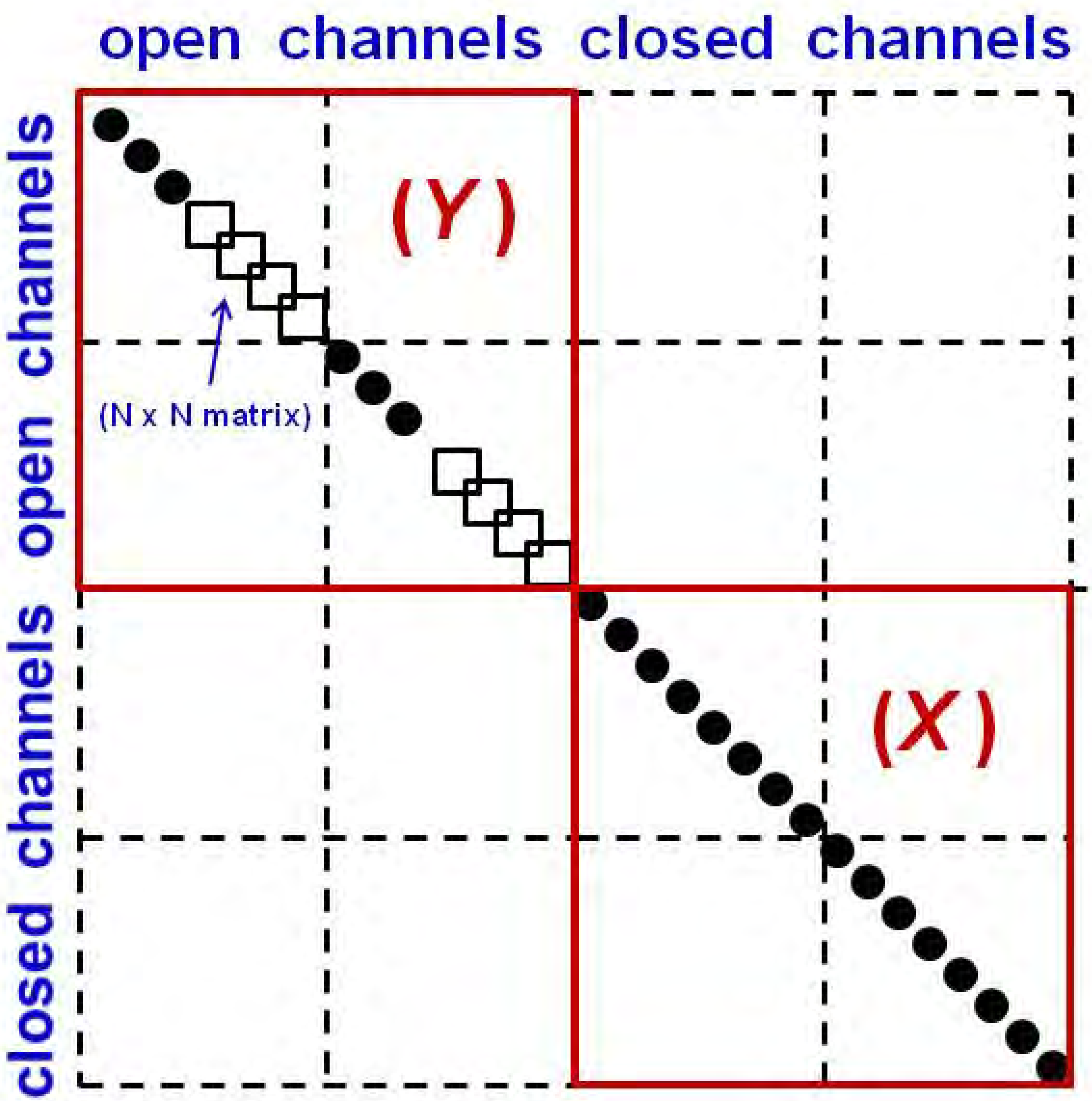
$$\langle \gamma' \varepsilon' | [1 - \boldsymbol{V}(E)\boldsymbol{P}(E)] K^{\mathbf{d}}(E) | \gamma_0 E \rangle = \langle \gamma' \varepsilon' | \boldsymbol{V}(E) | \gamma_0 E \rangle$$

where

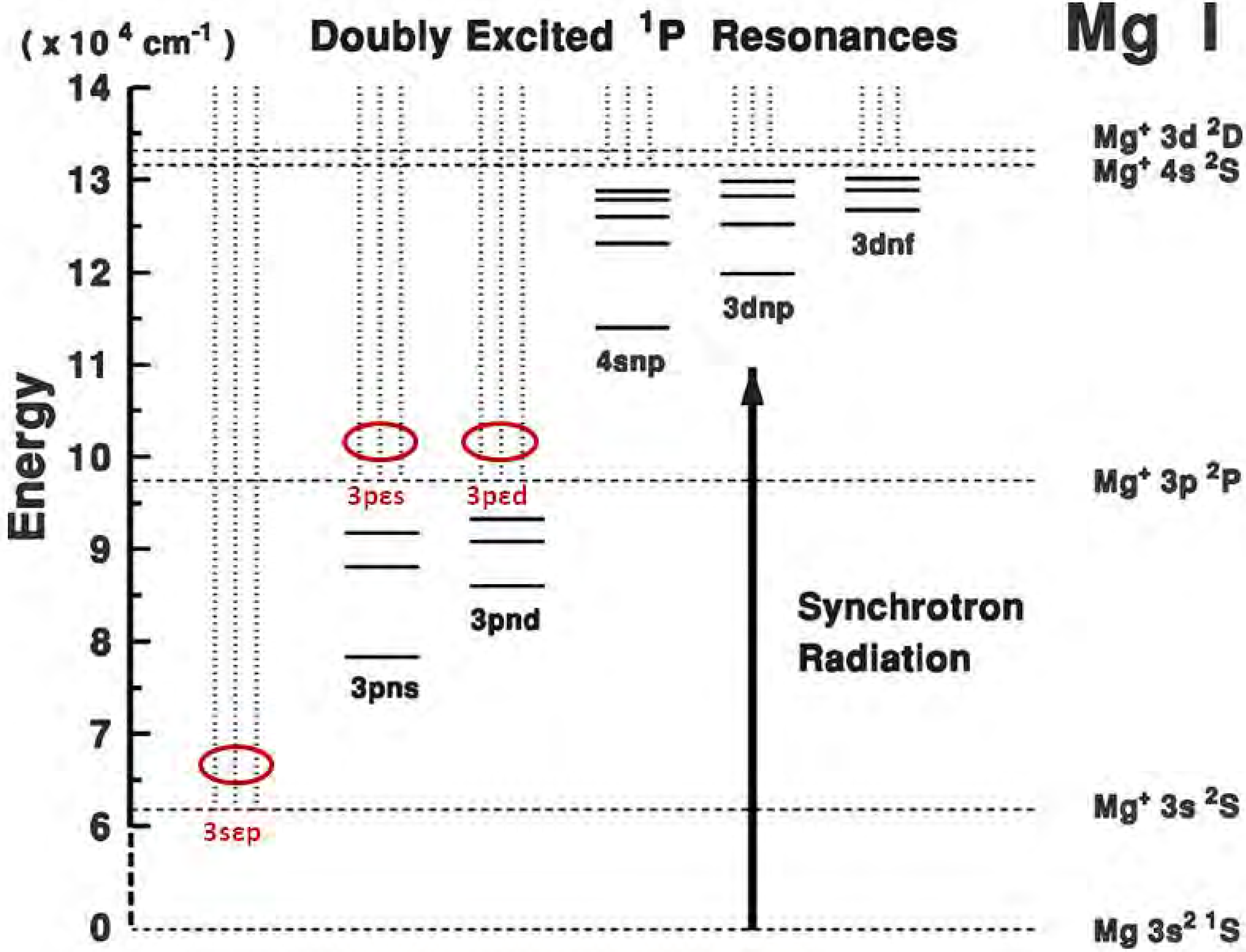
$$\boldsymbol{P}(E) = \boldsymbol{X}(E) + \boldsymbol{Y}(E)$$

$$\Longrightarrow \quad K^{\mathbf{d}}(E) = \frac{1}{[1 - \boldsymbol{V}(E)\boldsymbol{P}(E)]} \boldsymbol{V}(E)$$

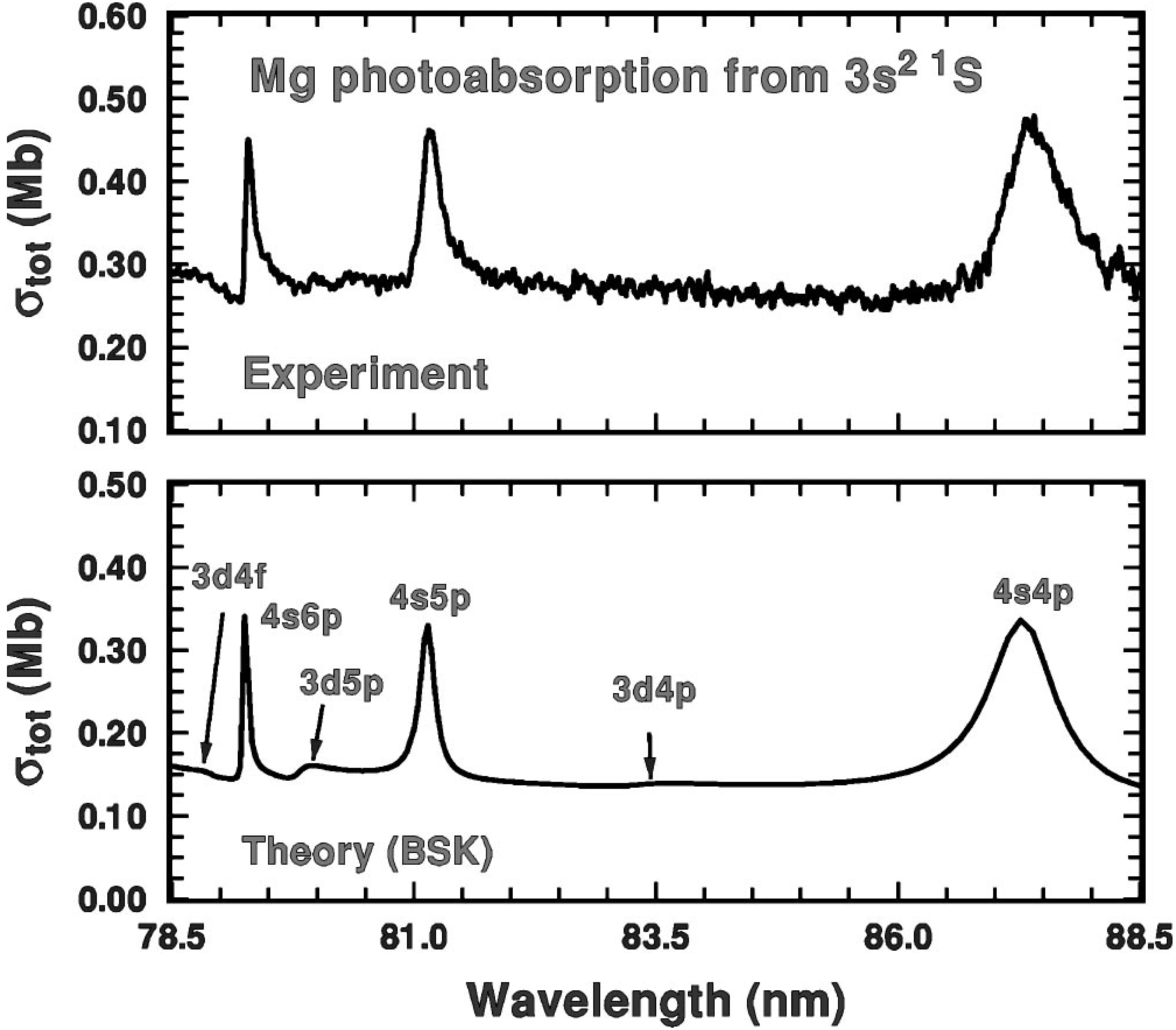
P matrix (= X + Y)



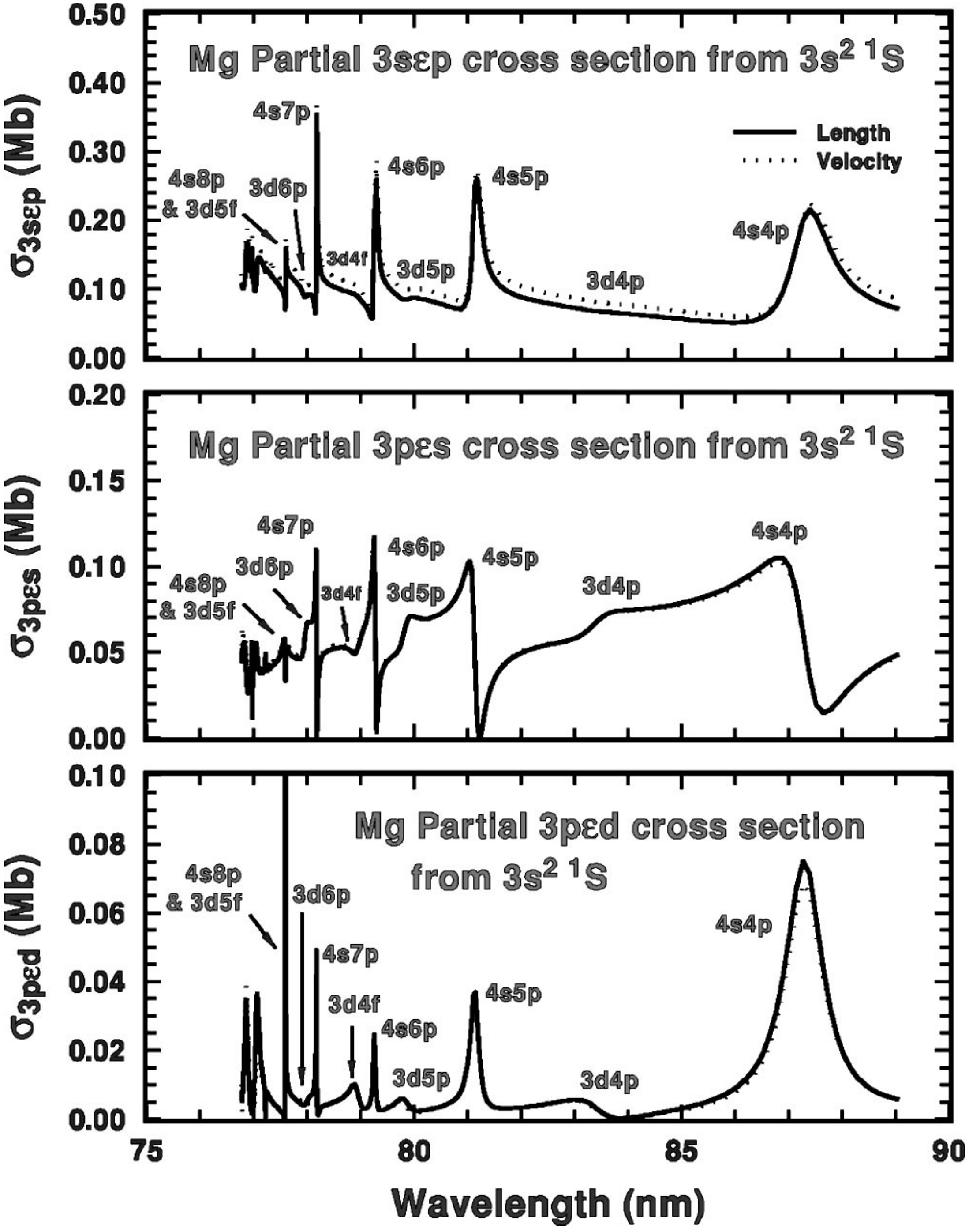
open channels closed channels
open channels
closed channels
(Y)
(X)
(N x N matrix)



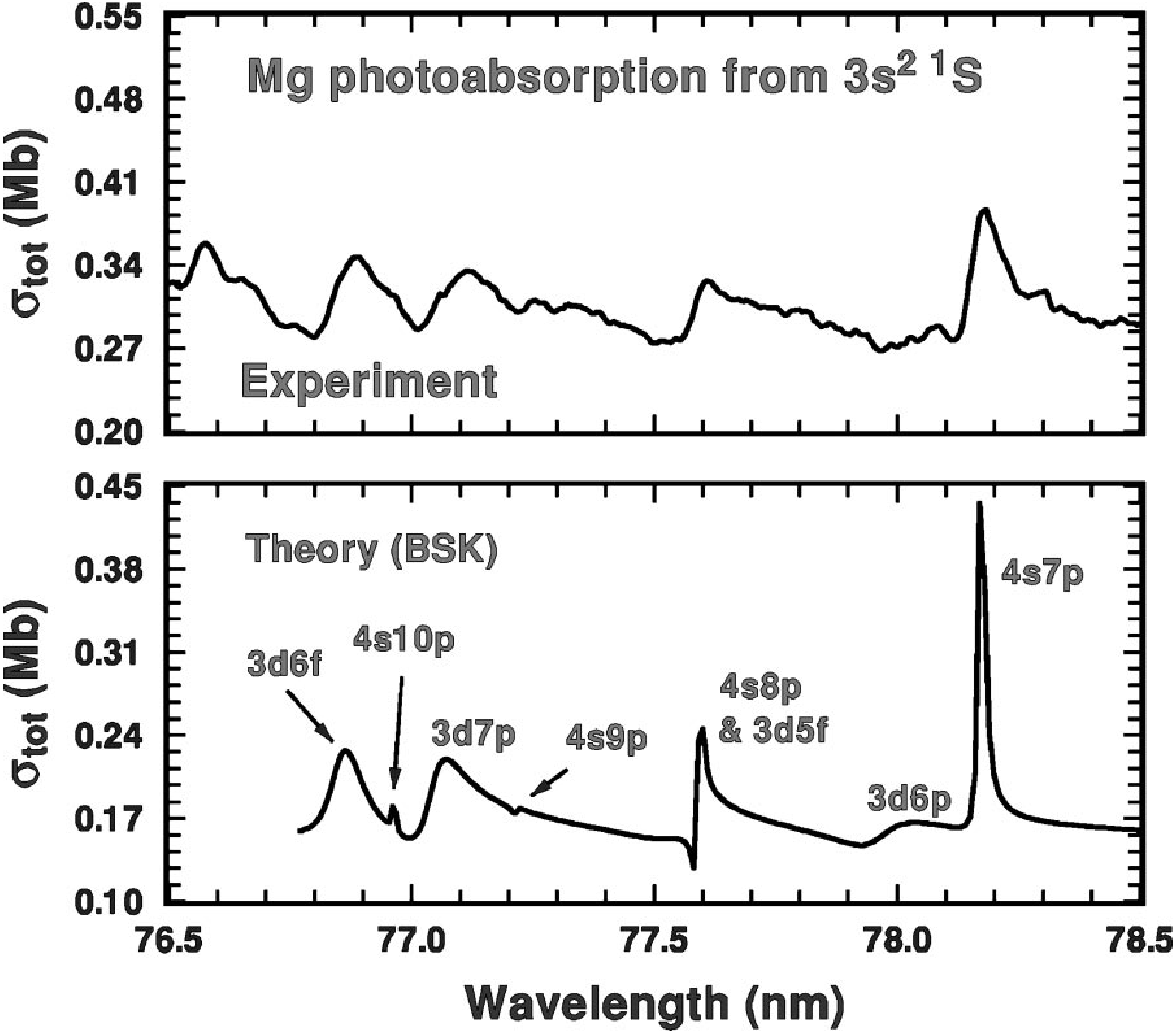
Phys. Rev. A 64, 052716 (2001).

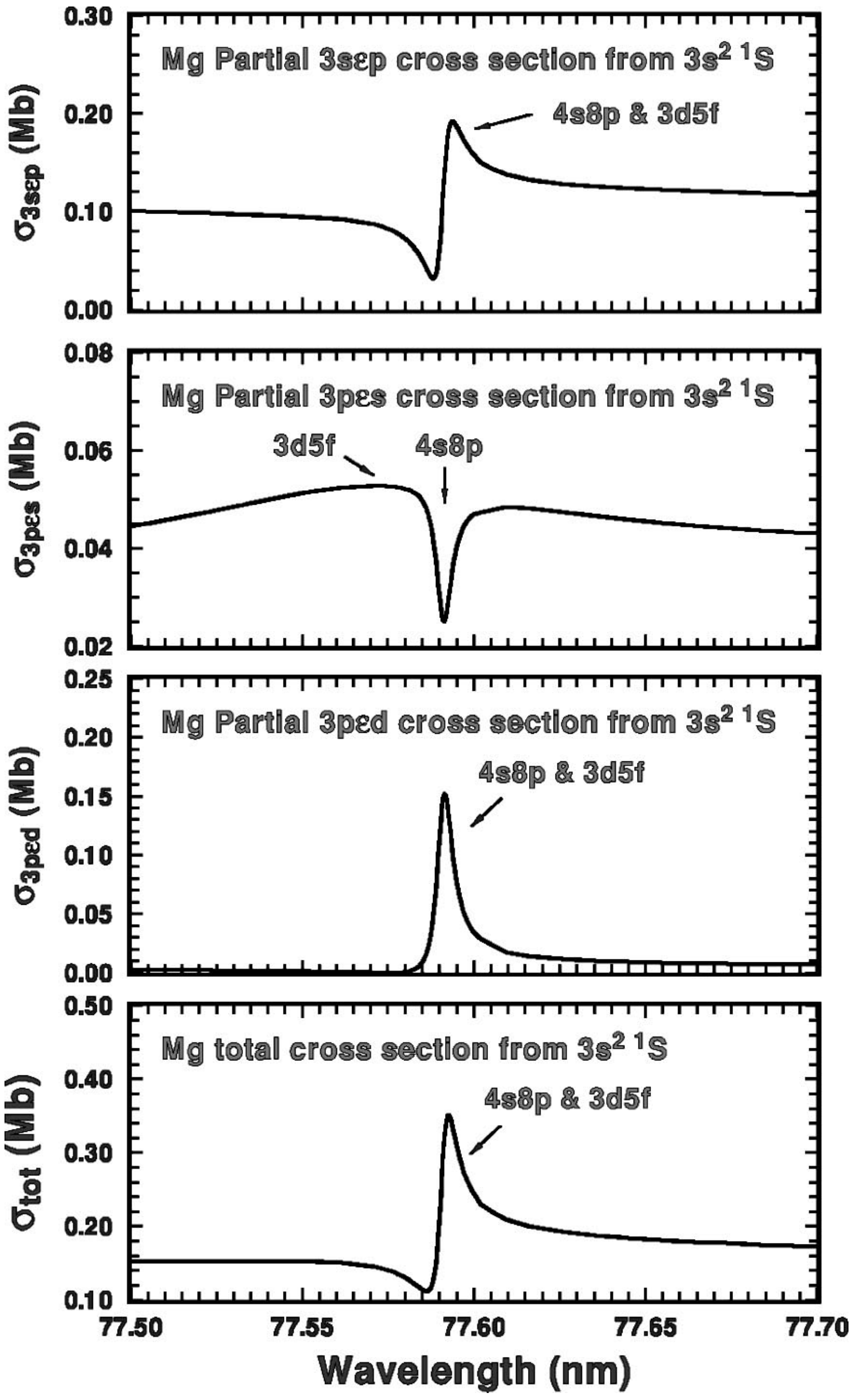


Mg photoabsorption from 3s^2 ^{1}S
Experiment
Theory (BSK)
σ_{tot} (Mb)
0.60
0.50
0.40
0.30
0.20
0.10
0.00
3d4f
4s6p
3d5p
4s5p
3d4p
4s4p
78.5
81.0
83.5
86.0
88.5
Wavelength (nm)

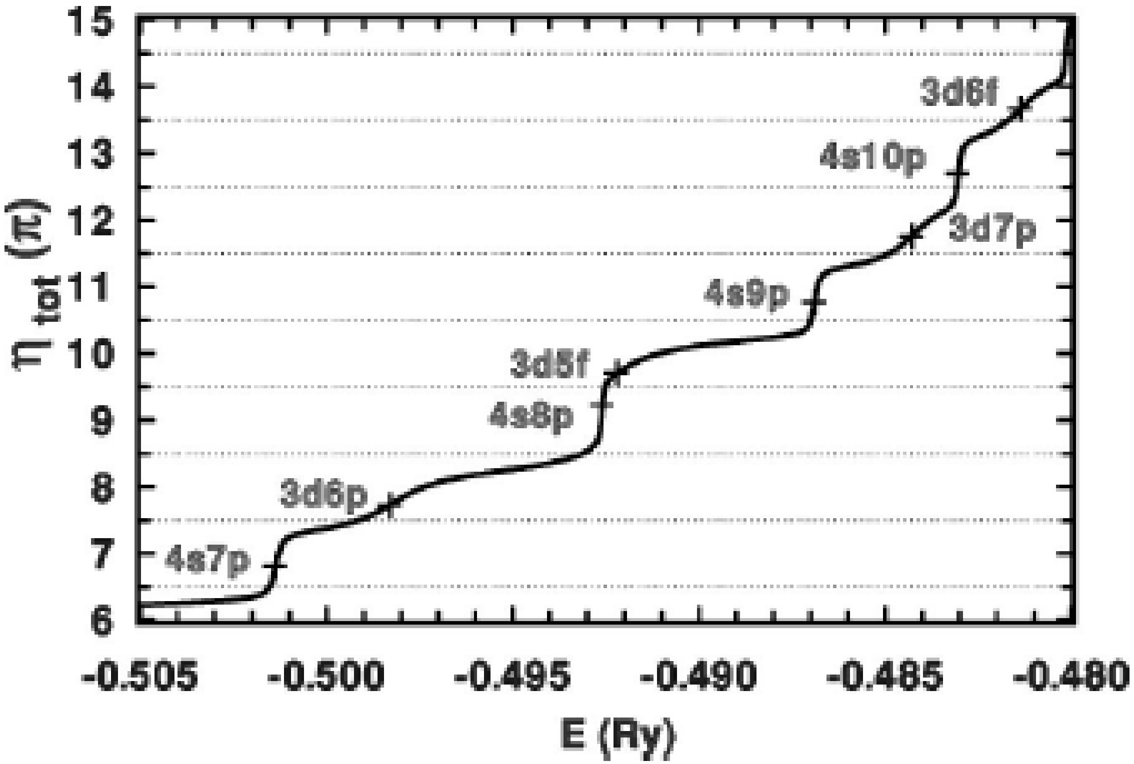


Mg Partial 3sεp cross section from 3s² ¹S
Length
Velocity
4s7p
4s6p
4s5p
4s8p
& 3d5f
3d6p
3d4f
3d5p
3d4p
4s4p
σ3sεp (Mb)
0.50
0.40
0.30
0.20
0.10
0.00
Mg Partial 3pεs cross section from 3s² ¹S
σ3pεs (Mb)
0.20
0.15
0.10
0.05
0.00
Mg Partial 3pεd cross section
from 3s² ¹S
σ3pεd (Mb)
0.10
0.08
0.06
0.04
0.02
0.00
75
80
85
90
Wavelength (nm)


Mg photoabsorption from 3s² ¹S
Experiment
Theory (BSK)
3d6f
4s10p
3d7p
4s9p
4s8p
& 3d5f
3d6p
4s7p
σtot (Mb)
0.55
0.48
0.41
0.34
0.27
0.20
0.45
0.38
0.31
0.24
0.17
0.10
76.5
77.0
77.5
78.0
78.5
Wavelength (nm)

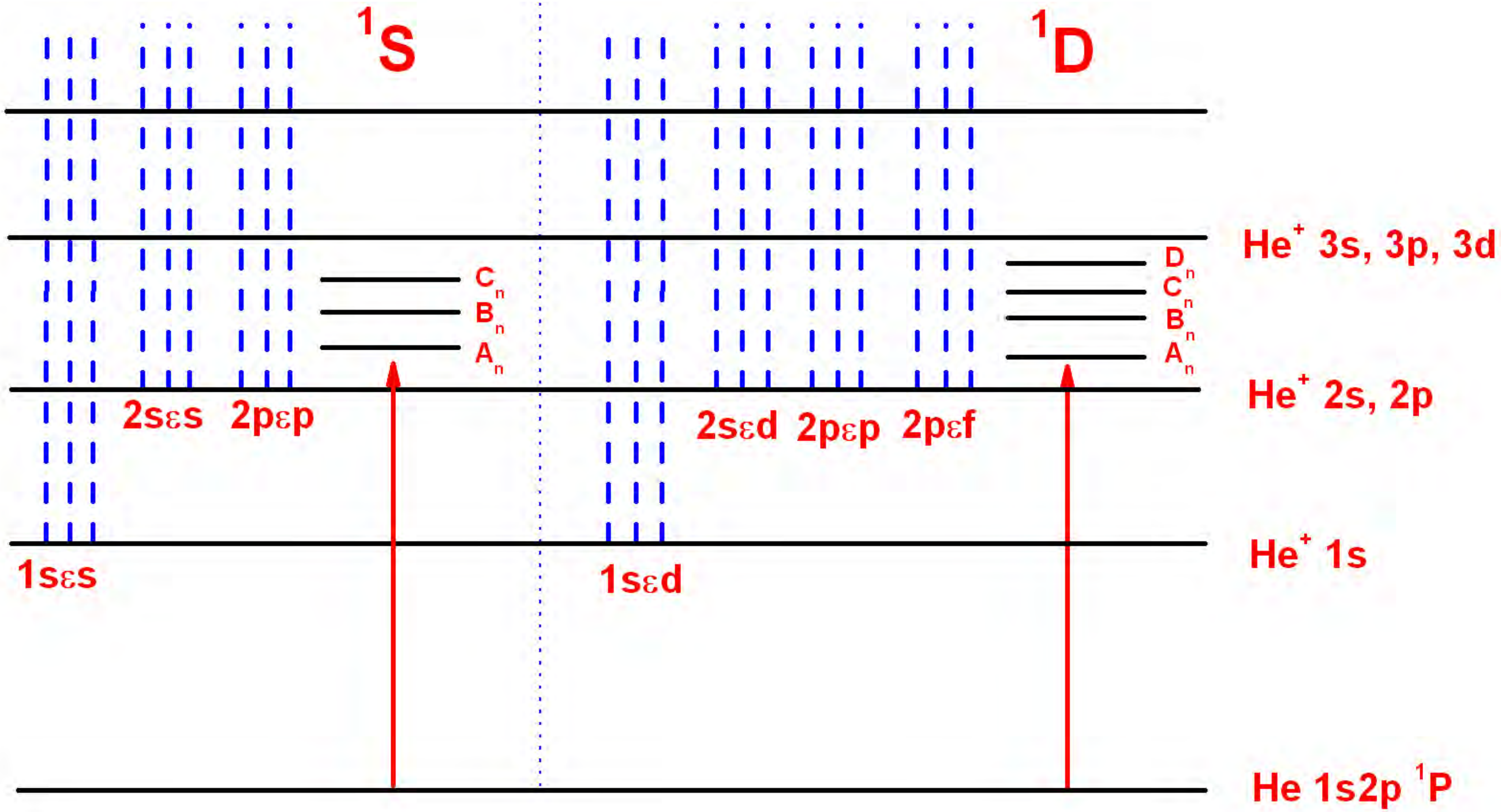


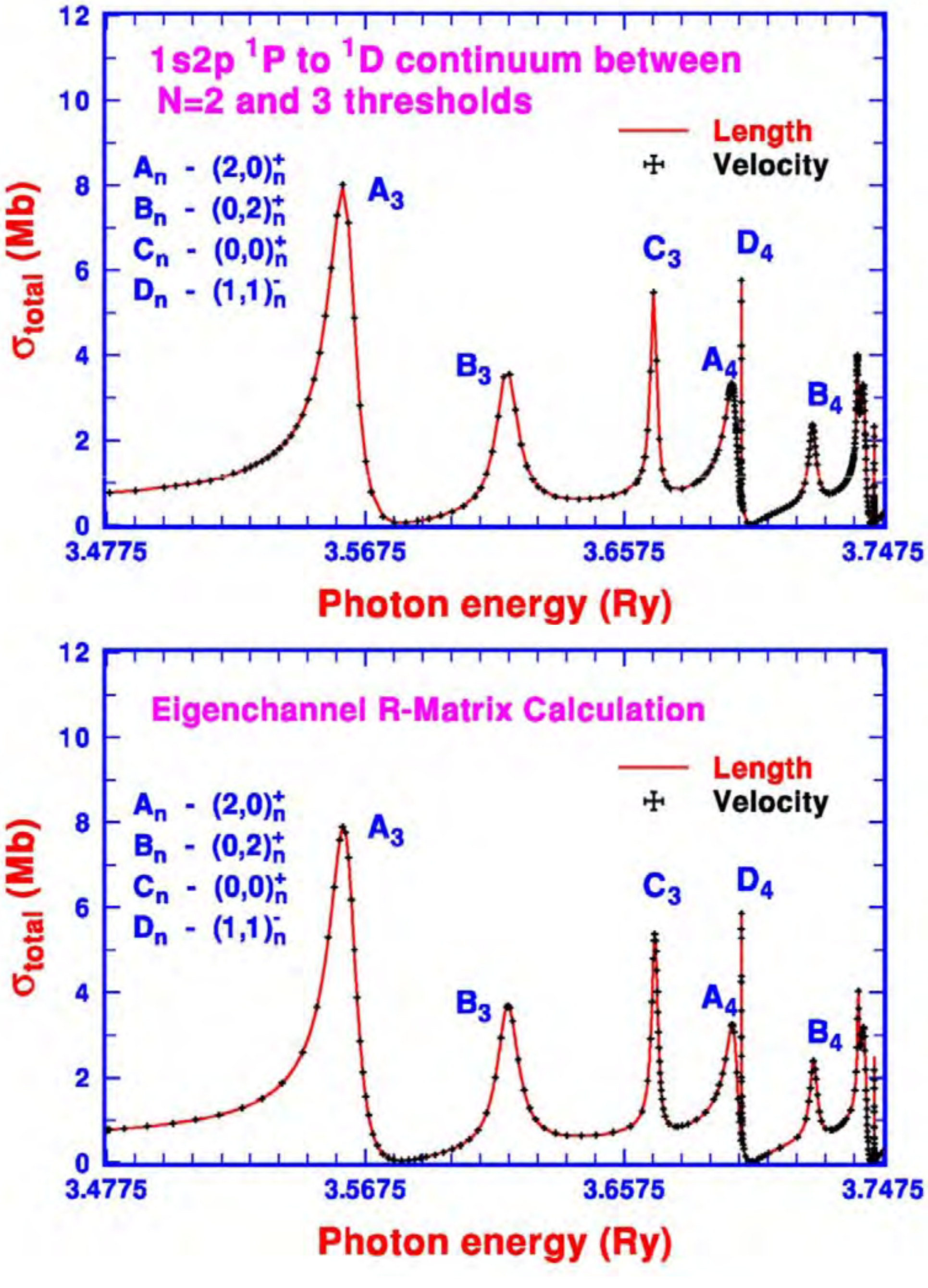
Mg Partial 3sεp cross section from 3s2 1S
4s8p & 3d5f
σ3sεp (Mb)
0.30
0.20
0.10
0.00
Mg Partial 3pεs cross section from 3s2 1S
3d5f
4s8p
σ3pεs (Mb)
0.08
0.06
0.04
0.02
Mg Partial 3pεd cross section from 3s2 1S
4s8p & 3d5f
σ3pεd (Mb)
0.25
0.20
0.15
0.10
0.05
0.00
Mg total cross section from 3s2 1S
4s8p & 3d5f
σtot (Mb)
0.50
0.40
0.30
0.20
0.10
77.50
77.55
77.60
77.65
77.70
Wavelength (nm)



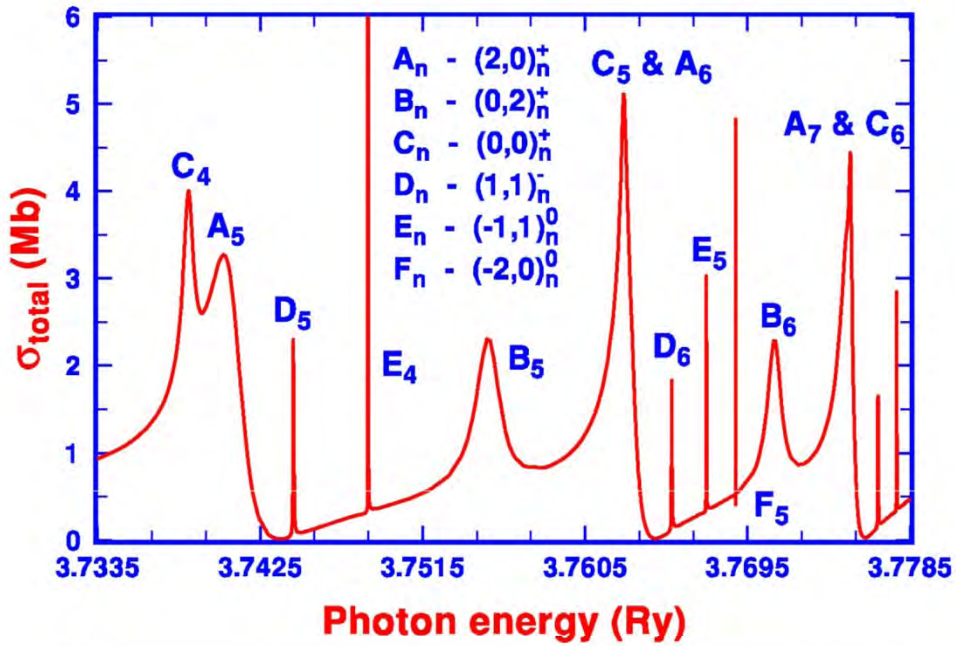
15
14
13
12
11
10
9
8
7
6
η tot (π)
3d6f
4s10p
3d7p
4s9p
3d5f
4s8p
3d6p
4s7p
-0.505
-0.500
-0.495
-0.490
-0.485
-0.480
E (Ry)

Overlapping doubly excited resonances

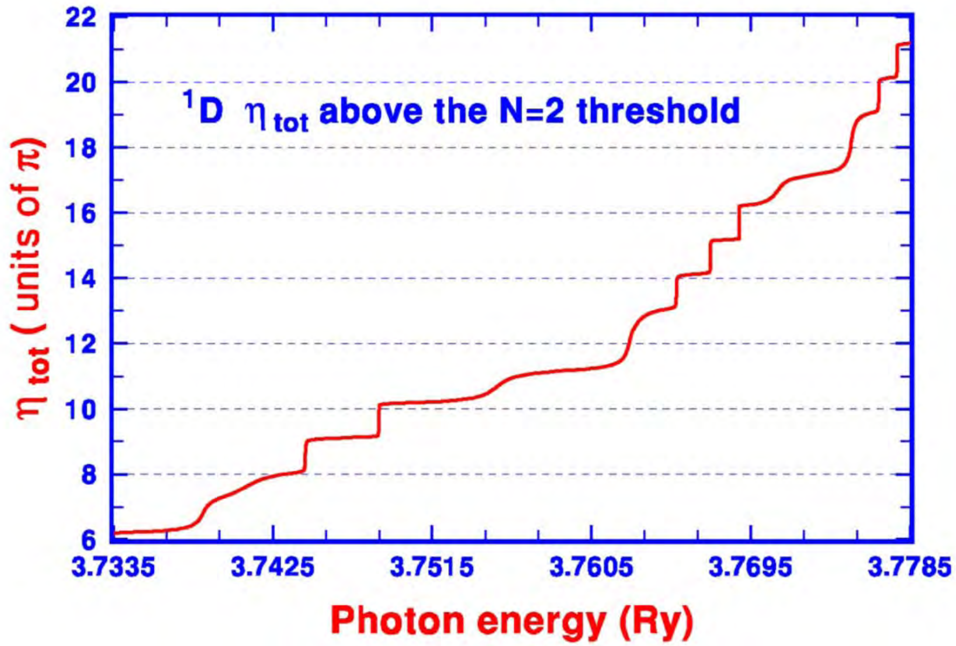




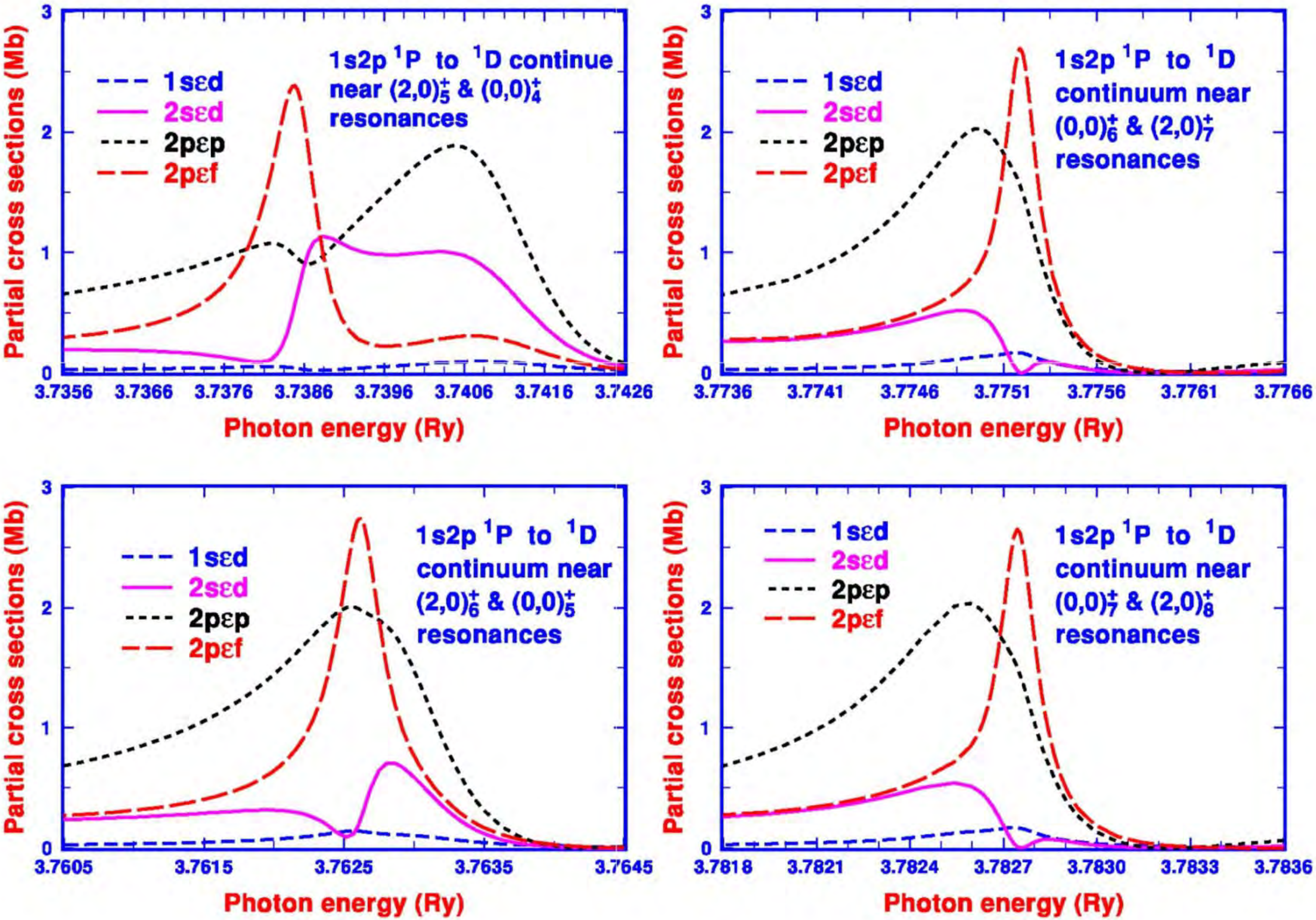
1s2p ^{1}P to ^{1}D continuum between
N=2 and 3 thresholds
Length
Velocity
A_n - $(2,0)_n^+$
B_n - $(0,2)_n^+$
C_n - $(0,0)_n^+$
D_n - $(1,1)_n^-$
A_3
B_3
C_3
D_4
A_4
B_4
σ_{total} (Mb)
0
2
4
6
8
10
12
3.4775
3.5675
3.6575
3.7475
Photon energy (Ry)
Eigenchannel R-Matrix Calculation
Length
Velocity
A_n - $(2,0)_n^+$
B_n - $(0,2)_n^+$
C_n - $(0,0)_n^+$
D_n - $(1,1)_n^-$
A_3
B_3
C_3
D_4
A_4
B_4
σ_{total} (Mb)
0
2
4
6
8
10
12
3.4775
3.5675
3.6575
3.7475
Photon energy (Ry)



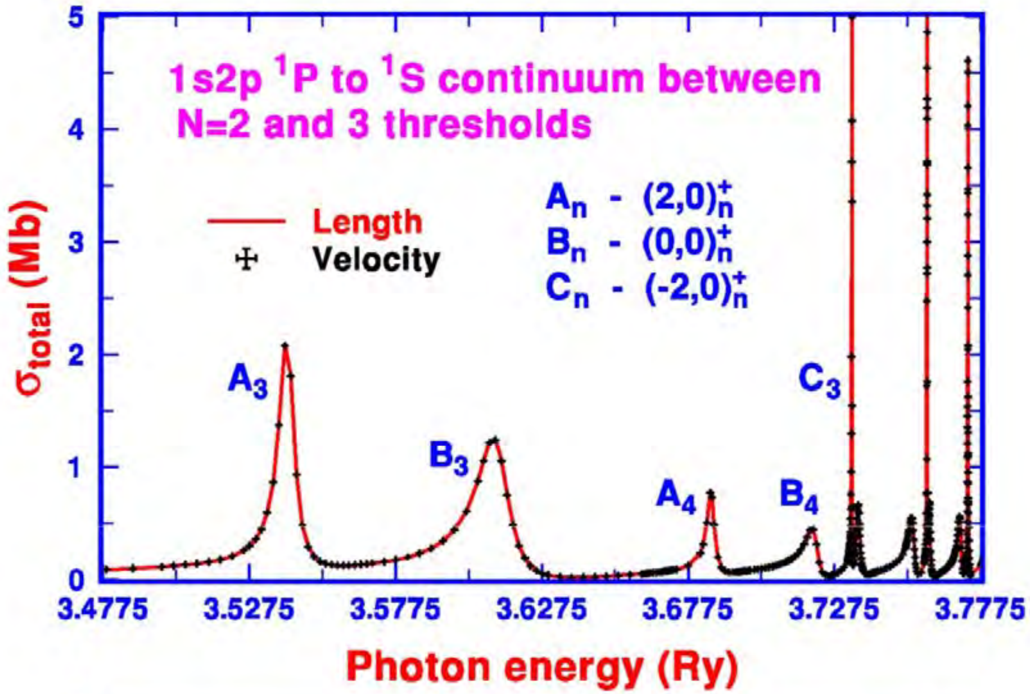
A_n - (2,0)^+_n
B_n - (0,2)^+_n
C_n - (0,0)^+_n
D_n - (1,1)^-_n
E_n - (-1,1)^0_n
F_n - (-2,0)^0_n
C4
A5
D5
E4
B5
C5 & A6
D6
E5
F5
B6
A7 & C6
σ_total (Mb)
0
1
2
3
4
5
6
3.7335
3.7425
3.7515
3.7605
3.7695
3.7785
Photon energy (Ry)



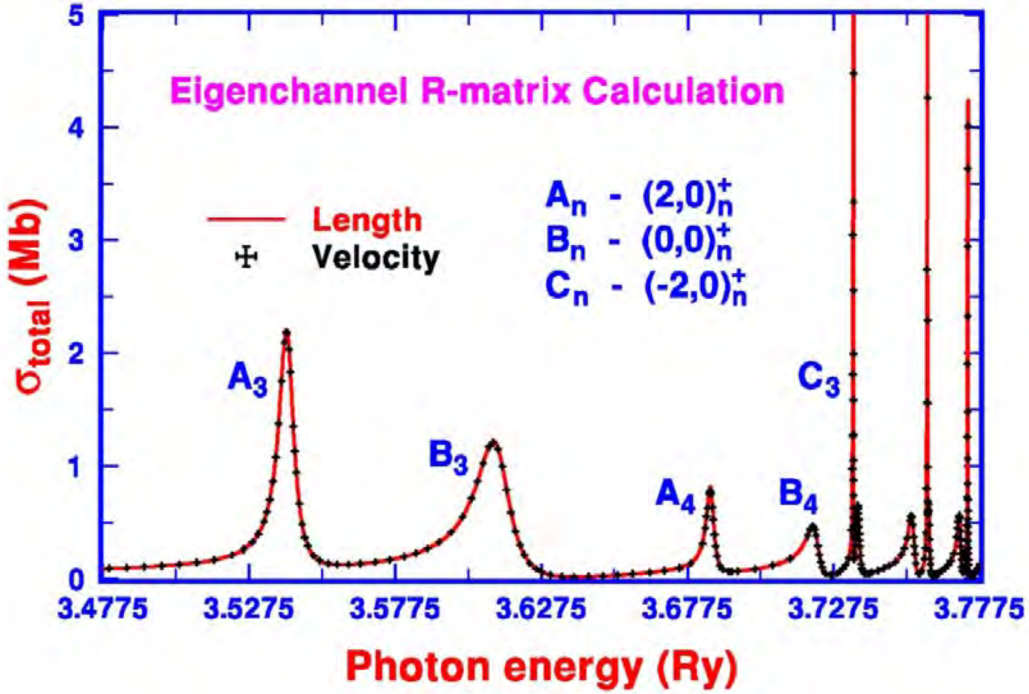
1D η_tot above the N=2 threshold
η_tot (units of π)
6
8
10
12
14
16
18
20
22
3.7335
3.7425
3.7515
3.7605
3.7695
3.7785
Photon energy (Ry)



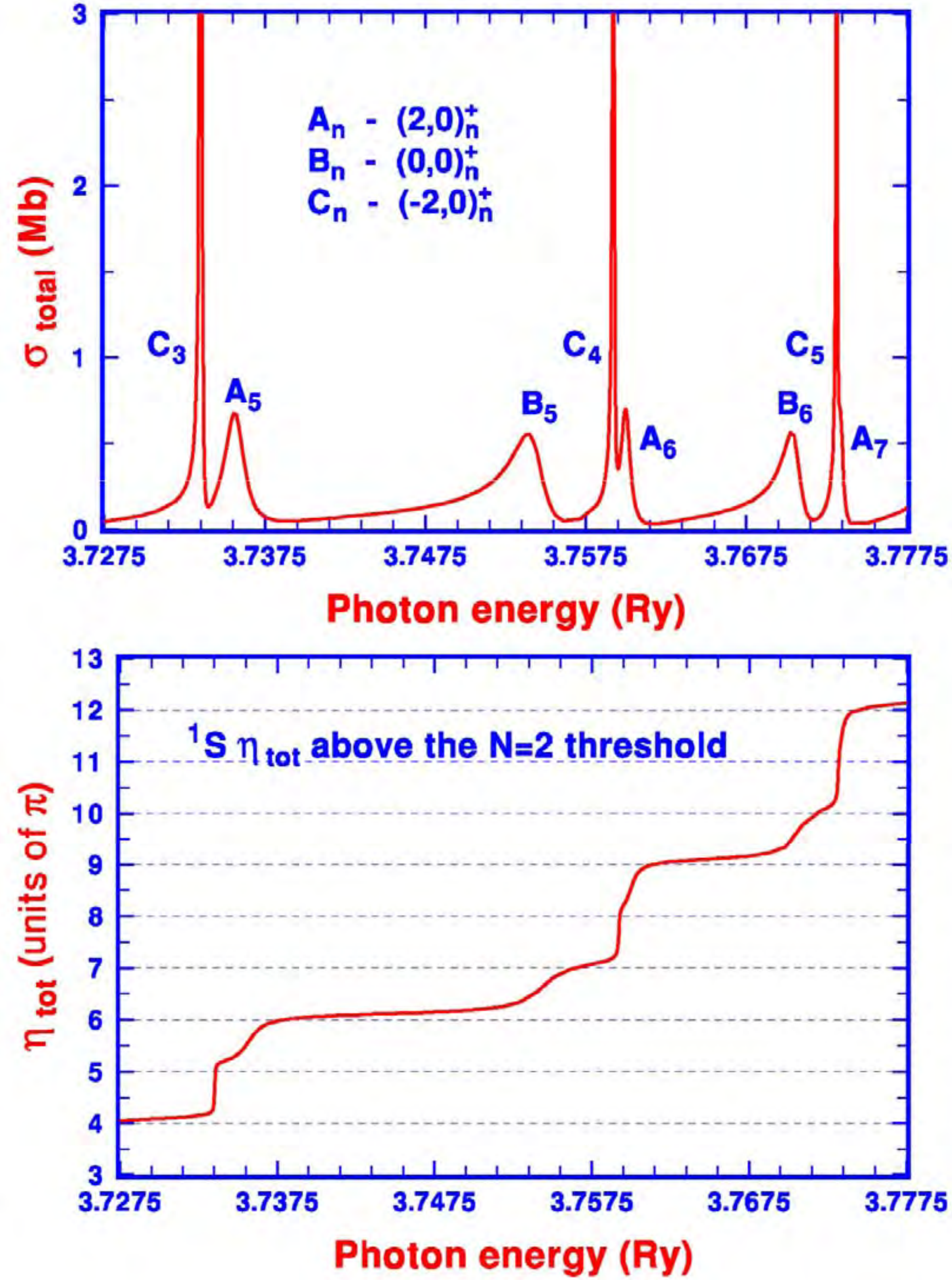
Partial cross sections (Mb)
1sεd
2sεd
2pεp
2pεf
1s2p ¹P to ¹D continue near (2,0)₅⁺ & (0,0)₄⁺ resonances
3.7356 3.7366 3.7376 3.7386 3.7396 3.7406 3.7416 3.7426
Photon energy (Ry)
1s2p ¹P to ¹D continuum near (0,0)₆⁺ & (2,0)₇⁺ resonances
3.7736 3.7741 3.7746 3.7751 3.7756 3.7761 3.7766
Photon energy (Ry)
1s2p ¹P to ¹D continuum near (2,0)₆⁺ & (0,0)₅⁺ resonances
3.7605 3.7615 3.7625 3.7635 3.7645
Photon energy (Ry)
1s2p ¹P to ¹D continuum near (0,0)₇⁺ & (2,0)₈⁺ resonances
3.7818 3.7821 3.7824 3.7827 3.7830 3.7833 3.7836
Photon energy (Ry)



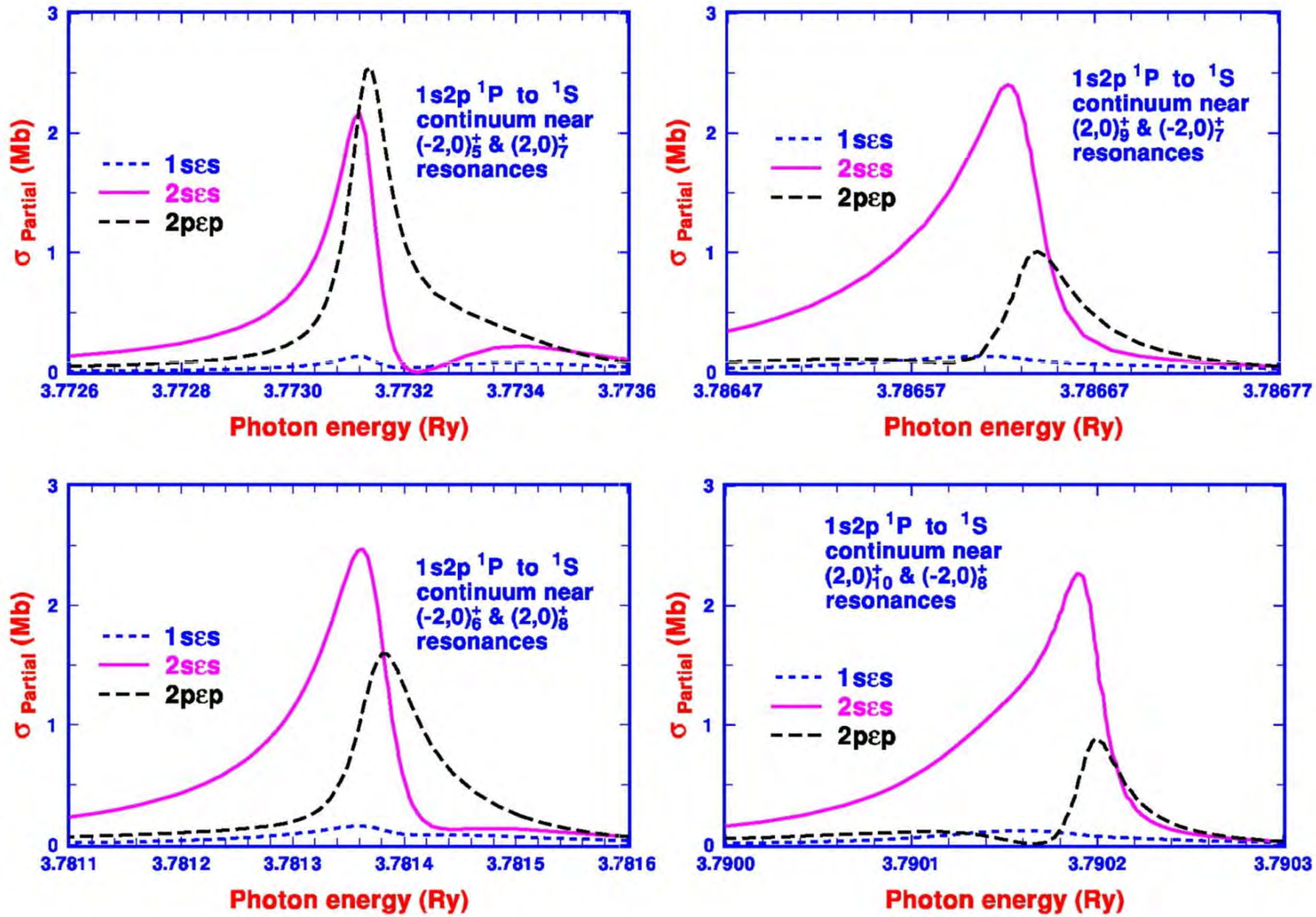
1s2p ^{1}P to ^{1}S continuum between
N=2 and 3 thresholds
Length
Velocity
A_n - $(2,0)^+_n$
B_n - $(0,0)^+_n$
C_n - $(-2,0)^+_n$
A_3
B_3
A_4
B_4
C_3
σ_{total} (Mb)
Photon energy (Ry)
0
1
2
3
4
5
3.4775
3.5275
3.5775
3.6275
3.6775
3.7275
3.7775



Eigenchannel R-matrix Calculation
Length
Velocity
A_n - $(2,0)^+_n$
B_n - $(0,0)^+_n$
C_n - $(-2,0)^+_n$
A_3
B_3
A_4
B_4
C_3
σ_{total} (Mb)
Photon energy (Ry)
0
1
2
3
4
5
3.4775
3.5275
3.5775
3.6275
3.6775
3.7275
3.7775



A_n - (2,0)+_n
B_n - (0,0)+_n
C_n - (-2,0)+_n
C3
A5
B5
C4
A6
C5
B6
A7
σ total (Mb)
Photon energy (Ry)
1S η tot above the N=2 threshold
η tot (units of π)
Photon energy (Ry)



σ Partial (Mb)
Photon energy (Ry)
1sεs
2sεs
2pεp
1s2p ^{1}P to ^{1}S
continuum near
$(-2,0)_5^+$ & $(2,0)_7^+$
resonances
3.7726
3.7728
3.7730
3.7732
3.7734
3.7736
1s2p ^{1}P to ^{1}S
continuum near
$(2,0)_9^+$ & $(-2,0)_7^+$
resonances
3.78647
3.78657
3.78667
3.78677
1s2p ^{1}P to ^{1}S
continuum near
$(-2,0)_6^+$ & $(2,0)_8^+$
resonances
3.7811
3.7812
3.7813
3.7814
3.7815
3.7816
1s2p ^{1}P to ^{1}S
continuum near
$(2,0)_{10}^+$ & $(-2,0)_8^+$
resonances
3.7900
3.7901
3.7902
3.7903
0
1
2
3

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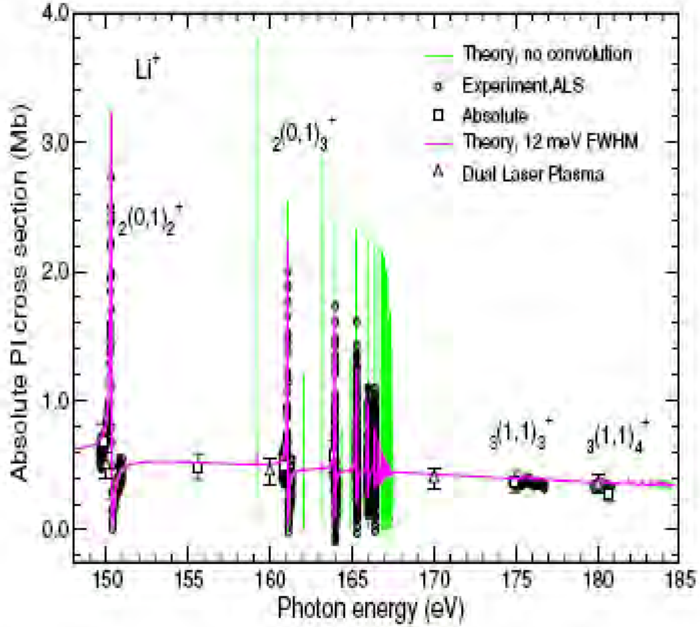
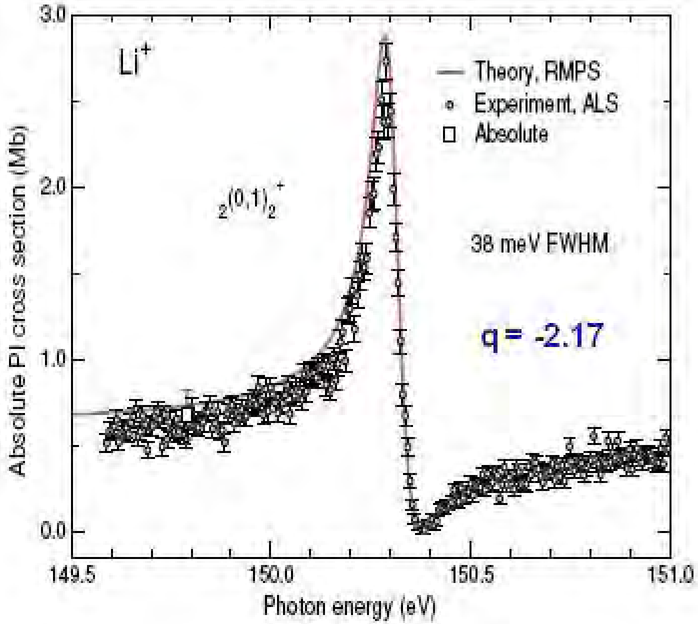
J. Phys. B: At. Mol. Opt. Phys. 39 (2006) 3957–3968 doi:10.1088/0953-4075/39/18/024

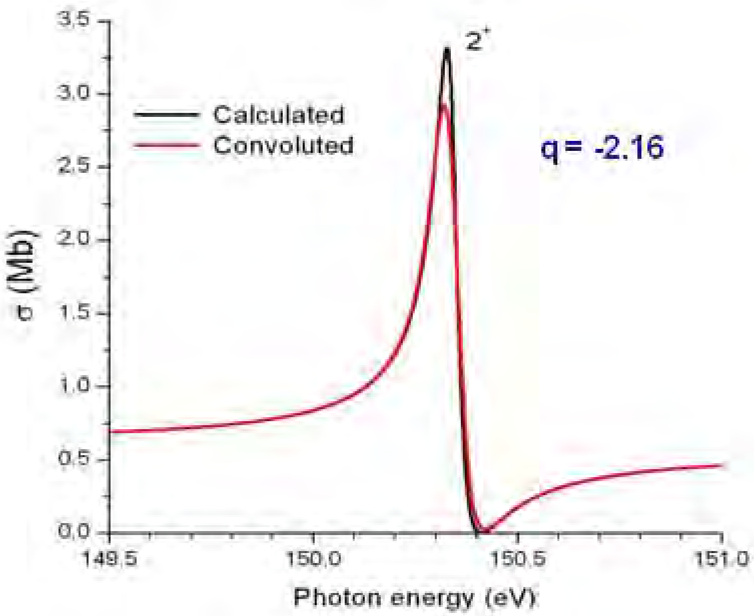
Doubly excited resonances in the photoionization spectrum of Li^+: experiment and theory

S W J Scully[1,9], I Álvarez[2], C Cisneros[2], E D Emmons[1], M F Gharaibeh[1], D Leitner[3], M S Lubell[4], A Müller[5], R A Phaneuf[1], R Püttner[6], A S Schlachter[3], S Schippers[5], W Shi[5,10], C P Ballance[7] and B M McLaughlin[8,9]

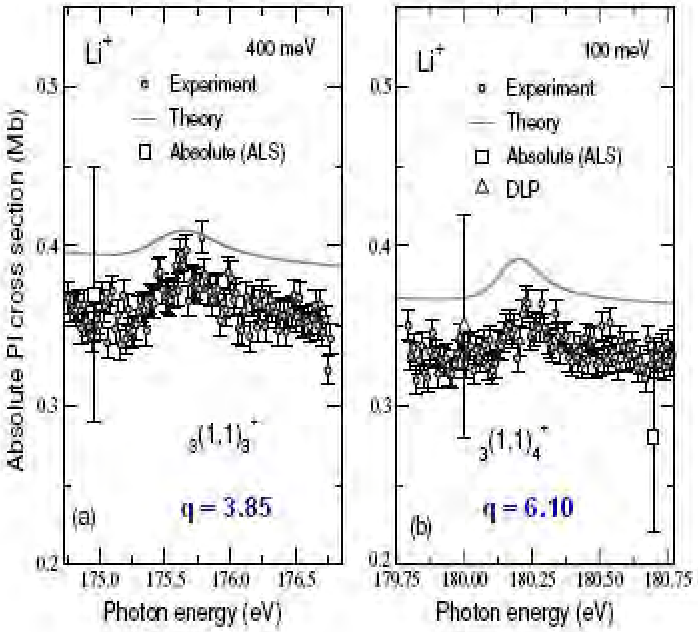


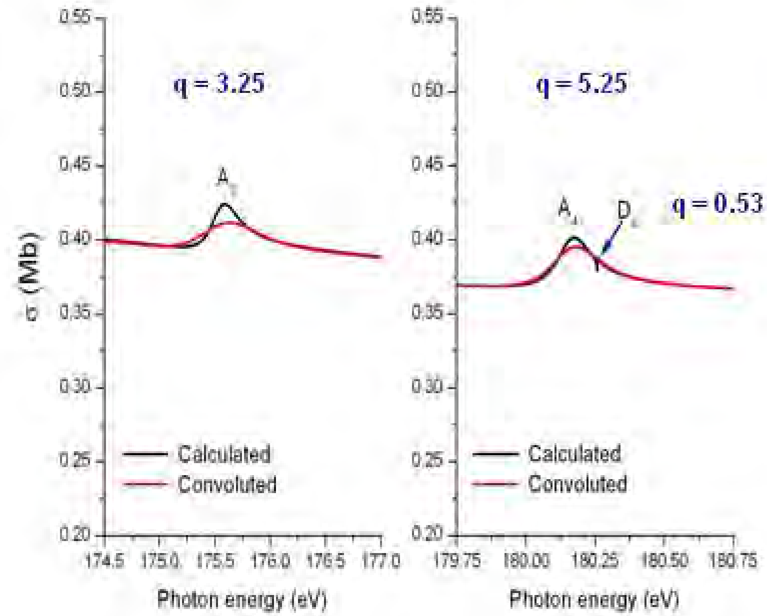


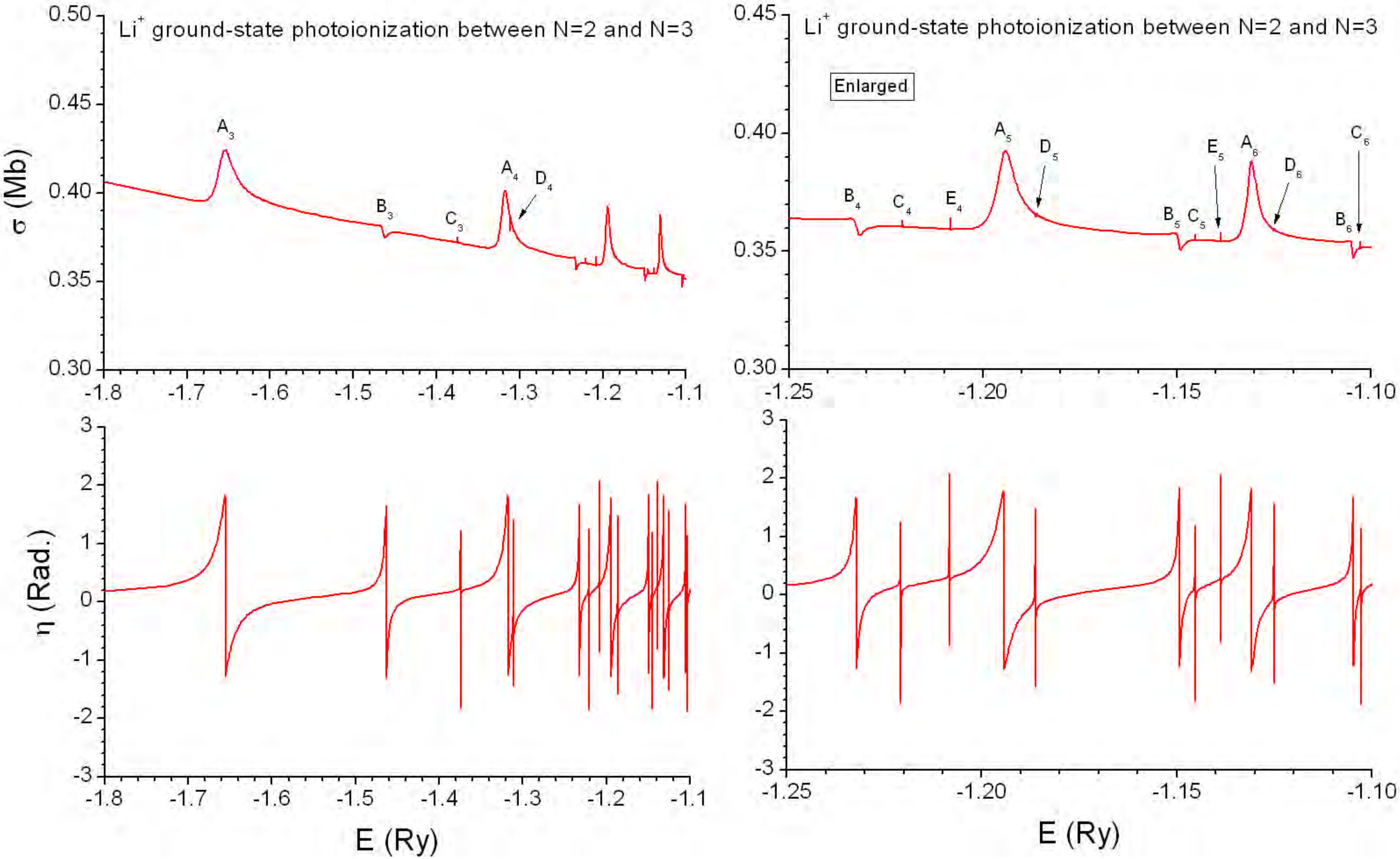
Li+
Theory, RMPS
Experiment, ALS
Absolute
2(0,1)2+
38 meV FWHM
q = -2.17
Absolute PI cross section (Mb)
Photon energy (eV)



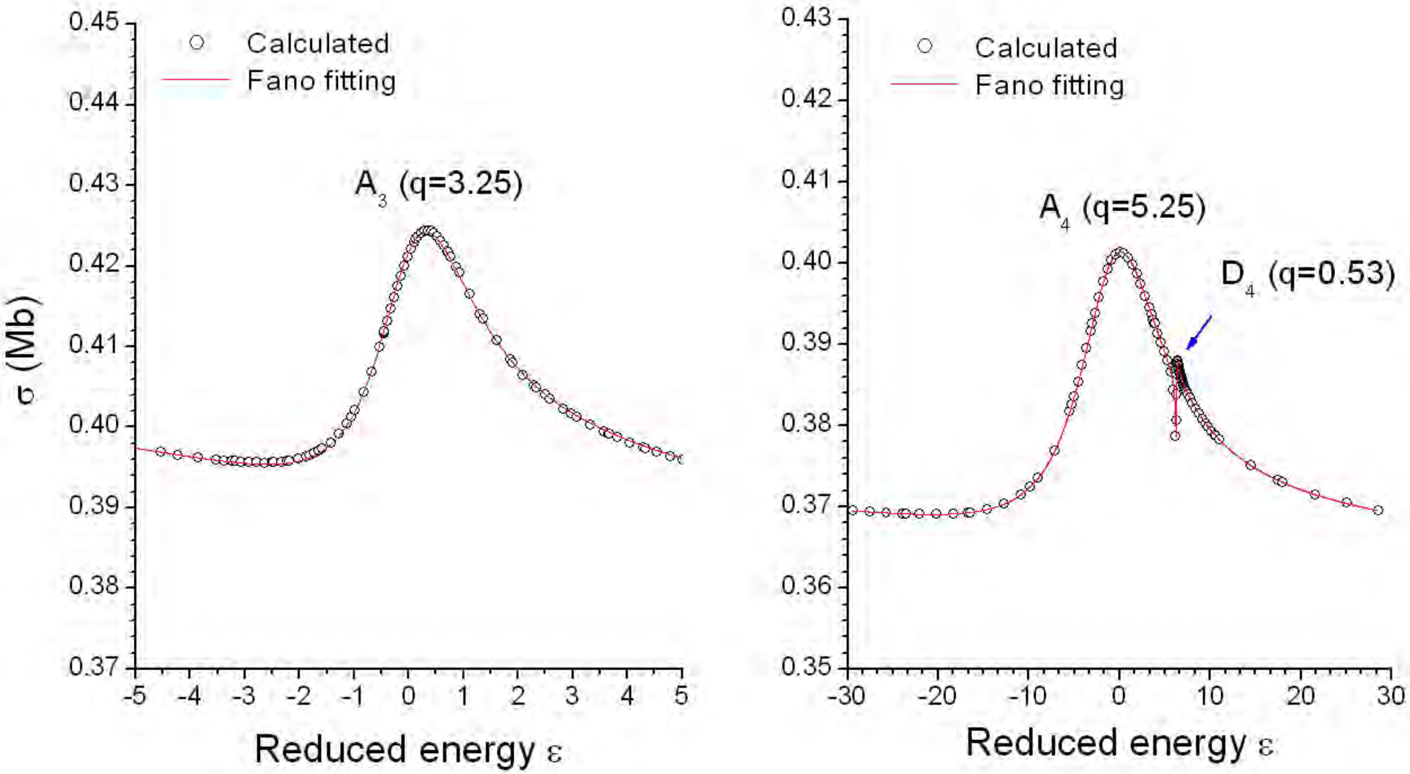
2+
Calculated
Convoluted
q = -2.16
σ (Mb)
Photon energy (eV)


Li+
400 meV
Experiment
Theory
Absolute (ALS)
Absolute PI cross section (Mb)
$_3(1,1)_3^+$
q = 3.85
(a)
Photon energy (eV)
Li+
100 meV
Experiment
Theory
Absolute (ALS)
DLP
$_3(1,1)_4^+$
q = 6.10
(b)
Photon energy (eV)

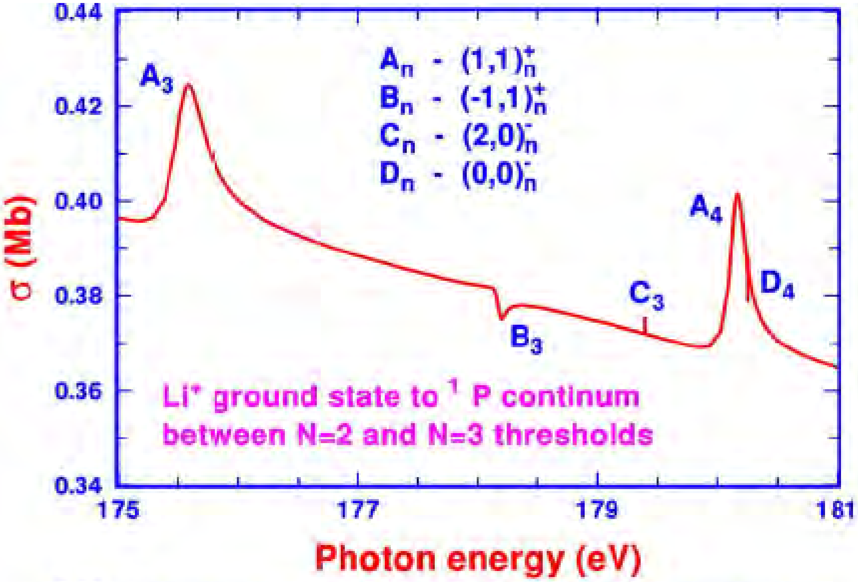

q = 3.25
A_3
σ (Mb)
Calculated
Convoluted
Photon energy (eV)
q = 5.25
A_4
D_4
q = 0.53
Calculated
Convoluted
Photon energy (eV)



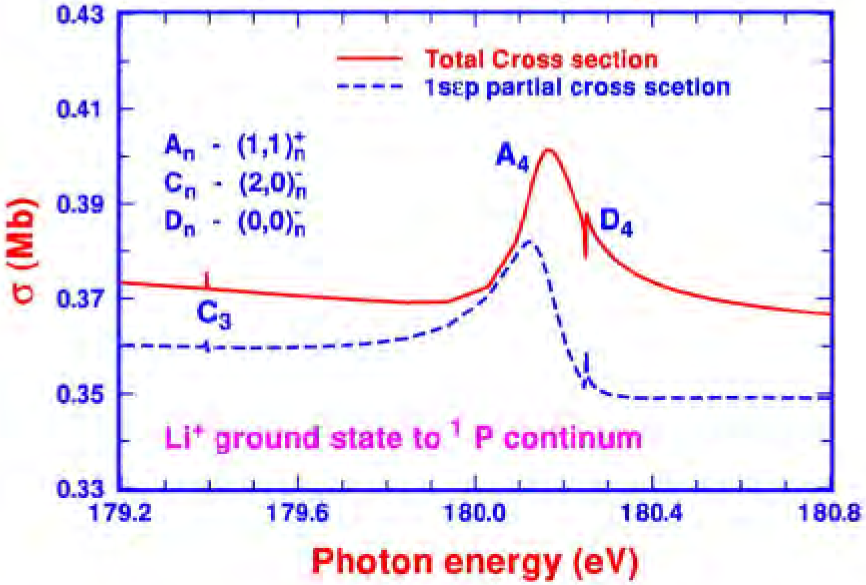
Li+ ground-state photoionization between N=2 and N=3
σ (Mb)
A3
B3
C3
A4
D4
η (Rad.)
E (Ry)
Li+ ground-state photoionization between N=2 and N=3
Enlarged
B4
C4
E4
A5
D5
B5
C5
E5
A6
D6
B6
C6
E (Ry)



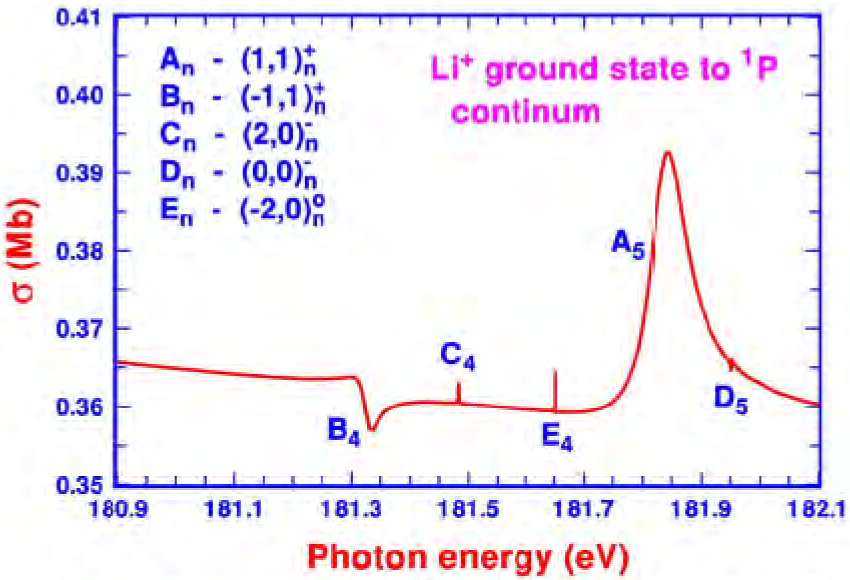
Calculated
Fano fitting
A3 (q=3.25)
σ (Mb)
0.45
0.44
0.43
0.42
0.41
0.40
0.39
0.38
0.37
-5 -4 -3 -2 -1 0 1 2 3 4 5
Reduced energy ε
Calculated
Fano fitting
A4 (q=5.25)
D4 (q=0.53)
0.43
0.42
0.41
0.40
0.39
0.38
0.37
0.36
0.35
-30 -20 -10 0 10 20 30
Reduced energy ε



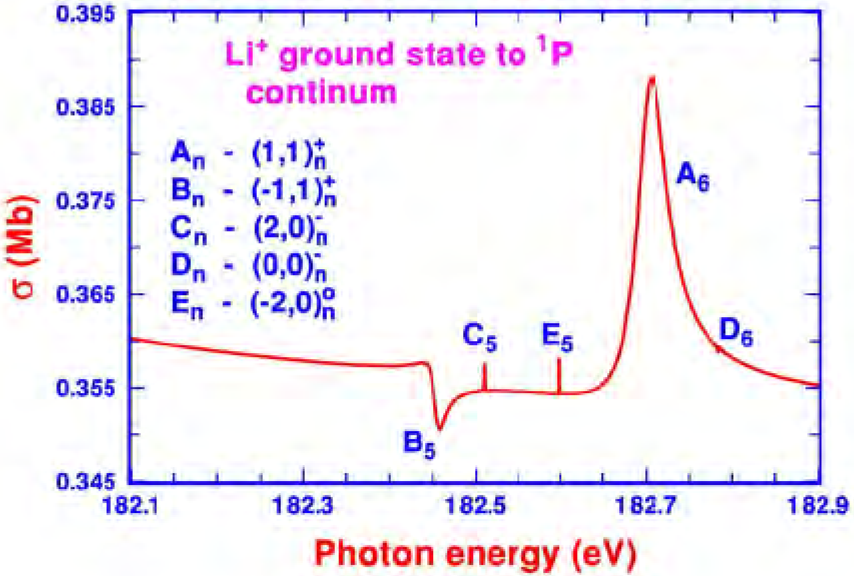
A3
An - (1,1)+n
Bn - (-1,1)+n
Cn - (2,0)-n
Dn - (0,0)-n
A4
D4
C3
B3
Li+ ground state to 1 P continuum
between N=2 and N=3 thresholds
σ (Mb)
0.44
0.42
0.40
0.38
0.36
0.34
175
177
179
181
Photon energy (eV)



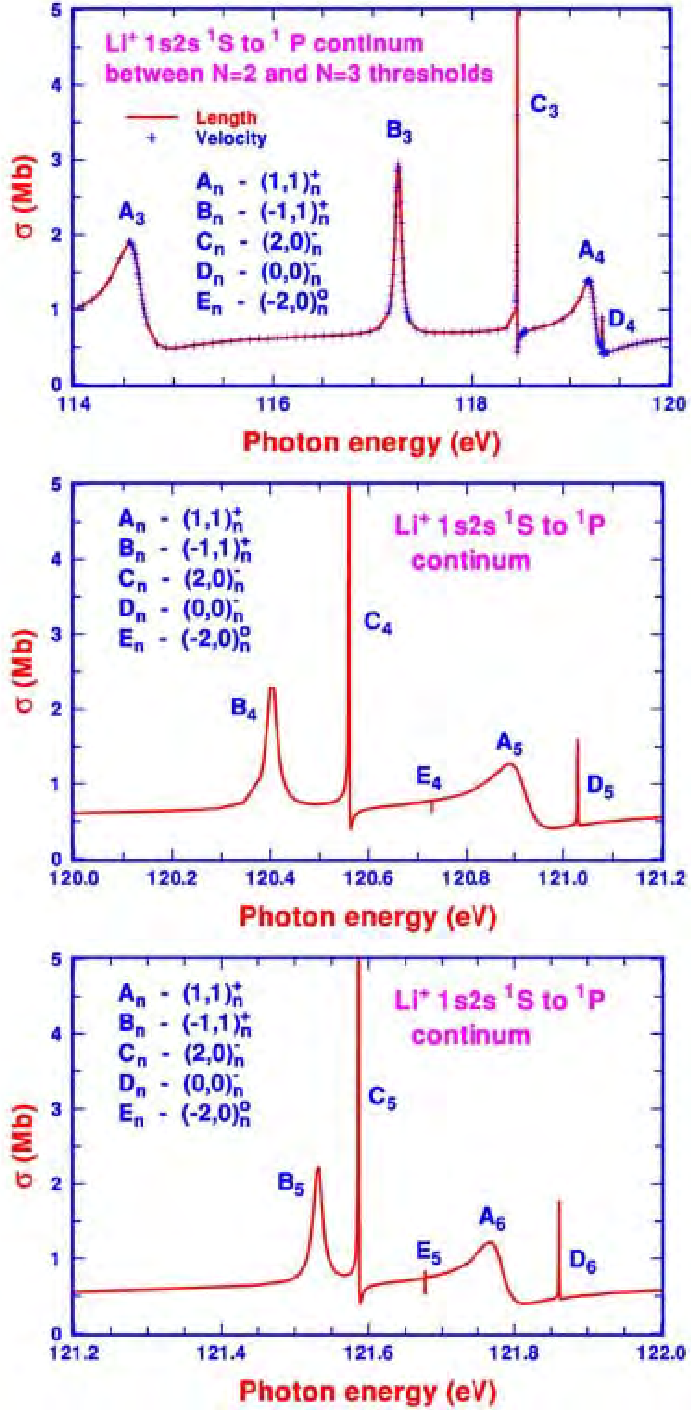
Total Cross section
1sεp partial cross scetion
An - (1,1)+n
Cn - (2,0)-n
Dn - (0,0)-n
A4
D4
C3
Li+ ground state to 1 P continuum
σ (Mb)
0.43
0.41
0.39
0.37
0.35
0.33
179.2
179.6
180.0
180.4
180.8
Photon energy (eV)



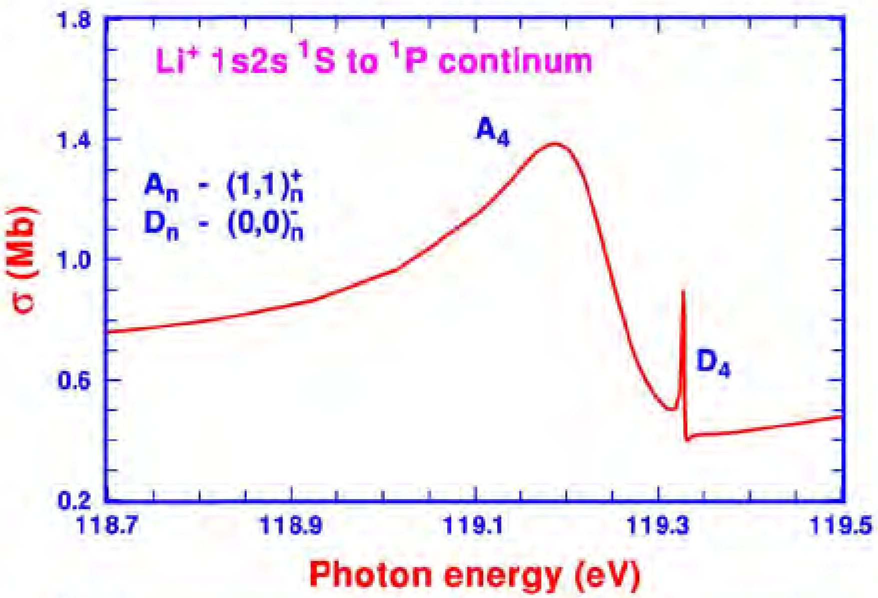
A_n - $(1,1)_n^+$
B_n - $(-1,1)_n^+$
C_n - $(2,0)_n^-$
D_n - $(0,0)_n^-$
E_n - $(-2,0)_n^o$
Li^+ ground state to ^1P continuum
A_5
B_4
C_4
D_5
E_4
σ (Mb)
Photon energy (eV)

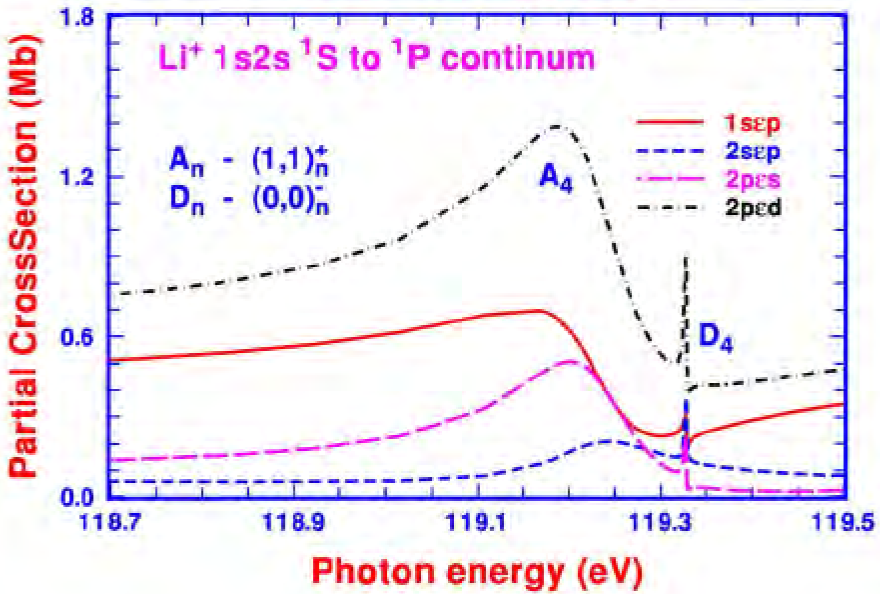


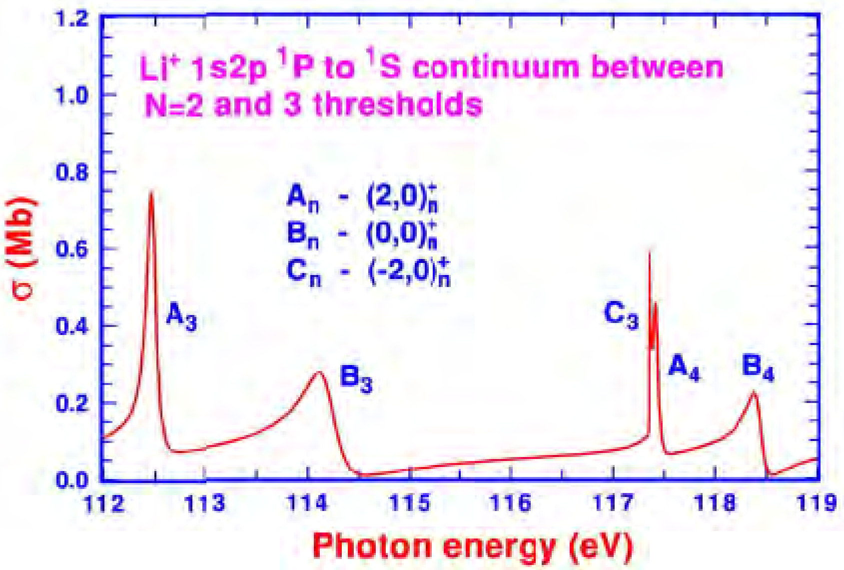
Li^+ ground state to ^1P continuum
A_n - $(1,1)_n^+$
B_n - $(-1,1)_n^+$
C_n - $(2,0)_n^-$
D_n - $(0,0)_n^-$
E_n - $(-2,0)_n^o$
A_6
B_5
C_5
D_6
E_5
σ (Mb)
Photon energy (eV)

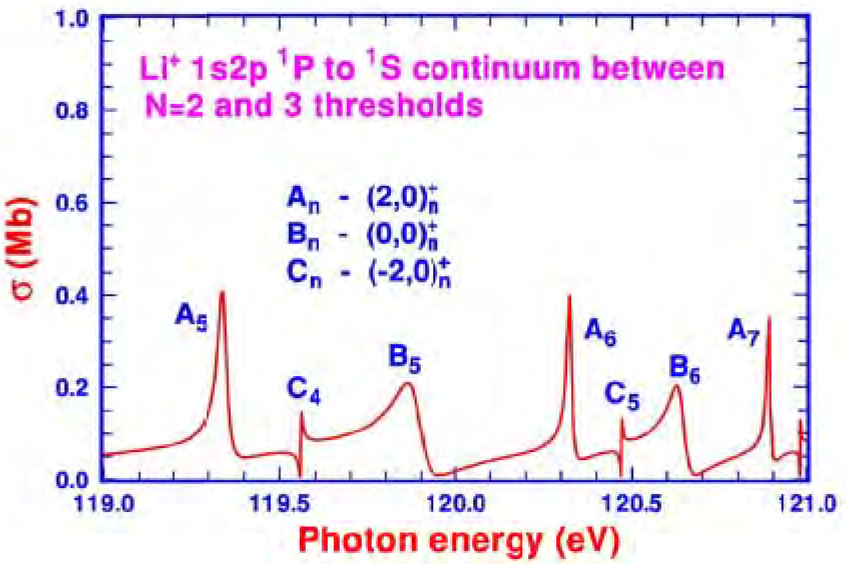


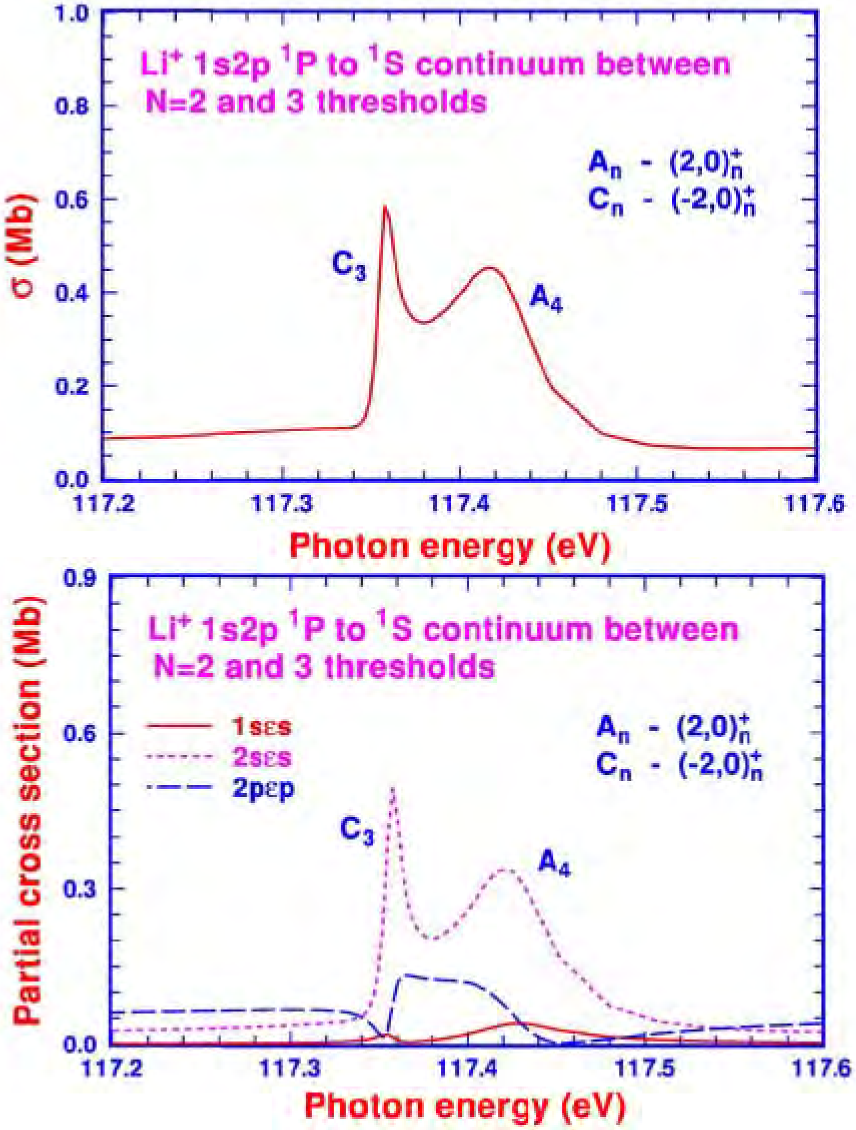
Li+ 1s2s 1S to 1 P continuum
between N=2 and N=3 thresholds
Length
Velocity
A3
B3
C3
A4
D4
An - (1,1)+n
Bn - (-1,1)+n
Cn - (2,0)-n
Dn - (0,0)-n
En - (-2,0)on
σ (Mb)
Photon energy (eV)
114
116
118
120
0
1
2
3
4
5
Li+ 1s2s 1S to 1P
continuum
An - (1,1)+n
Bn - (-1,1)+n
Cn - (2,0)-n
Dn - (0,0)-n
En - (-2,0)on
B4
C4
E4
A5
D5
σ (Mb)
Photon energy (eV)
120.0
120.2
120.4
120.6
120.8
121.0
121.2
0
1
2
3
4
5
Li+ 1s2s 1S to 1P
continuum
An - (1,1)+n
Bn - (-1,1)+n
Cn - (2,0)-n
Dn - (0,0)-n
En - (-2,0)on
B5
C5
E5
A6
D6
σ (Mb)
Photon energy (eV)
121.2
121.4
121.6
121.8
122.0
0
1
2
3
4
5


Li+ 1s2s 1S to 1P continum
A4
An - (1,1)+n
Dn - (0,0)-n
D4
σ (Mb)
1.8
1.4
1.0
0.6
0.2
118.7
118.9
119.1
119.3
119.5
Photon energy (eV)

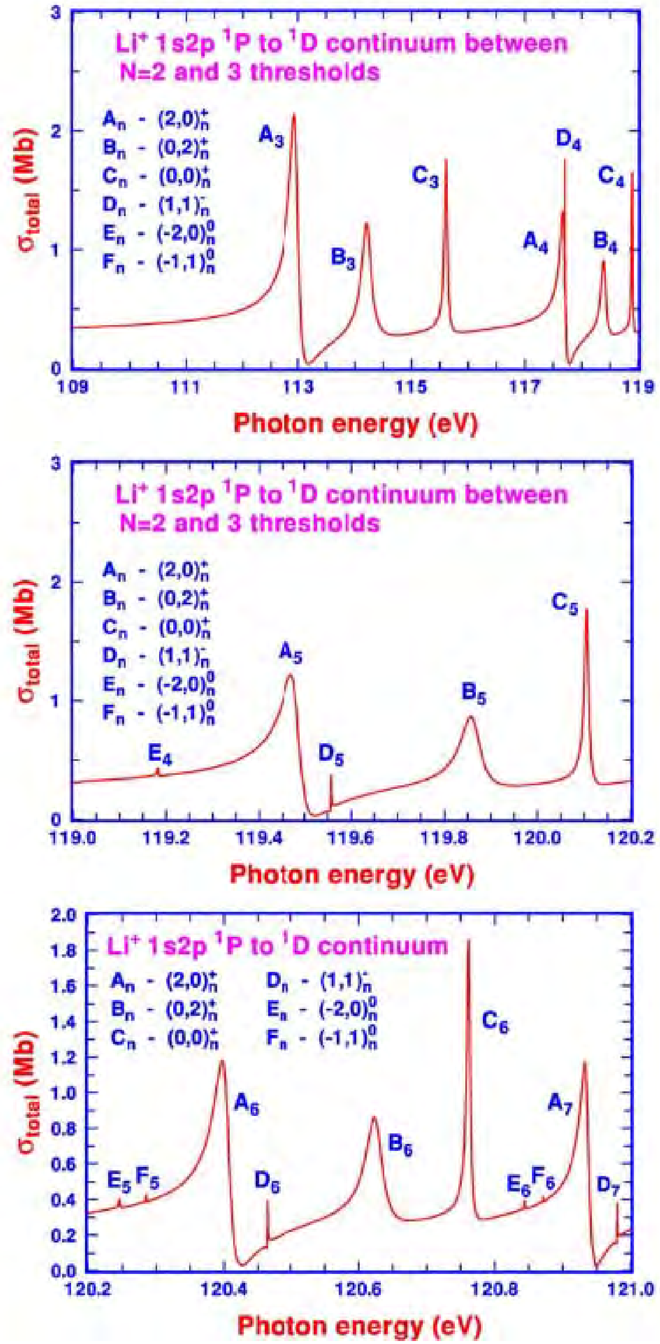

Li+ 1s2s 1S to 1P continum
1sεp
2sεp
2pεs
2pεd
An - (1,1)+n
Dn - (0,0)-n
A4
D4
Partial CrossSection (Mb)
1.8
1.2
0.6
0.0
118.7
118.9
119.1
119.3
119.5
Photon energy (eV)

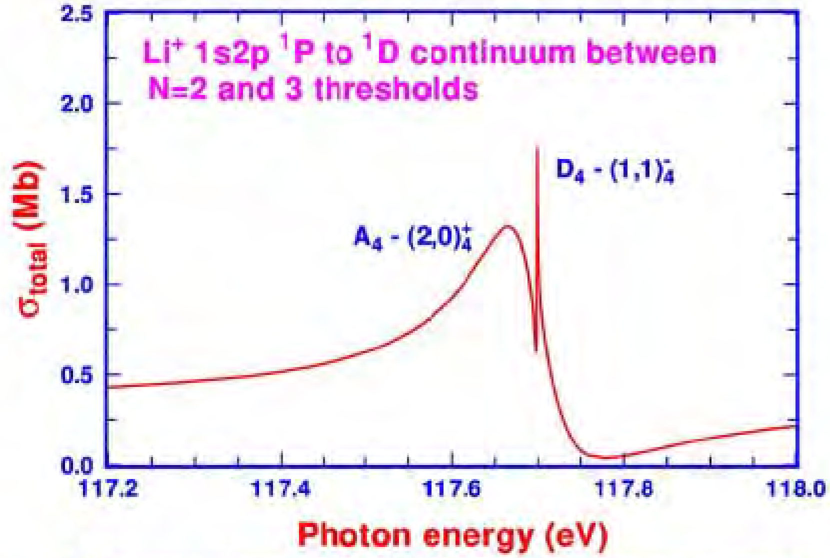

Li+ 1s2p 1P to 1S continuum between
N=2 and 3 thresholds
An - (2,0)n+
Bn - (0,0)n+
Cn - (-2,0)n+
A3
B3
C3
A4
B4
σ (Mb)
Photon energy (eV)
0.0
0.2
0.4
0.6
0.8
1.0
1.2
112
113
114
115
116
117
118
119


Li+ 1s2p 1P to 1S continuum between
N=2 and 3 thresholds
An - (2,0)n+
Bn - (0,0)n+
Cn - (-2,0)n+
A5
C4
B5
A6
C5
B6
A7
σ (Mb)
Photon energy (eV)
0.0
0.2
0.4
0.6
0.8
1.0
119.0
119.5
120.0
120.5
121.0

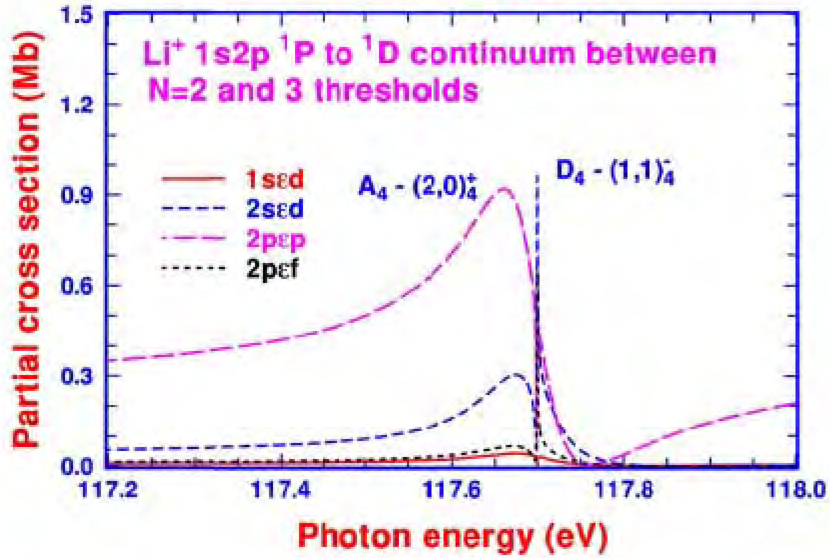


Li+ 1s2p 1P to 1S continuum between
N=2 and 3 thresholds
An - (2,0)+n
Cn - (-2,0)+n
C3
A4
σ (Mb)
1.0
0.8
0.6
0.4
0.2
0.0
117.2
117.3
117.4
117.5
117.6
Photon energy (eV)
Li+ 1s2p 1P to 1S continuum between
N=2 and 3 thresholds
1sεs
2sεs
2pεp
An - (2,0)+n
Cn - (-2,0)+n
C3
A4
Partial cross section (Mb)
0.9
0.6
0.3
0.0
117.2
117.3
117.4
117.5
117.6
Photon energy (eV)

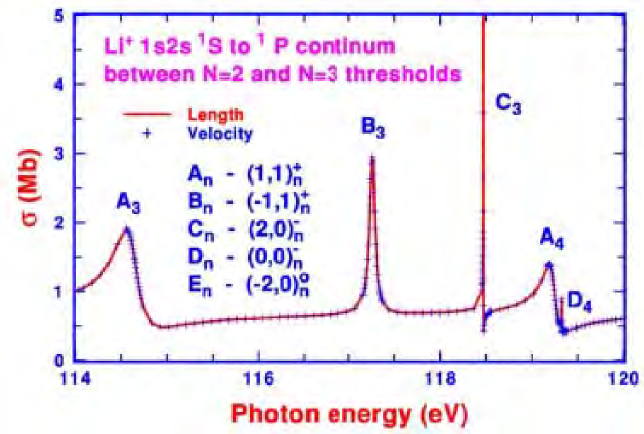

Li+ 1s2p 1P to 1D continuum between
N=2 and 3 thresholds
An - (2,0)+n
Bn - (0,2)+n
Cn - (0,0)+n
Dn - (1,1)-n
En - (-2,0)0n
Fn - (-1,1)0n
A3
B3
C3
A4
D4
B4
C4
σtotal (Mb)
Photon energy (eV)
109
111
113
115
117
119
0
1
2
3
Li+ 1s2p 1P to 1D continuum between
N=2 and 3 thresholds
An - (2,0)+n
Bn - (0,2)+n
Cn - (0,0)+n
Dn - (1,1)-n
En - (-2,0)0n
Fn - (-1,1)0n
E4
A5
D5
B5
C5
σtotal (Mb)
Photon energy (eV)
119.0
119.2
119.4
119.6
119.8
120.0
120.2
0
1
2
3
Li+ 1s2p 1P to 1D continuum
An - (2,0)+n
Bn - (0,2)+n
Cn - (0,0)+n
Dn - (1,1)-n
En - (-2,0)0n
Fn - (-1,1)0n
E5 F5
A6
D6
B6
C6
E6 F6
A7
D7
σtotal (Mb)
Photon energy (eV)
120.2
120.4
120.6
120.8
121.0
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0

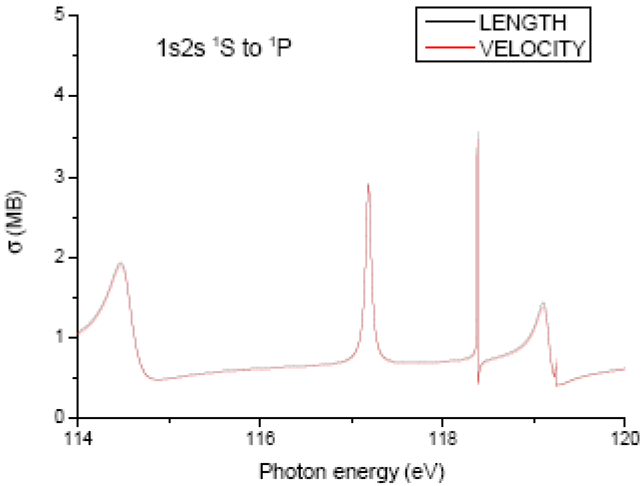


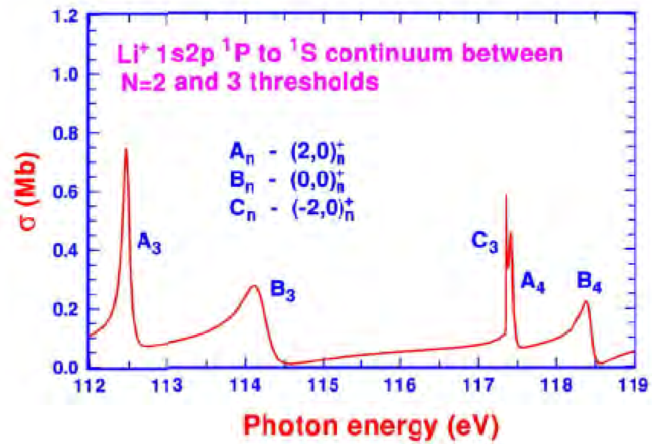
Li+ 1s2p 1P to 1D continuum between
N=2 and 3 thresholds
D4 - (1,1)-4
A4 - (2,0)+4
σtotal (Mb)
Photon energy (eV)



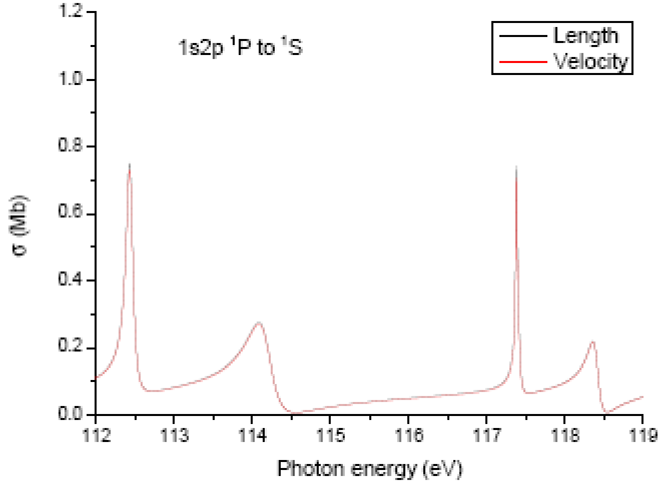
Li+ 1s2p 1P to 1D continuum between
N=2 and 3 thresholds
1sεd
2sεd
2pεp
2pεf
A4 - (2,0)+4
D4 - (1,1)-4
Partial cross section (Mb)
Photon energy (eV)


Li+ 1s2s 1S to 1 P continum
between N=2 and N=3 thresholds
Length
Velocity
A3
B3
C3
A4
D4
An - (1,1)+n
Bn - (-1,1)+n
Cn - (2,0)-n
Dn - (0,0)-n
En - (-2,0)on
σ (Mb)
Photon energy (eV)

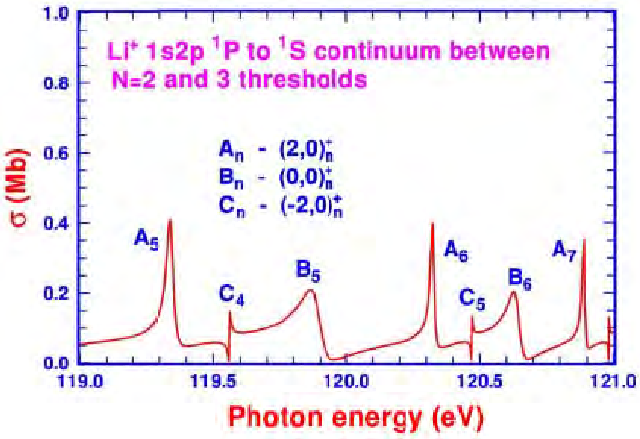

1s2s 1S to 1P
LENGTH
VELOCITY
σ (MB)
Photon energy (eV)



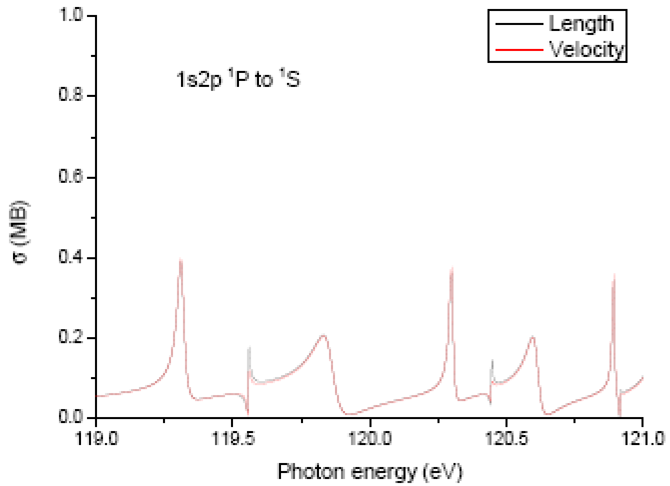
Li+ 1s2p 1P to 1S continuum between
N=2 and 3 thresholds
An - (2,0)+n
Bn - (0,0)+n
Cn - (-2,0)+n
A3
B3
C3
A4
B4
σ (Mb)
Photon energy (eV)



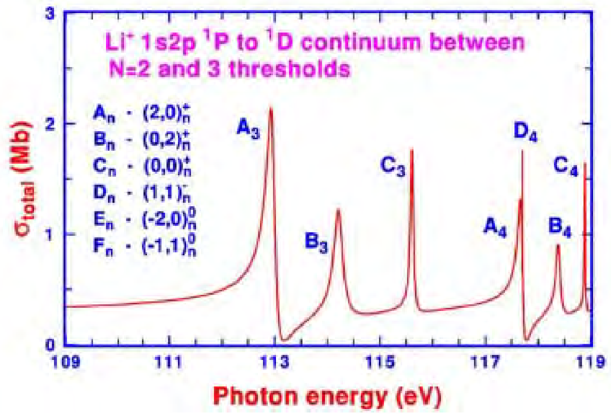
1s2p 1P to 1S
Length
Velocity
σ (Mb)
Photon energy (eV)



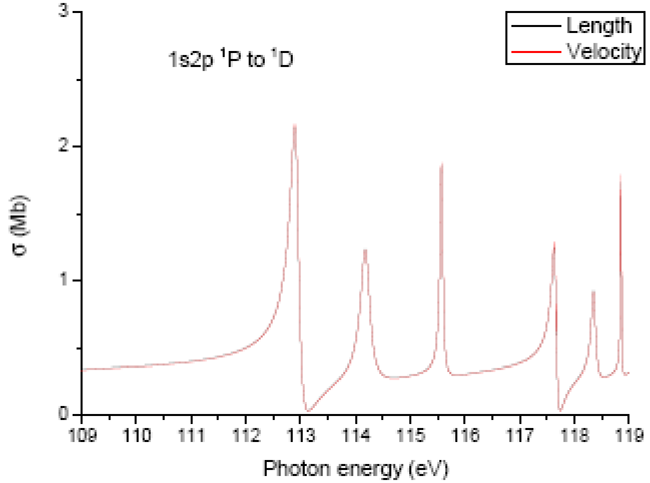
Li+ 1s2p 1P to 1S continuum between
N=2 and 3 thresholds
A5
C4
B5
A6
C5
B6
A7
σ (Mb)
Photon energy (eV)



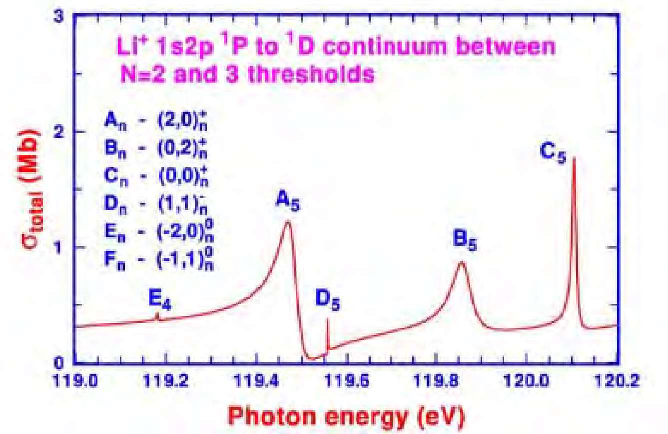
Length
Velocity
1s2p 1P to 1S
σ (MB)
Photon energy (eV)

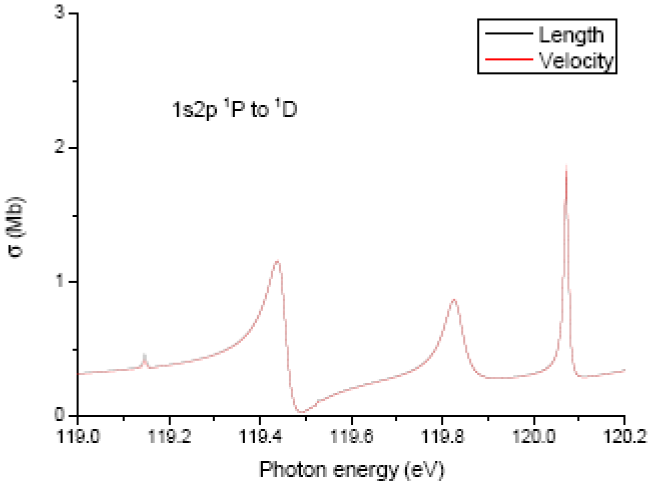


Li⁺ 1s2p ¹P to ¹D continuum between
N=2 and 3 thresholds
A_n - $(2,0)_n^+$
B_n - $(0,2)_n^+$
C_n - $(0,0)_n^+$
D_n - $(1,1)_n^-$
E_n - $(-2,0)_n^0$
F_n - $(-1,1)_n^0$
A_3
B_3
C_3
A_4
D_4
B_4
C_4
σ_{total} (Mb)
Photon energy (eV)



1s2p ¹P to ¹D
Length
Velocity
σ (Mb)
Photon energy (eV)

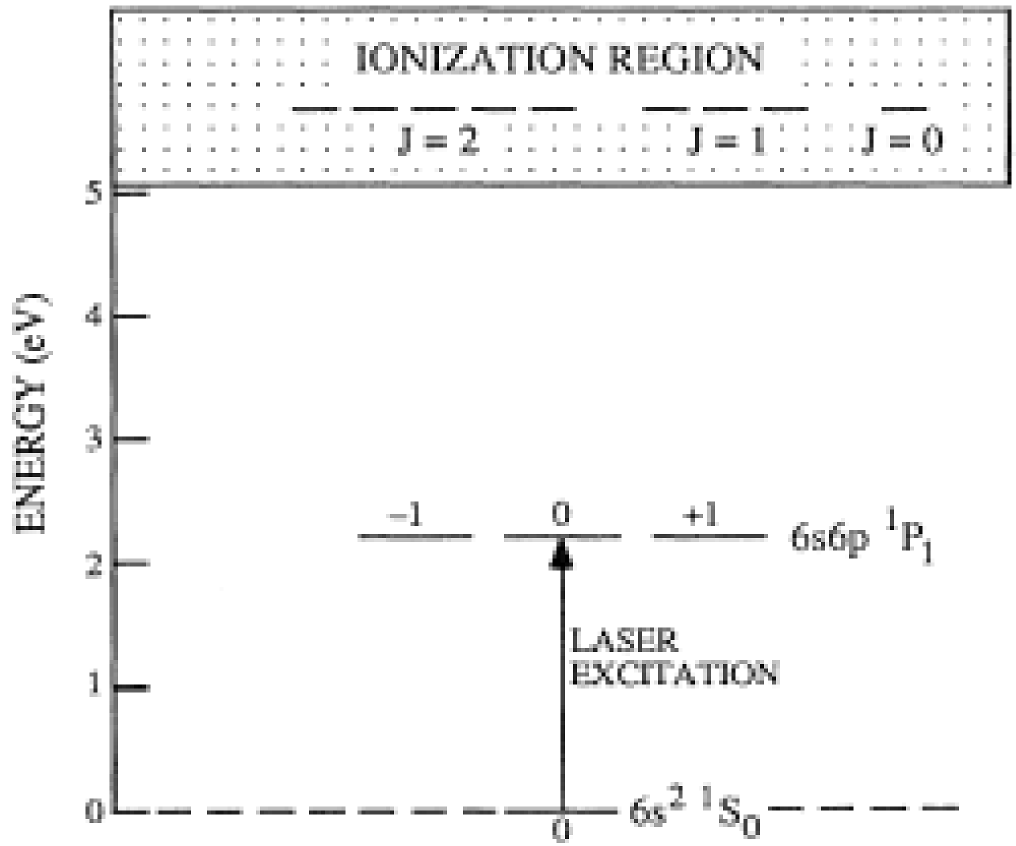

Li+ 1s2p 1P to 1D continuum between N=2 and 3 thresholds
An - (2,0)+n
Bn - (0,2)+n
Cn - (0,0)+n
Dn - (1,1)-n
En - (-2,0)0n
Fn - (-1,1)0n
A5
B5
C5
D5
E4
σtotal (Mb)
Photon energy (eV)
0
1
2
3
119.0
119.2
119.4
119.6
119.8
120.0
120.2


Length
Velocity
1s2p 1P to 1D
σ (Mb)
Photon energy (eV)
0
1
2
3
119.0
119.2
119.4
119.6
119.8
120.0
120.2

Absolute Cross Sections for the Photoionization of the $6s6p$ ^1P Excited State of Barium

L.-W. He, C. E. Burkhardt, M. Ciocca, and J. J. Leventhal
Department of Physics, University of Missouri–St. Louis, St. Louis, Missouri 63121

S. T. Manson
Department of Physics and Astronomy, Georgia State University, Atlanta, Georgia 30303
(Received 8 July 1991)



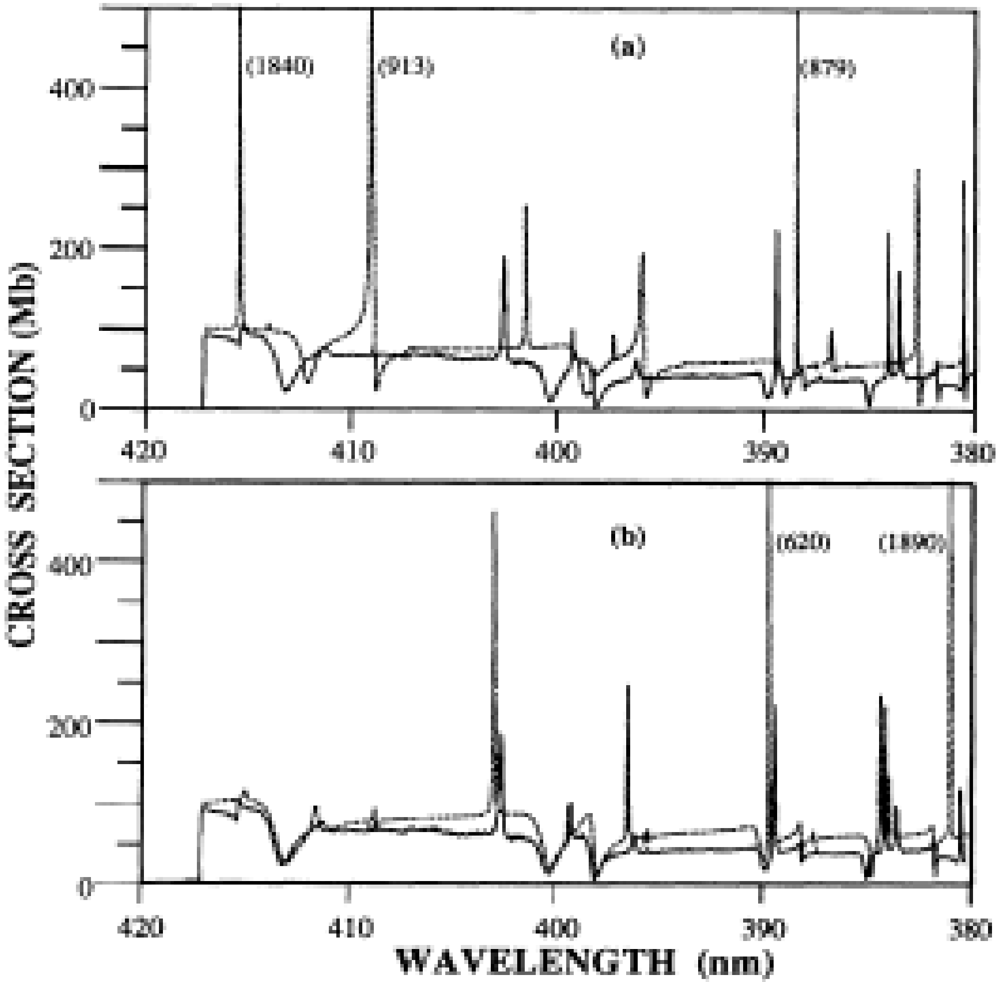


FIG. 2. Photoionization cross section of Ba $6s6p\,^1P$ state near threshold. The solid lines are the data reported in this work. The dashed lines represent the calculations of (a) Ref. [10] and (b) Ref. [11].

Ba 6s6p $^{1}P_{J=1}$ $\Longrightarrow$ $^{1,3}L^{e}_{J=0}$, $^{1,3}L^{e}_{J=2}$

Open chs:

6sεs $^{1}S^{e}_{J=0}$, 6sεd $^{1,3}D^{e}_{J=2}$

Closed chs:

5dnd $^{1}S^{e}_{J=0}$ & $^{3}P^{e}_{J=0}$,

5dns $^{1,3}D^{e}_{J=2}$, 5dnd $^{1,3}D^{e}_{J=2}$ & $^{3}P^{e}_{J=2}$, 5dng $^{1,3}D^{e}_{J=2}$

Atomic photoionization in changing plasma environment

$$H(\mathbf{r}_1, \mathbf{r}_2, \ldots; D) = \Sigma_i\, h_0(\mathbf{r}_i; D) + \Sigma_{i>j}\, e^2/\mathbf{r}_{ij}\,,$$

where $h_0(\mathbf{r}; D) = (p^2/2m) - (Z\, e^2/\,\mathbf{r})\, e^{-r/D}$,

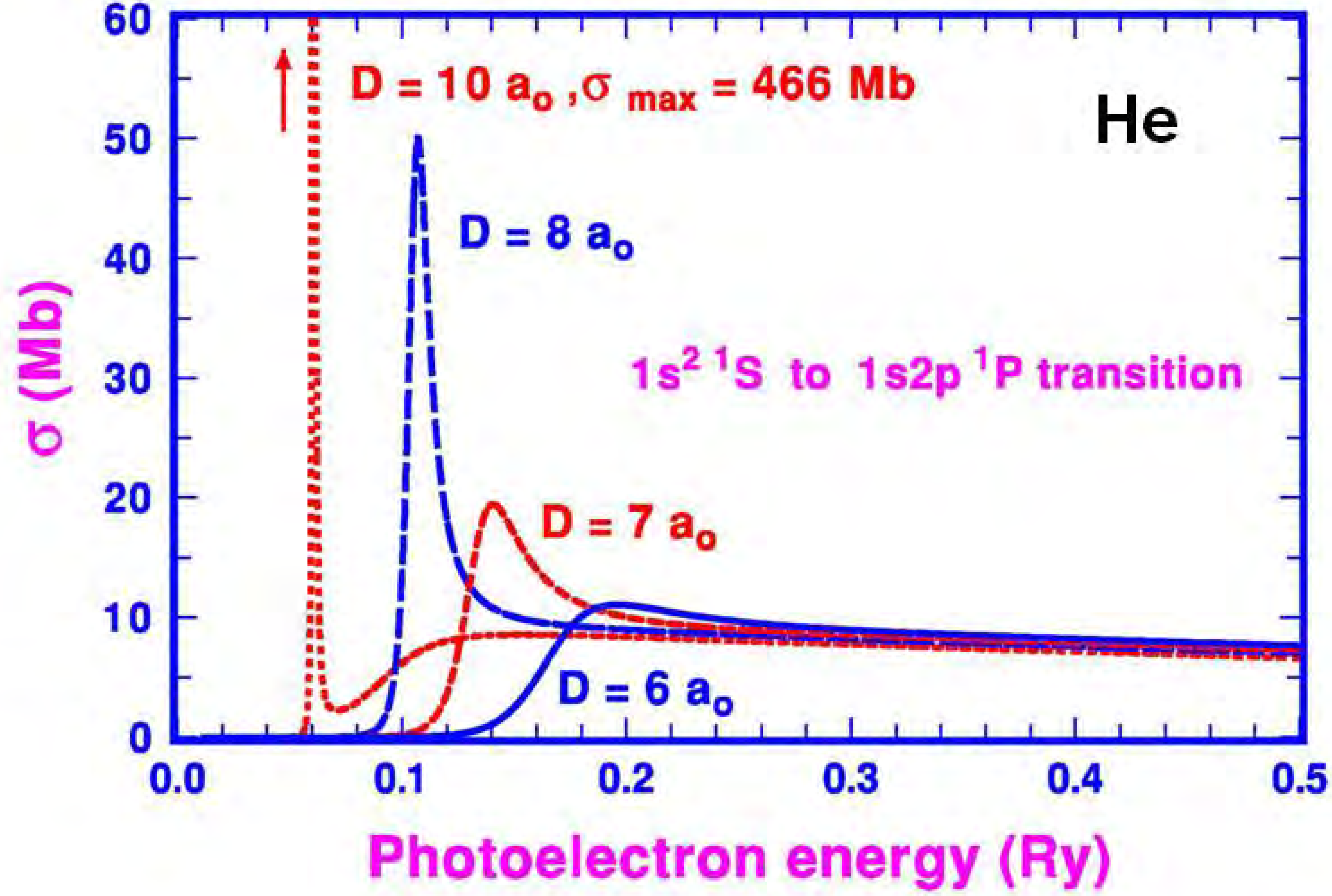
p: electron momentum, *D* :Debye length given by

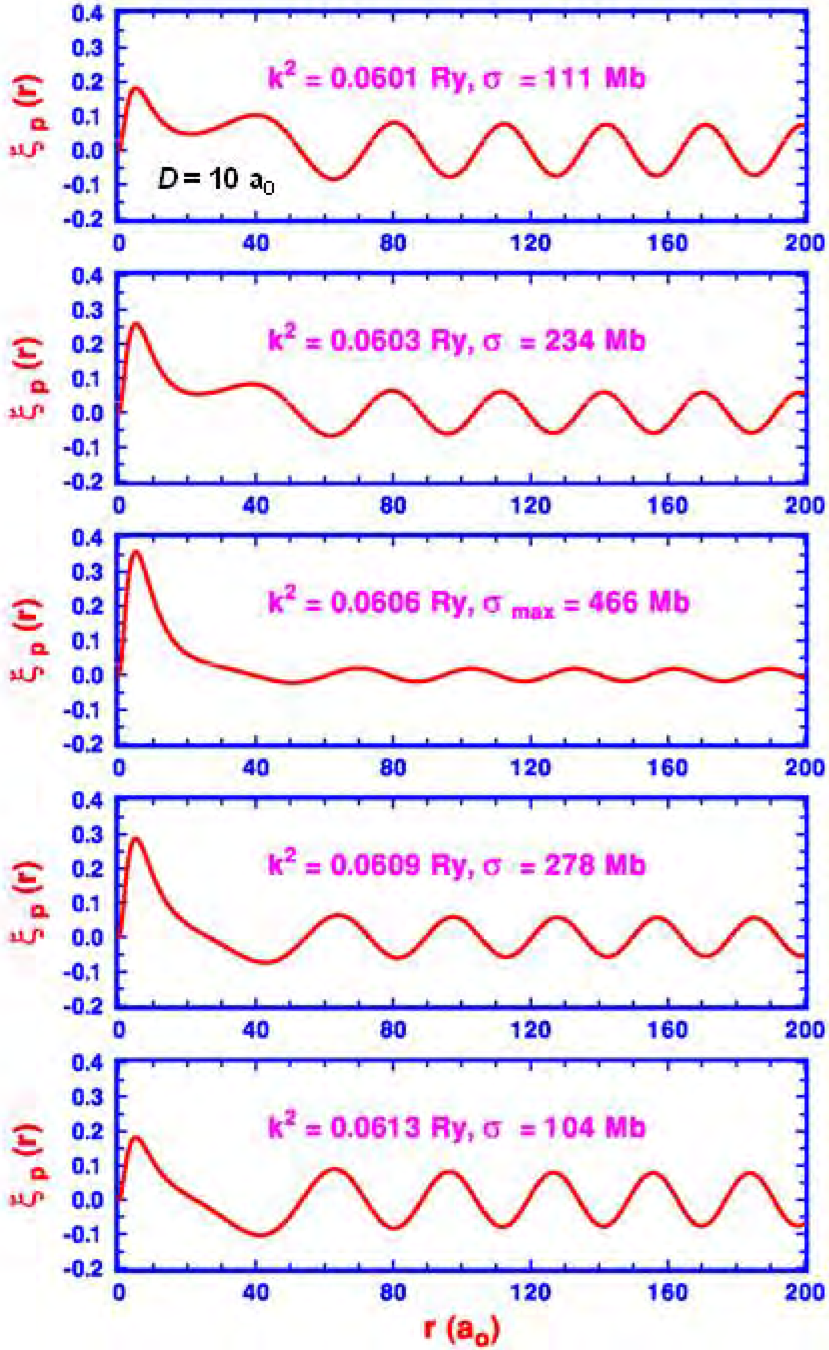
$$D = 1.304 \times 10^9\, (T/n)^{1/2},$$ (in unit of a_0)

T: plasma temperature (in degree Kelvin)

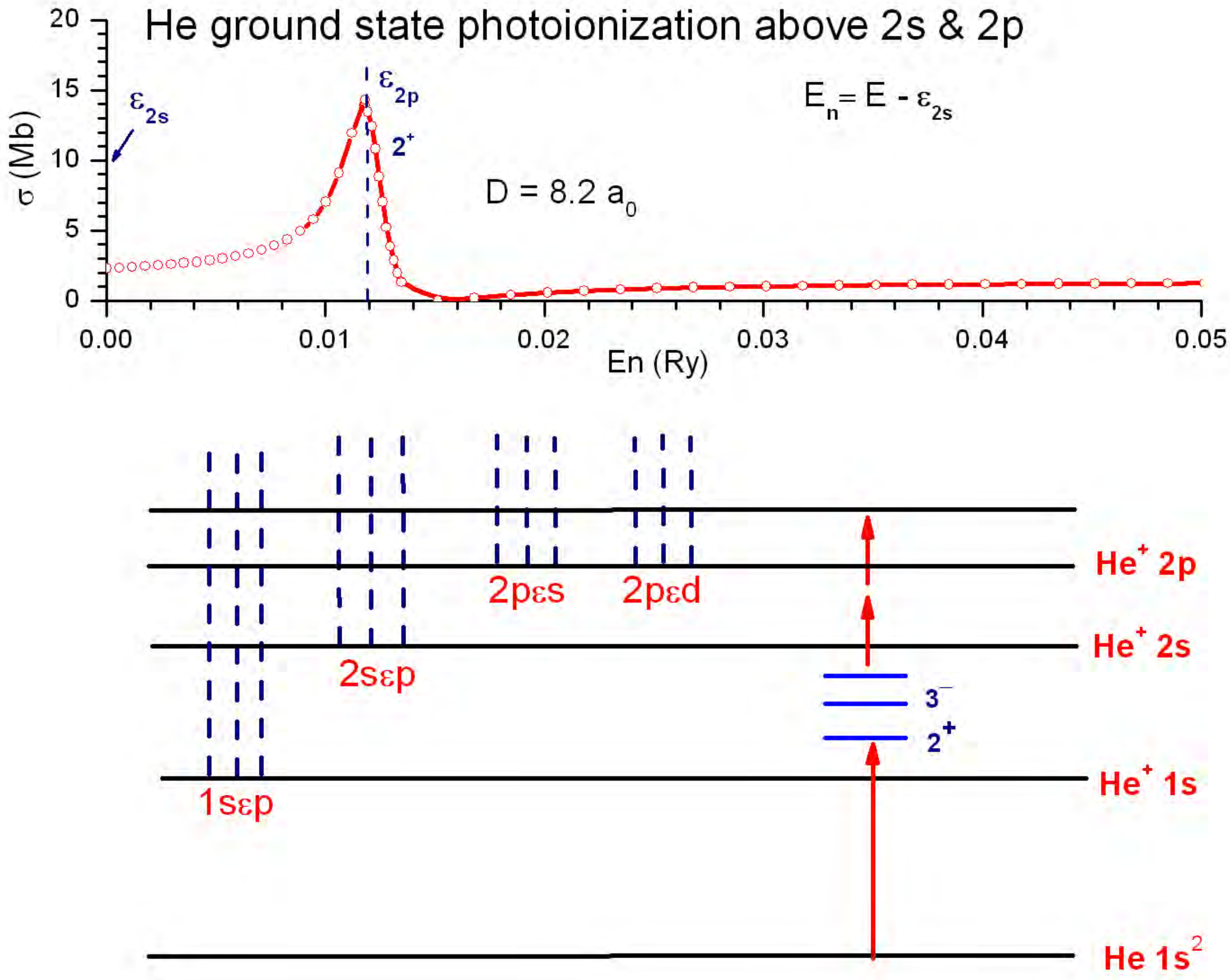
n: density (in cm^{-3})

Phys. Rev. A88,023406 (2013)

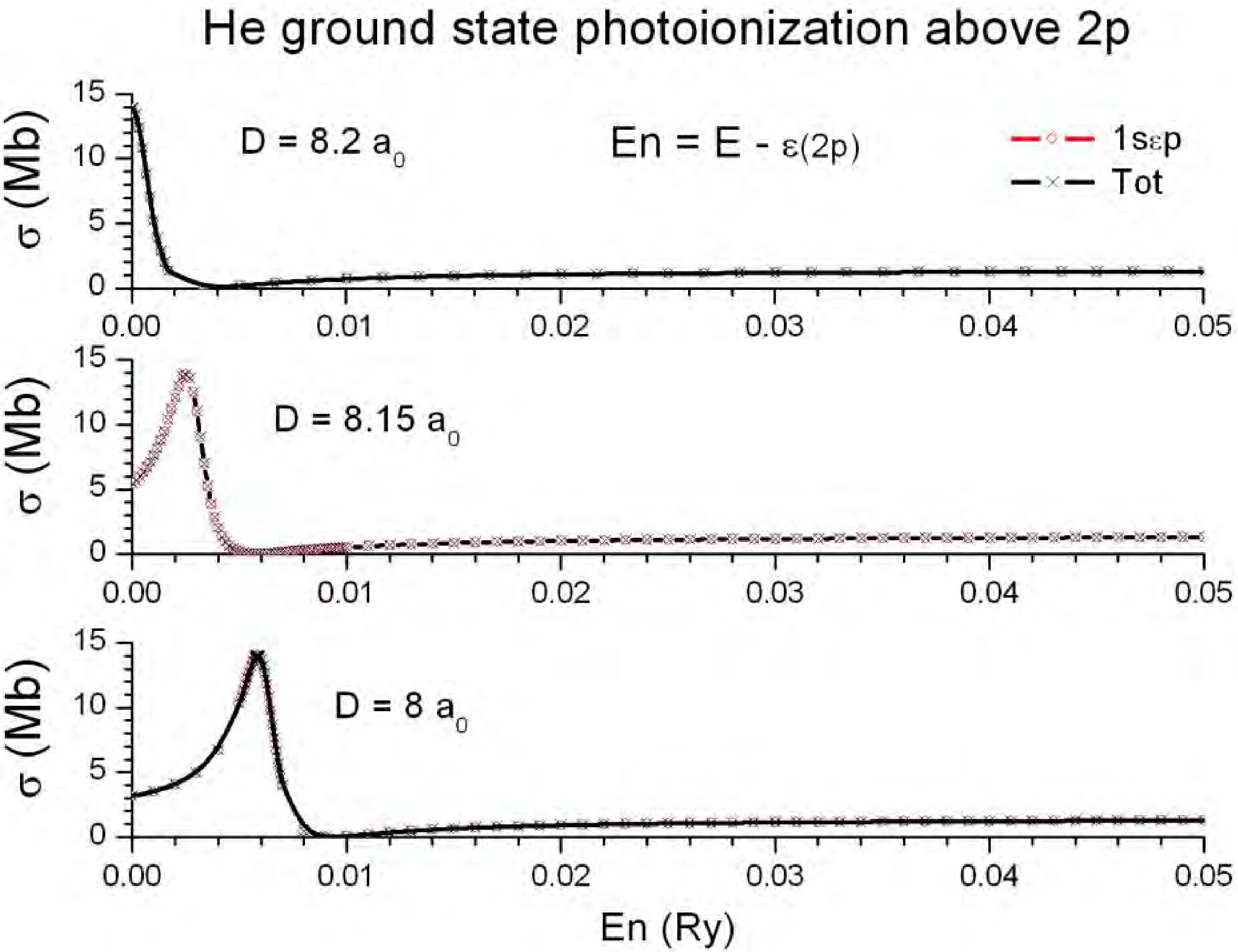




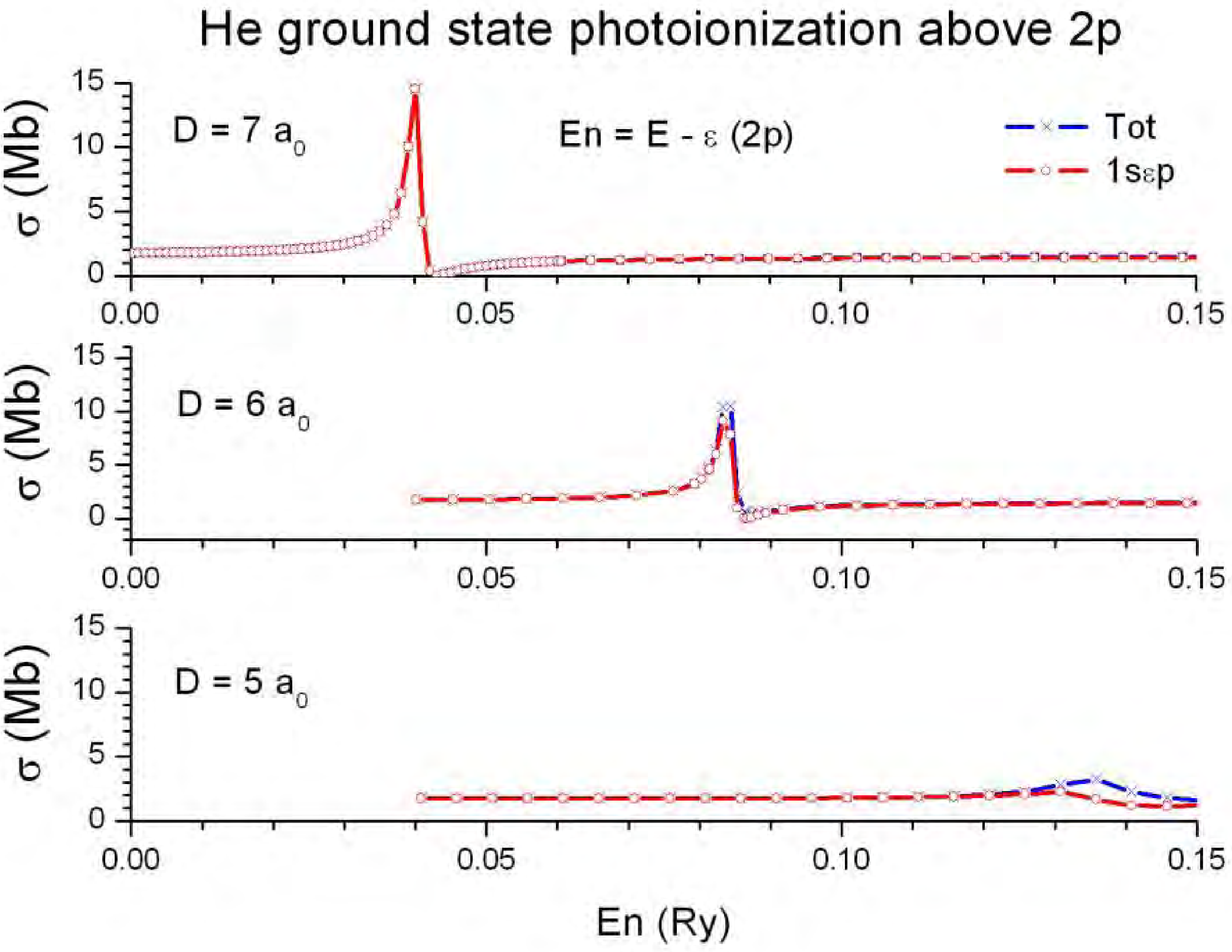
k² = 0.0601 Ry, σ = 111 Mb
D = 10 a0
k² = 0.0603 Ry, σ = 234 Mb
k² = 0.0606 Ry, σ max = 466 Mb
k² = 0.0609 Ry, σ = 278 Mb
k² = 0.0613 Ry, σ = 104 Mb
ξp (r)
r (a0)



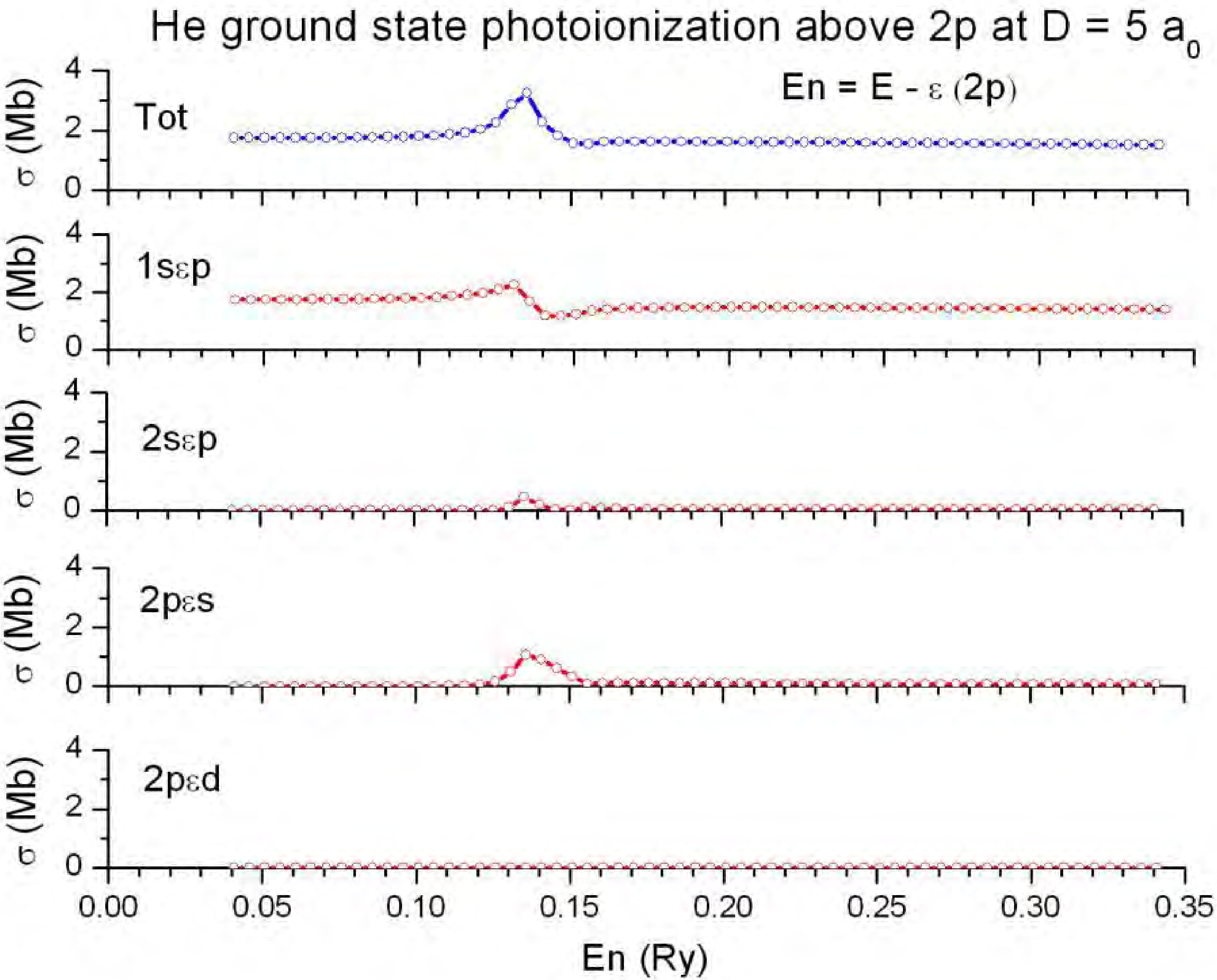
He ground state photoionization above 2s & 2p
σ (Mb)
20
15
10
5
0
ε2s
ε2p
2+
En= E - ε2s
D = 8.2 a0
0.00
0.01
0.02
0.03
0.04
0.05
En (Ry)
He+ 2p
2pεs
2pεd
He+ 2s
2sεp
3−
2+
He+ 1s
1sεp
He 1s2



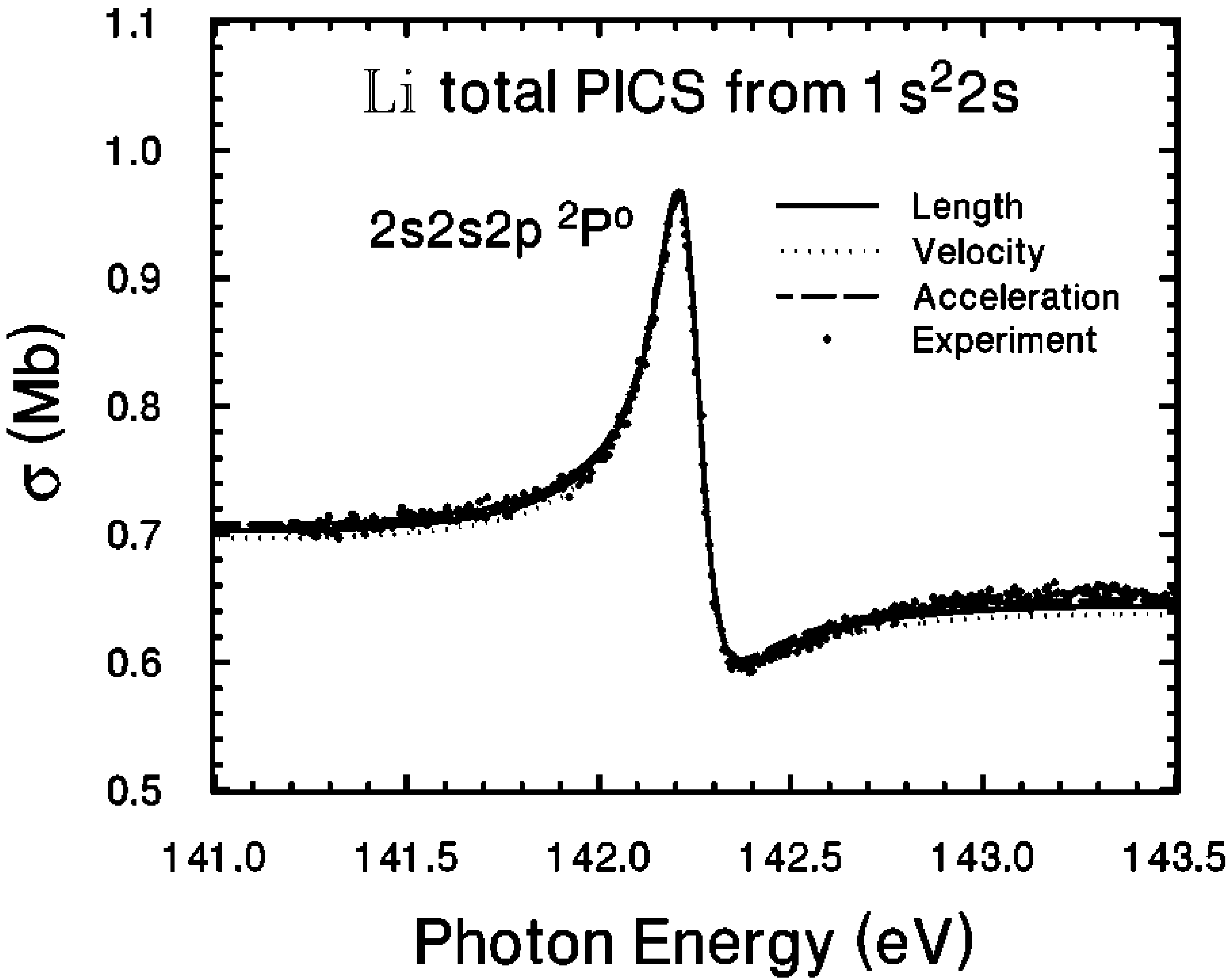
He ground state photoionization above 2p
D = 8.2 a0
En = E - ε(2p)
1sεp
Tot
σ (Mb)
D = 8.15 a0
D = 8 a0
0
5
10
15
0.00
0.01
0.02
0.03
0.04
0.05
En (Ry)

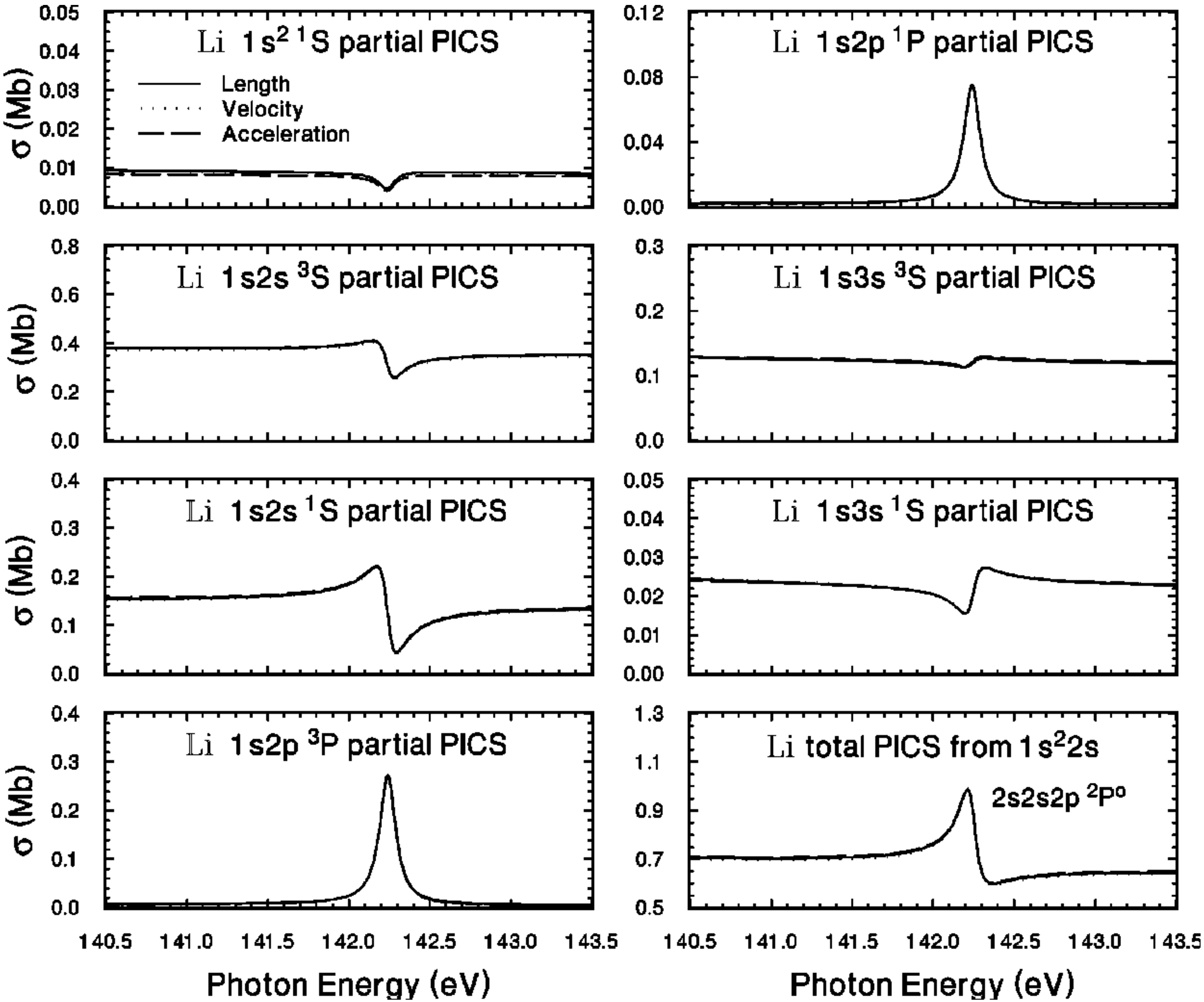


He ground state photoionization above 2p
σ (Mb)
D = 7 a0
En = E - ε (2p)
Tot
1sεp
D = 6 a0
D = 5 a0
0
5
10
15
0.00
0.05
0.10
0.15
En (Ry)


He ground state photoionization above 2p at D = 5 a0
En = E - ε (2p)
Tot
1sεp
2sεp
2pεs
2pεd
σ (Mb)
0
2
4
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35
En (Ry)

Triply excited lithium: Phys. Rev. A 63, 020702 (2001).





Li 1s2 1S partial PICS
Length
Velocity
Acceleration
Li 1s2p 1P partial PICS
Li 1s2s 3S partial PICS
Li 1s3s 3S partial PICS
Li 1s2s 1S partial PICS
Li 1s3s 1S partial PICS
Li 1s2p 3P partial PICS
Li total PICS from 1s22s
2s2s2p 2Po
σ (Mb)
Photon Energy (eV)