Complex - rotation Method for Atomic Photoionization

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Divalent atoms

Atom	Z	Ground-state configuration
Be	4	$[1s^2]\ 2s^2$
Mg	12	$[1s^2\ 2s^2\ 2p^6]\ 3s^2$
Ca	20	$[1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6]\ 4s^2$
Sr	38	$[1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^6]\ 5s^2$
Ba	56	$[1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^6\ 5s^2\ 4d^{10}\ 5p^6]\ 6s^2$

Divalent Atoms

- **Effective one-particle Hamiltonian :**

$$h_\ell^{eff} = \left(-\frac{1}{2}\frac{d^2}{dr^2} - \frac{Z}{r} + \frac{1}{2}\frac{\ell(\ell+1)}{r^2}\right) + V_\ell^{FCHF}(r) + V_p(r),$$

where $V_\ell^{FCHF}(r)$ is the frozen-core Hartree-Fock (FCHF) potential and

$$V_p = -\frac{\alpha_0}{r^4}\left(1 - \exp^{(r/r_0)^6}\right)$$

is a parametrized long-range dipole core-polarization potential.

- **One-particle radial equation:**

$$h_\ell^{eff}(r)\,\chi_{n\ell}(r) = \varepsilon_{n\ell}\,\chi_{n\ell}(r),$$

where the solution $\chi_{n\ell}(r)$ is expanded in terms of a set of B-splines defined between $r = 0$ and $r = R$, i.e.,

$$\chi_{n\ell}(r) = \sum_{i=1}^{N} C_i\, B_i(r).$$

Forzen-core Hartree-Fock Potential

$$V_\ell^{FCHF}\, f_\ell(r) = \sum_{n_0\ell_0}^{core} 2\left(\frac{2\ell_0+1}{2\ell+1}\right)^{1/2} (\ell||\, V^0(\chi_{n_0\ell_0}, \chi_{n_0\ell_0}; r\,||\,\ell)\, f_\ell(r)$$

$$-\frac{1}{2\ell+1}\sum_{n_0\ell_0}^{core}\sum_\nu (-1)^\nu\, (\ell||\, V^\nu(\chi_{n_0\ell_0}, f_{\ell_0}; r\,||\,\ell_0)\, \chi_{n_0\ell_0}(r),$$

where

$$(\ell||\, V^\nu(a, b; r\,||\,\ell') = (\ell||\, C^{[\nu]}\,||\,\ell')(\ell_a||\, C^{[\nu]}\,||\,\ell_b)$$

$$\int_0^\infty ds\, a(s)\, b(s) \frac{r_<^\nu}{r_>^{\nu+1}}$$

and $(\ell||\, C^{[\nu]}\,||\,\ell')$ is the reduced matrix element of the tensor operator C^ν for spherical harmonics given by

$$(\ell||\, C^{[\nu]}\,||\,\ell') = (-1)^\ell[(2\ell+1)(2\ell'+1)]^{1/2}\begin{pmatrix}\ell & \nu & \ell'\\ 0 & 0 & 0\end{pmatrix}.$$

Complex B-splines

- *Modified* complex radial function:

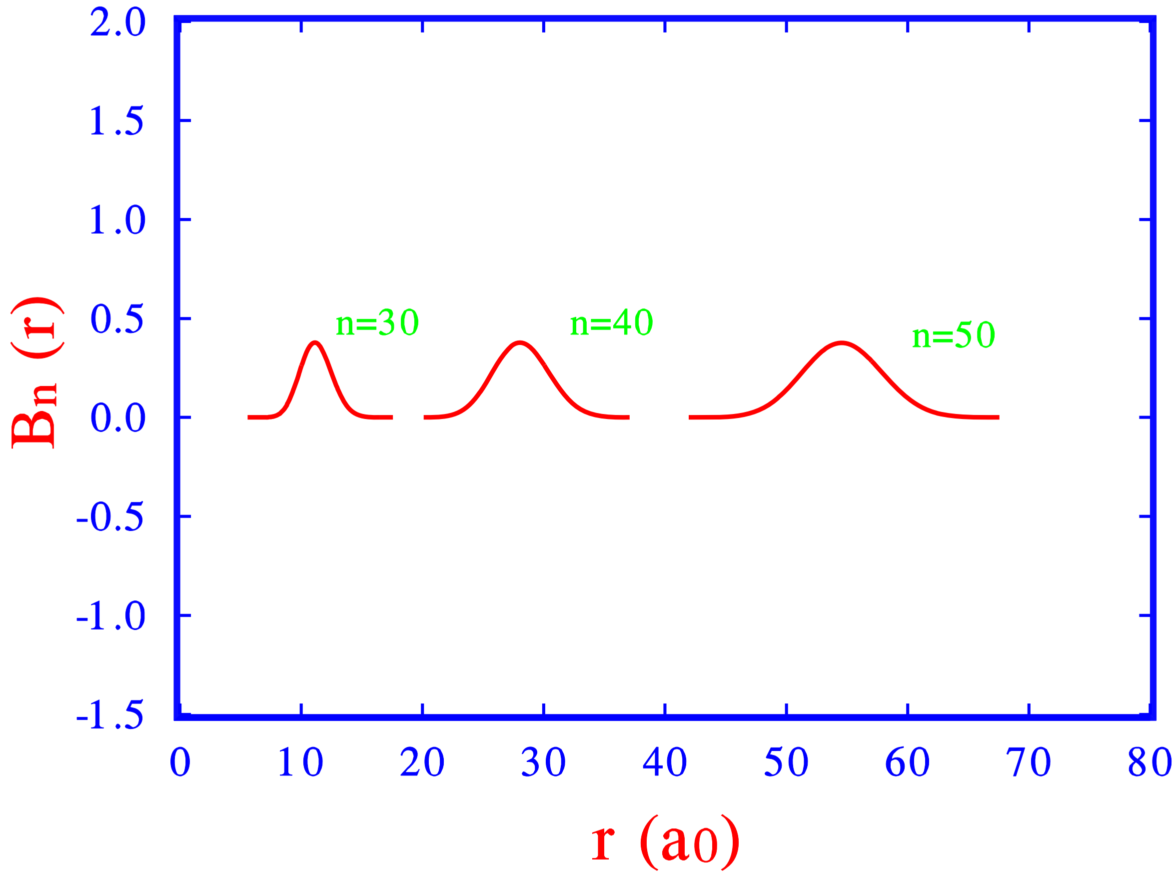
$$\tilde{\chi}_{\varepsilon\ell}(z) = \sum_{i=1}^{N} C_i \tilde{B}_i(z),$$

where $z = re^{-i\theta}$, $\tilde{B}_i = B_i(z)\, e^{-\beta z}$ and β is a variational parameter.

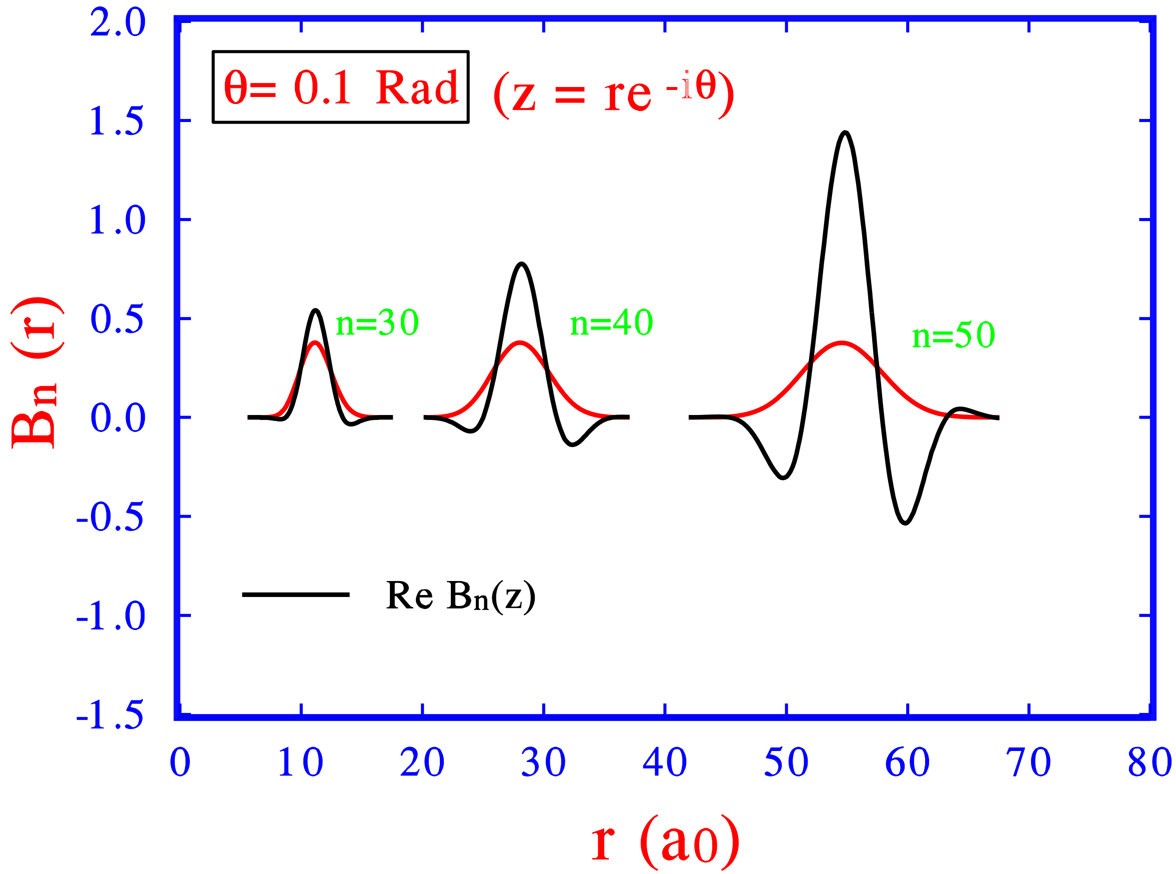
- Two-electron configuration:

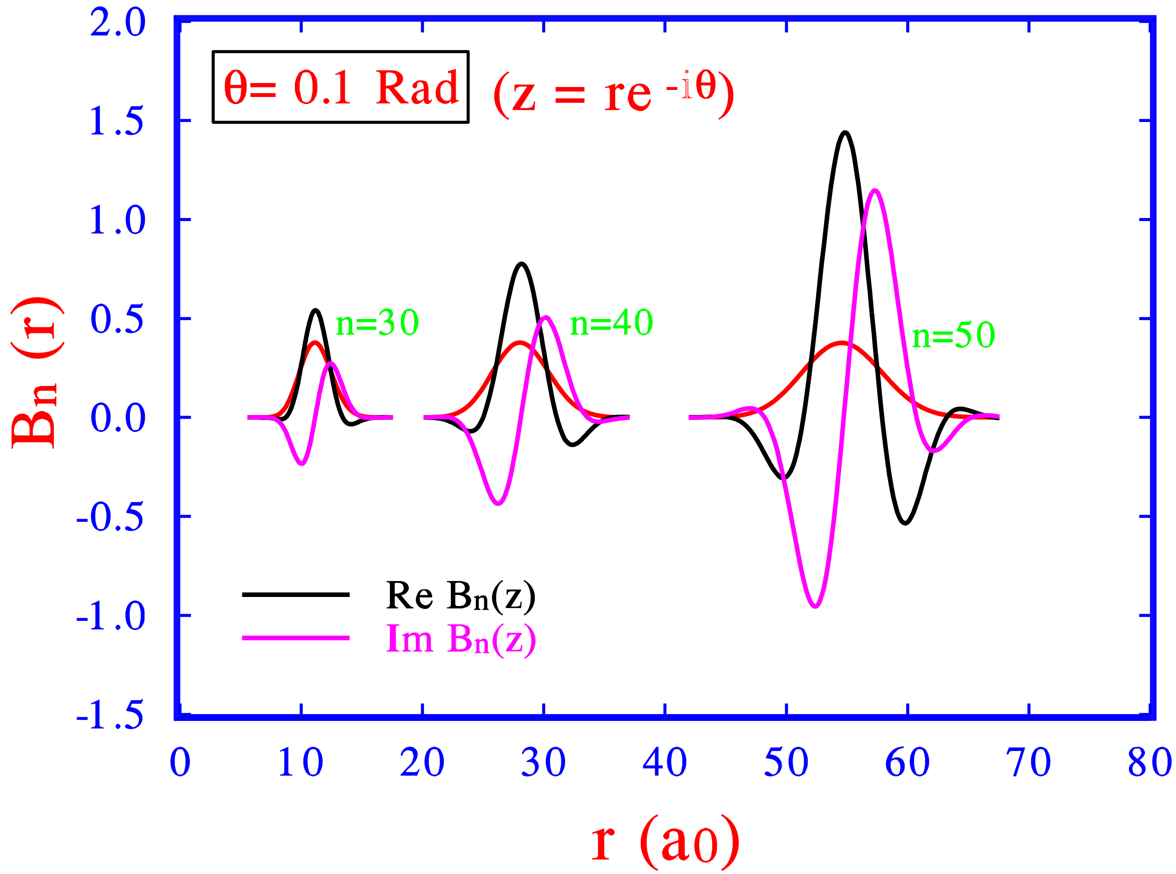
$|n_o\,\ell_o, \varepsilon_\nu\,\ell_\nu(\theta,\beta)\rangle$ – *complex* open channel

$|n_c\,\ell_c, n_\nu\,\ell_\nu\rangle$ – *real* closed channel



2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
0
10
20
30
40
50
60
70
80
n=30
n=40
n=50
Bn (r)
r (a0)


θ= 0.1 Rad
(z = re -iθ)
n=30
n=40
n=50
Re Bn(z)
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
0
10
20
30
40
50
60
70
80
Bn (r)
r (a0)



θ= 0.1 Rad
(z = re -iθ)
n=30
n=40
n=50
Re Bn(z)
Im Bn(z)
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
0
10
20
30
40
50
60
70
80
Bn (r)
r (a0)

Complex Zero-order Eigenstate

Nonrelativistic complex eigenvalue problem:

$$\langle \phi_\mu^{(0)}(\theta) | H_{nr} | \phi_\nu^{(0)}(\theta) \rangle = \delta_{\mu\nu} \, E_\mu^{(0)}(\theta),$$

where

$$\phi_\mu^{(0)}(\theta) = \sum_j C^{(closed)}_{n'_j\ell'_j n_j\ell_j} \, |n'_j\ell'_j, n_j\ell_j\rangle$$
$$+ \sum_k C^{(open)}_{n'_k\ell'_k\varepsilon_k\ell_k} |n'_k\ell'_k\varepsilon_k\ell_k(\theta, \beta_k)\rangle$$

is the *complex* zero-order eigenstate and

$$E_\mu^{(0)}(\theta) = E^{(0)}_{\mu,res} - i\Gamma_\mu^{(0)}/2$$

is the *complex* energy eigenvalue.

J. Phys. B: At. Mol. Opt. Phys. **34** (2001) 165–174

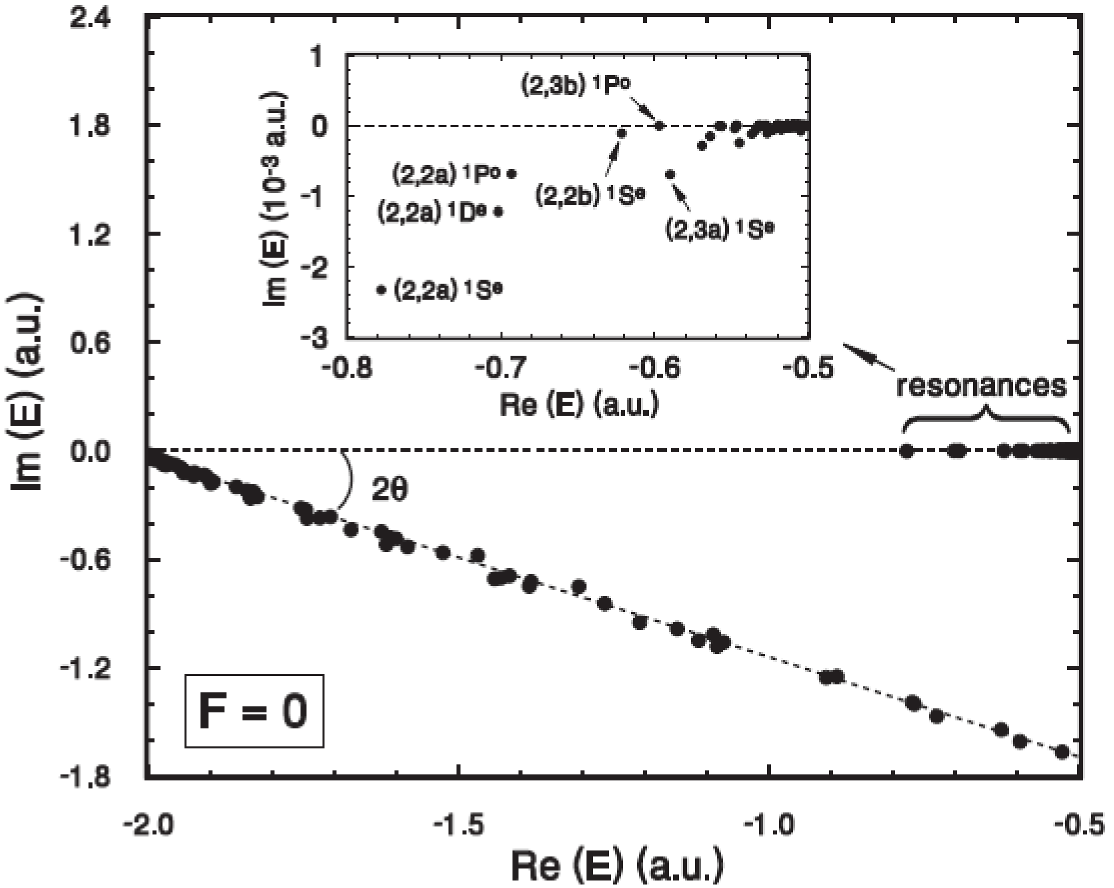


Figure 2. The energy spectrum from a saddle-point complex-rotation calculation in the field-free case. Seven angular symmetries and 892 terms are used in the wavefunction. Our calculated widths are very stable when the angle θ is varied from 0.3 to 0.6 rad.

Inner-projection Technique

$$\langle n_0\ell_0\,\varepsilon_\nu\ell_\nu(\theta,\beta)|H_{nr}|n_0'\ell_0'\,\varepsilon_\nu'\ell_\nu'(\theta,\beta')\rangle = \sum_{n_\nu,n_\nu'} O_{\varepsilon_\nu,n_\nu} \langle n_0\ell_0\,n_\nu\ell_\nu|H_{nr}|n_0'\ell_0'\,n_\nu'\ell_\nu'\rangle\,O^t_{n_\nu',\varepsilon_\nu'},$$

where the overlap integral

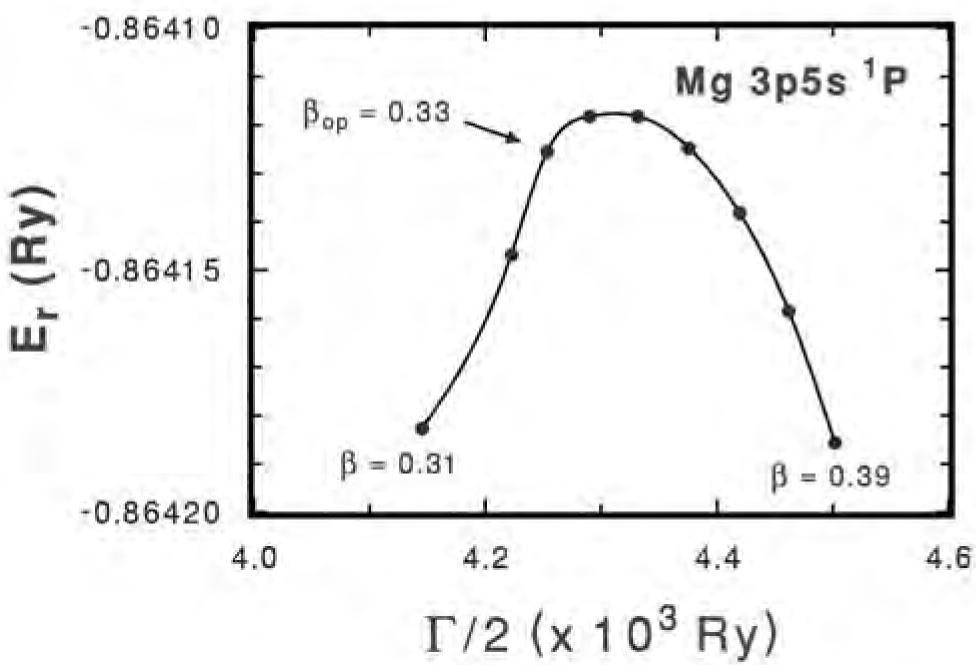
$$O_{\varepsilon_\nu,n_\nu} = \langle n_0\ell_0\,\varepsilon_\nu\ell_\nu(\theta,\beta)|n_0\ell_0\,n_\nu\ell_\nu\rangle$$

and $O^t_{n_\nu',\varepsilon_\nu'}$ is its corresponding transpose

$$O^t_{n_\nu',\varepsilon_\nu'} = \langle n_0'\ell_0'\,n_\nu'\ell_\nu'|n_0'\ell_0'\,\varepsilon_\nu'\ell_\nu'(\theta,\beta')\rangle.$$

Stabilization Condition

$$\left(\frac{\partial\,|E_\mu^{(0)}(\theta)|}{\partial\beta}\right) = 0$$



Hamiltonian Matrix

- **Total Hamiltonian:**

$$H = H_{nr} + H_{so},$$

where H_{so} is the spin-orbit interaction.

- **Complex eigenvalue problem:**

$$\langle \Psi_\mu(\theta) | H | \Psi_\nu(\theta) \rangle = \delta_{\mu\nu} E_\mu(\theta),$$

where

$$\Psi_\mu(\theta) = \sum_\nu C_\nu^{(\mu)} \phi_\nu^{(0)}(\theta)$$

is the *complex* eigenstate and

$$E_\mu(\theta) = E_{res}^\mu - i\Gamma_\mu/2$$

is the *complex* energy eigenvalue.

Photoionization Cross Section

$$\sigma(E) = \sum_{\nu} \sigma_{\nu}(E)$$

where

$$\sigma_{\nu}(E) = 4\pi\alpha\,\Delta E^{\gamma}\,Im\,\frac{\langle\Phi_0|D|\Psi_{\nu}(\theta)\rangle^2}{E_{\nu}(\theta) - E},$$

$\Delta E = E - E_0$: transition energy

dipole-length: $D = \hat{\epsilon} \cdot (\vec{r}_1 + \vec{r}_2)$ and $\gamma = 1$

dipole-velocity: $D = \hat{\epsilon} \cdot (\vec{\nabla}_1 + \vec{\nabla}_2)$ and $\gamma = -1$

Parametrized Photoionization Cross Section

- **Complex dipole matrix:**

$$\langle \Phi_0 | D | \Psi_\nu(\theta) \rangle = B_\nu + iC_\nu$$

- **Fano profile:**

$$\sigma(E) = \sigma_0(E) + \sum_\nu \sigma_\nu,$$

where $\sigma_0(E)$ is the background cross section, and

$$\sigma_\nu(E) = \sigma_b^\nu \left[\frac{(q_\nu + \varepsilon_\nu)^2}{1 + \varepsilon_\nu^2} - 1 \right],$$

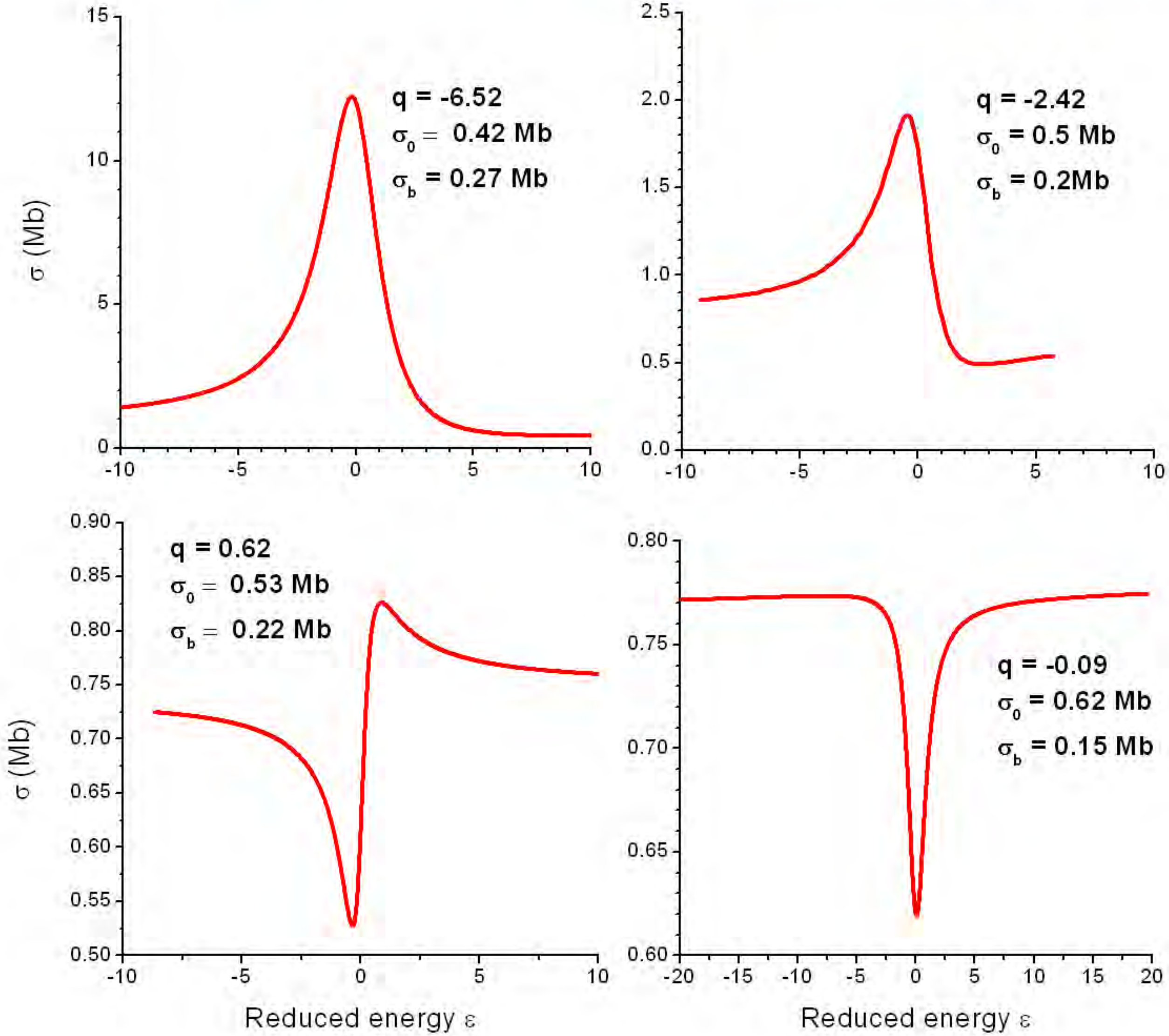
where

$\varepsilon_\nu = (E - E_{res}^\nu)/\frac{1}{2}\Gamma_\nu$: reduced energy,

$q_\nu = -B_\nu/C_\nu$: Fano q-parameter,

$\sigma_b^\nu = 8\pi\alpha\Delta E^\gamma C_\nu^2/\Gamma_\nu$: background.

Fano profiles: $\sigma(\varepsilon) = \sigma_0 + \sigma_b(q+\varepsilon)^2/(1+\varepsilon^2)$



Convolution

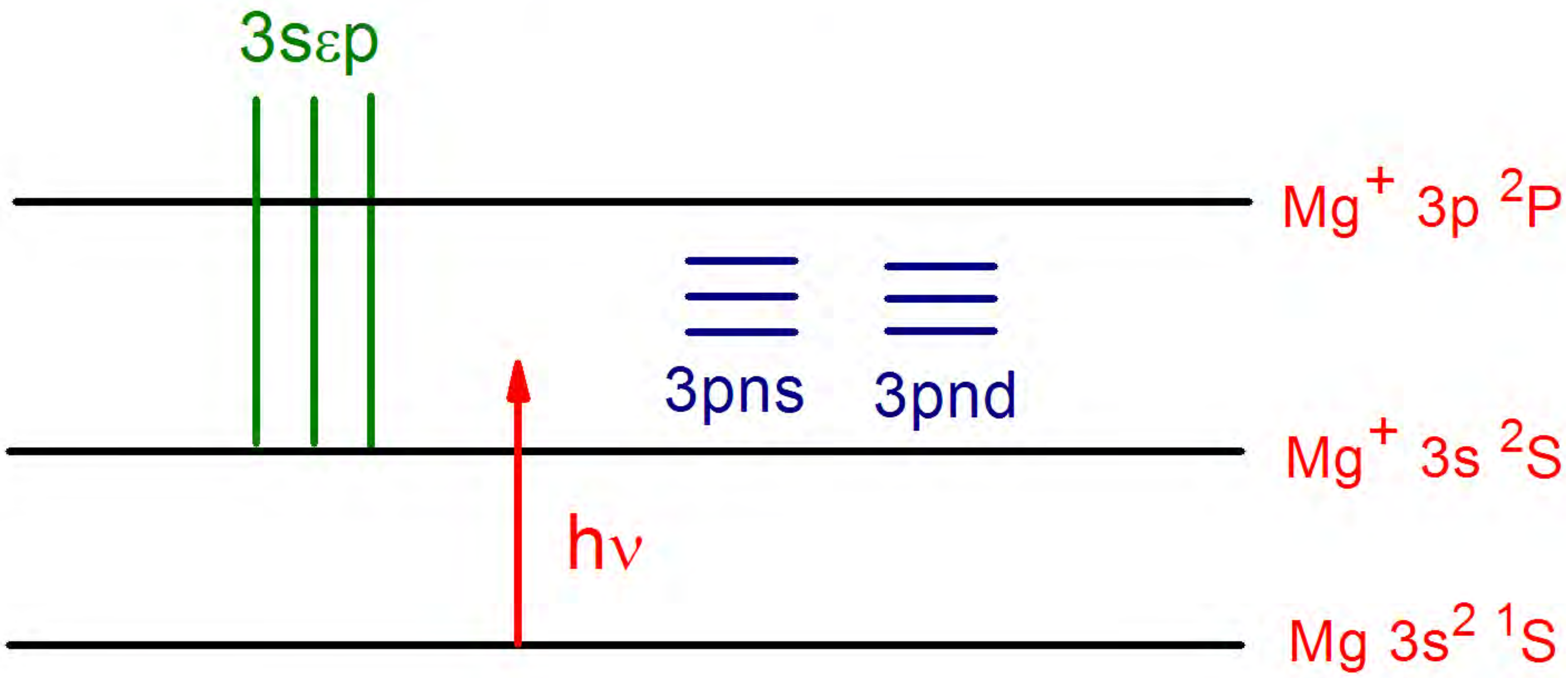
$$\sigma_c(E) = \int_{-\infty}^{+\infty} \sigma(E')\, g(E'-E\,;\Omega)\, dE'$$

where g is a normalized Gaussian

$$g(E\,;\Omega) = e^{-E^2/\Delta^2} / (\pi\,\Delta^2)^{1/2}, \quad \Delta = \Omega / [2\,(ln\,2)^{1/2}]$$

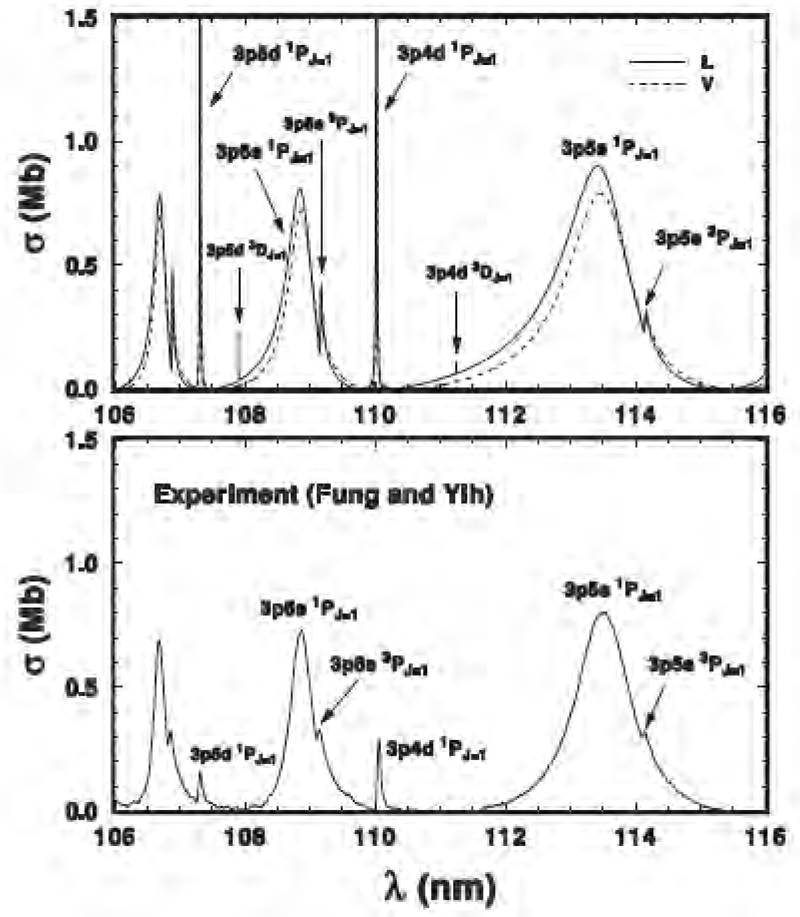
The energy resolution Ω is given by the full width at half maximum (FWHM) of the distribution function.

Mg doubly excited $^{1,3}L^{o}_{J=1}$ resonances



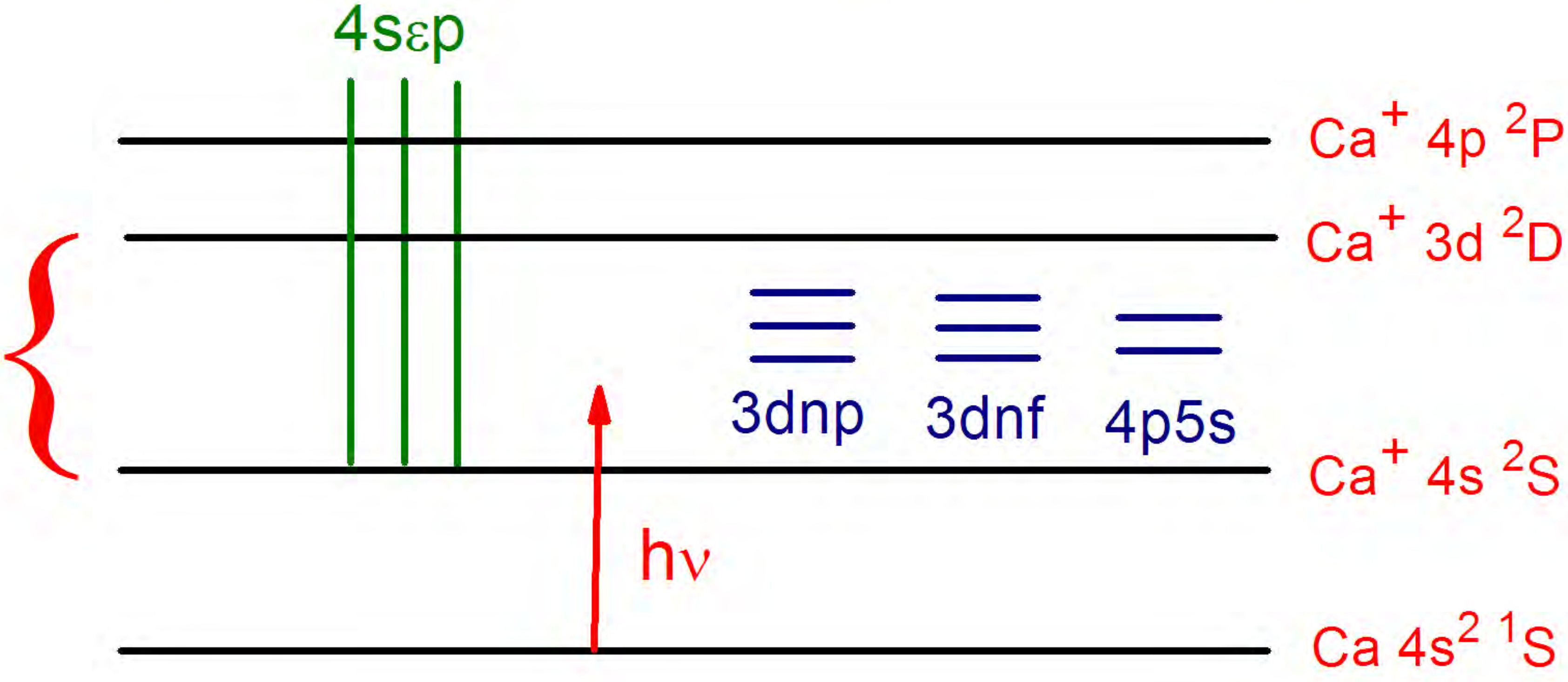
Open chs: $3s\varepsilon p\ ^{1,3}P$

Closed chs: $3pns\ ^{1,3}P$, $3pnd\ ^{1,3}P$ & ^{3}D



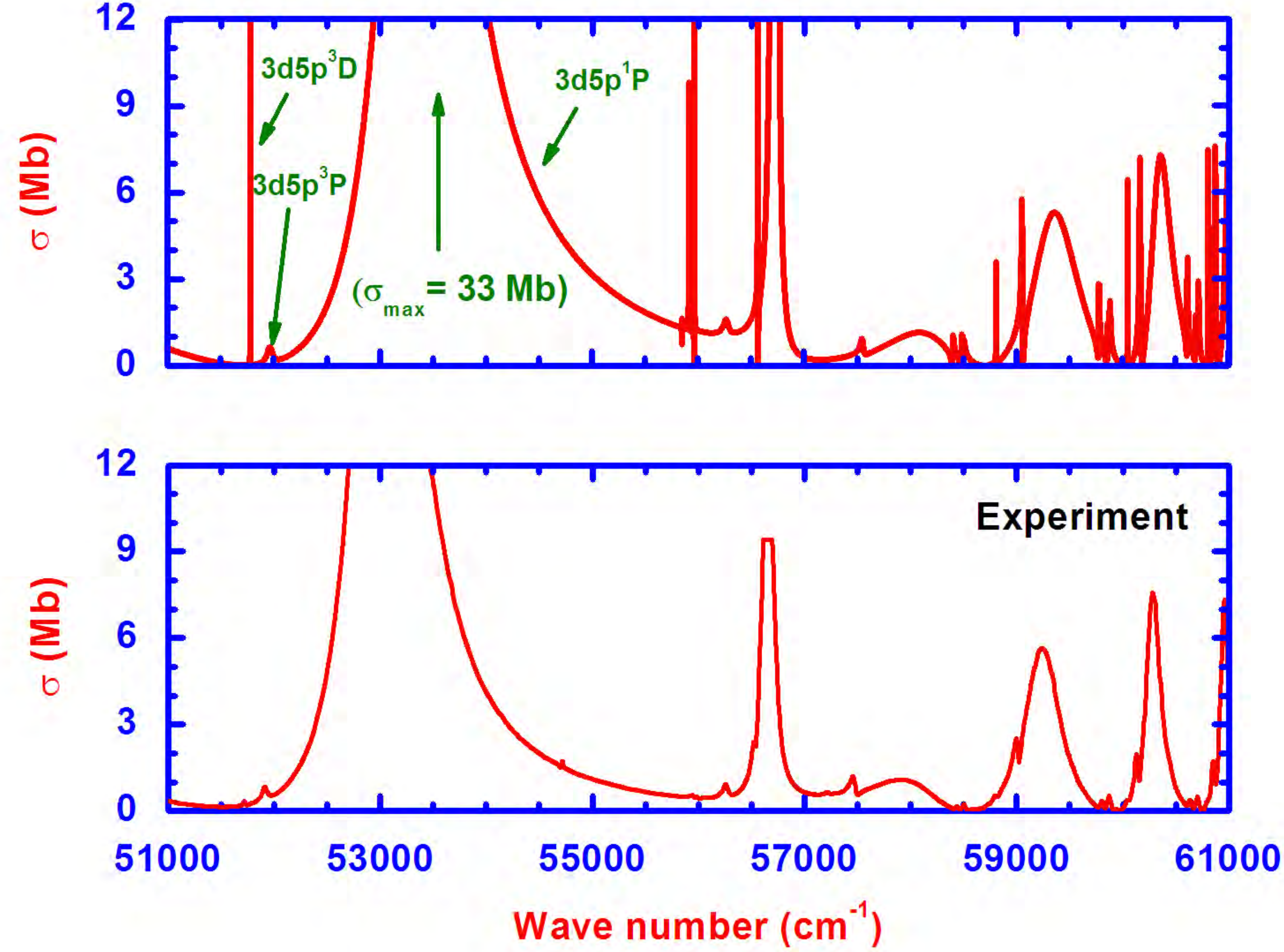
Experiment (Fung and Yih)
σ (Mb)
λ (nm)
L
V

Ca doubly excited $^{1,3}L^{o}_{J=1}$ resonances

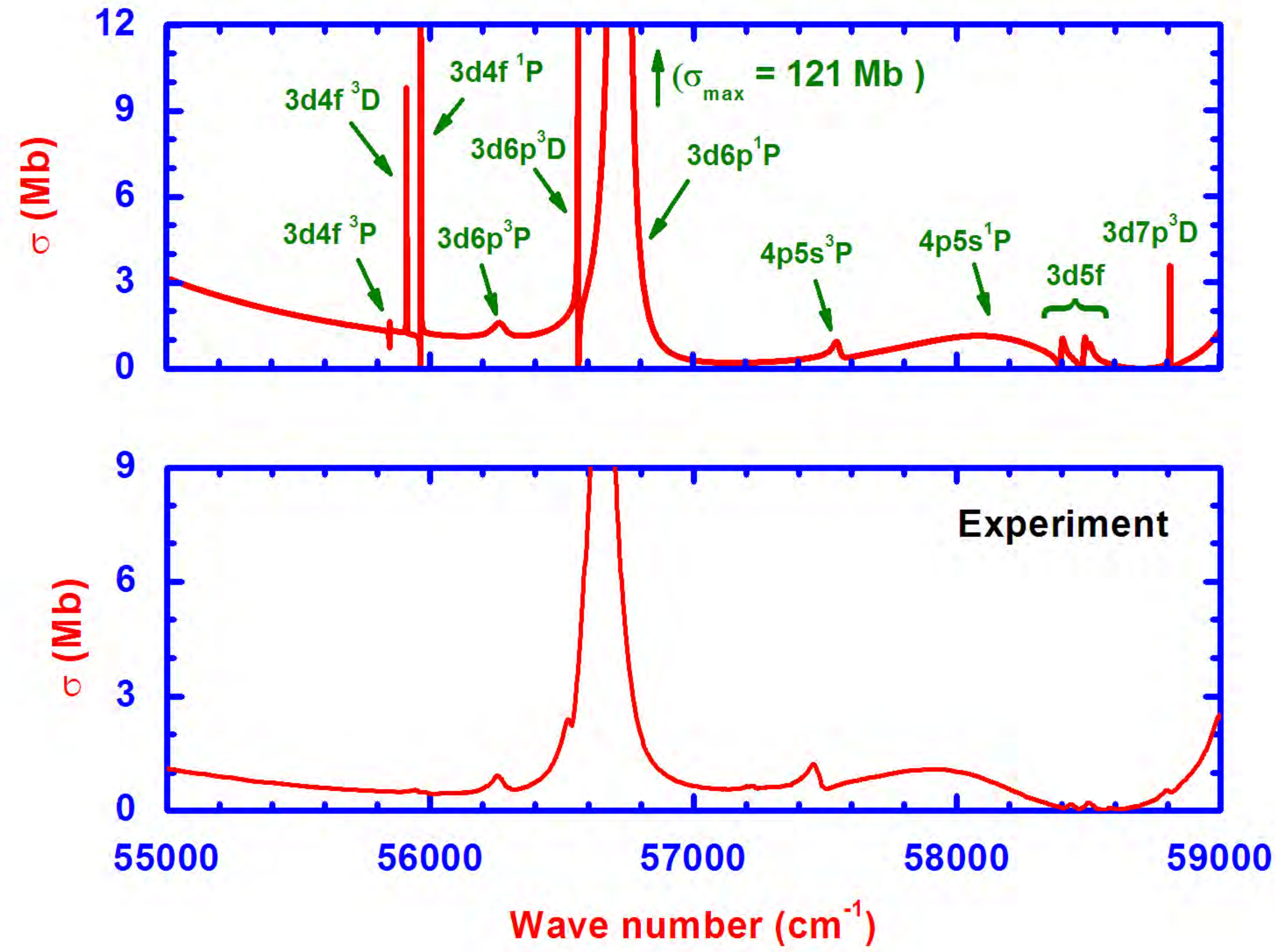


Open chs (2): 4sεp $^{1,3}P$

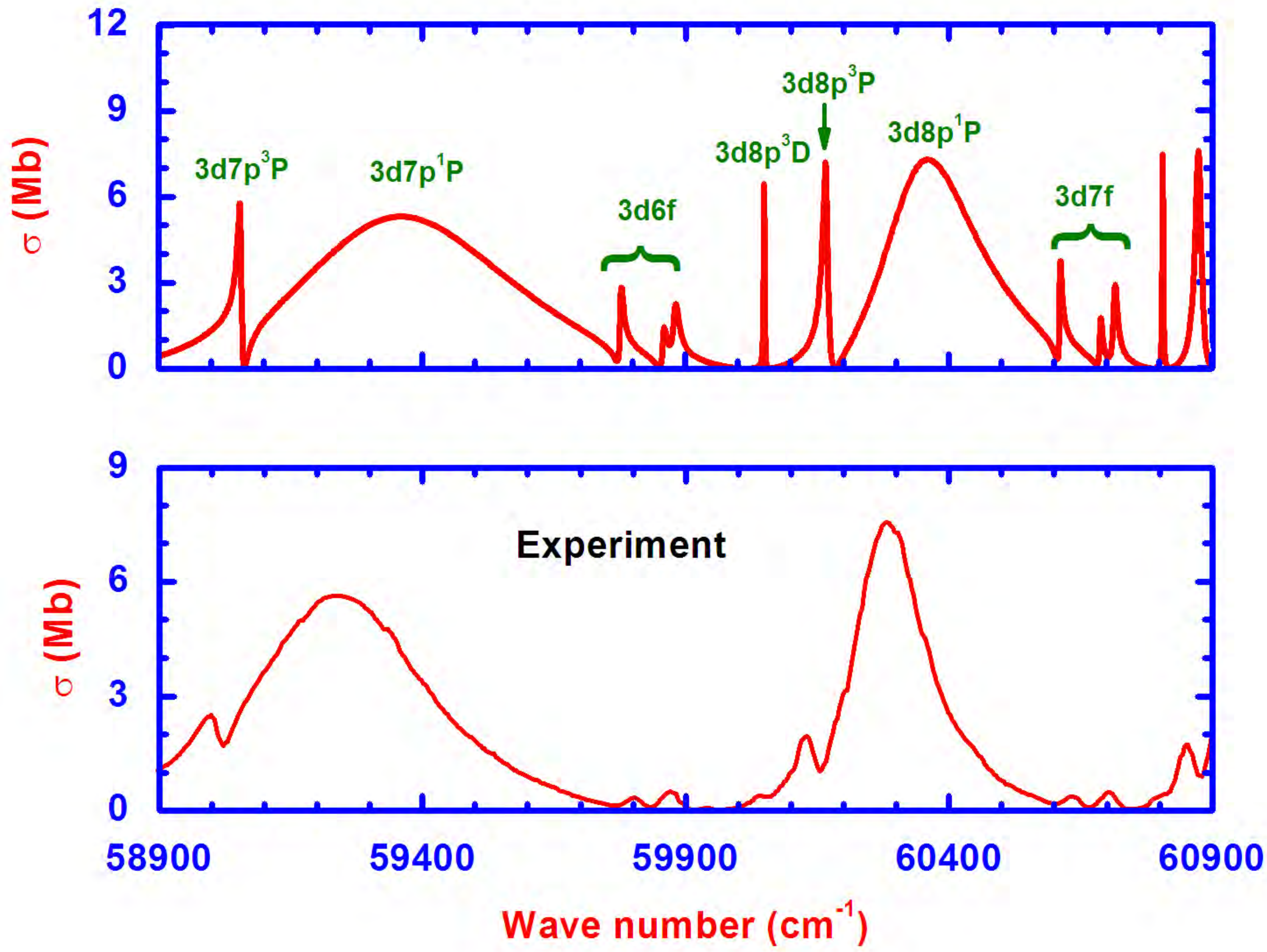
Closed chs (8): 4p5s $^{1,3}P$, 3dnp $^{1,3}P$ & ^{3}D, 3dnf $^{1,3}P$ & ^{3}D



3d5p^{3}D
3d5p^{3}P
3d5p^{1}P
(σ_{max} = 33 Mb)
Experiment
σ (Mb)
σ (Mb)
0
3
6
9
12
51000
53000
55000
57000
59000
61000
Wave number (cm^{-1})

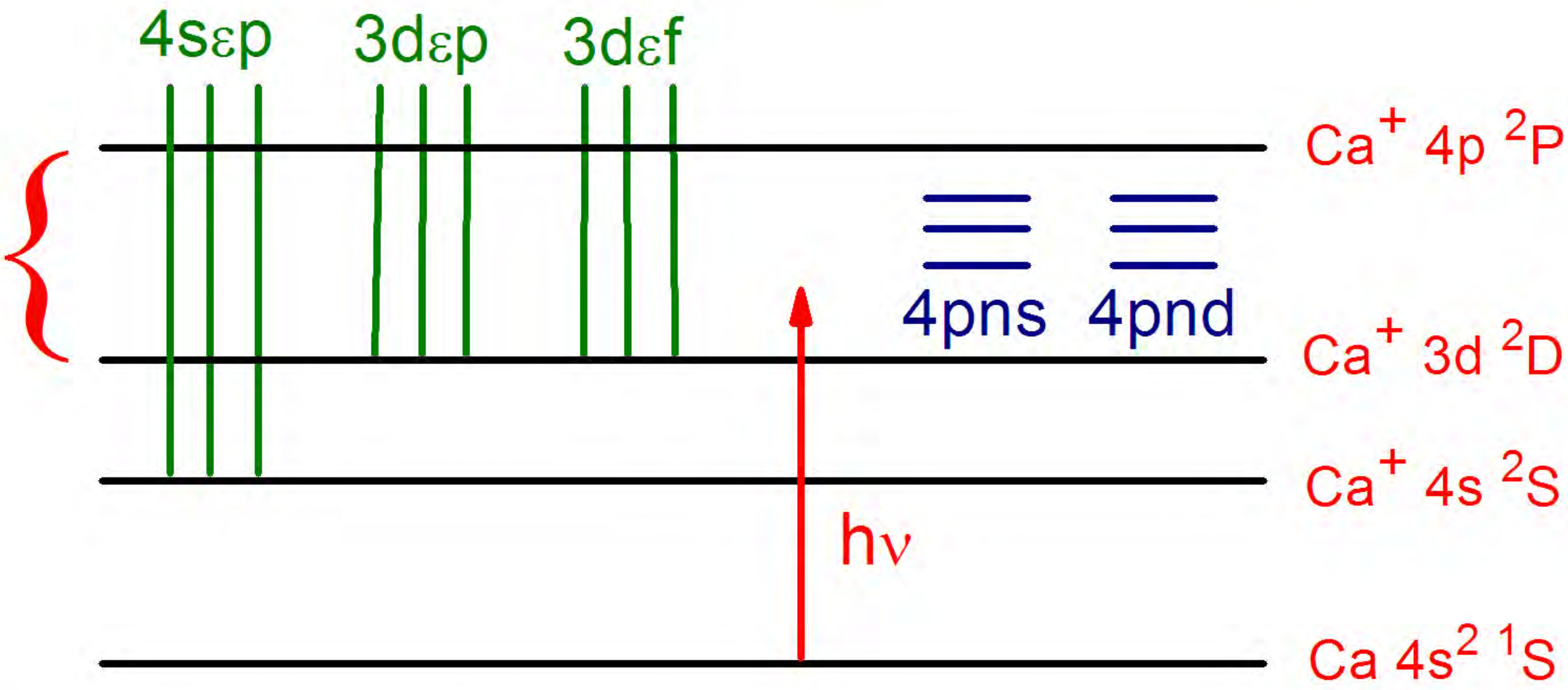


3d4f 3D
3d4f 1P
3d6p3D
3d6p1P
(σmax = 121 Mb)
3d4f 3P
3d6p3P
4p5s3P
4p5s1P
3d5f
3d7p3D
Experiment
σ (Mb)
Wave number (cm-1)



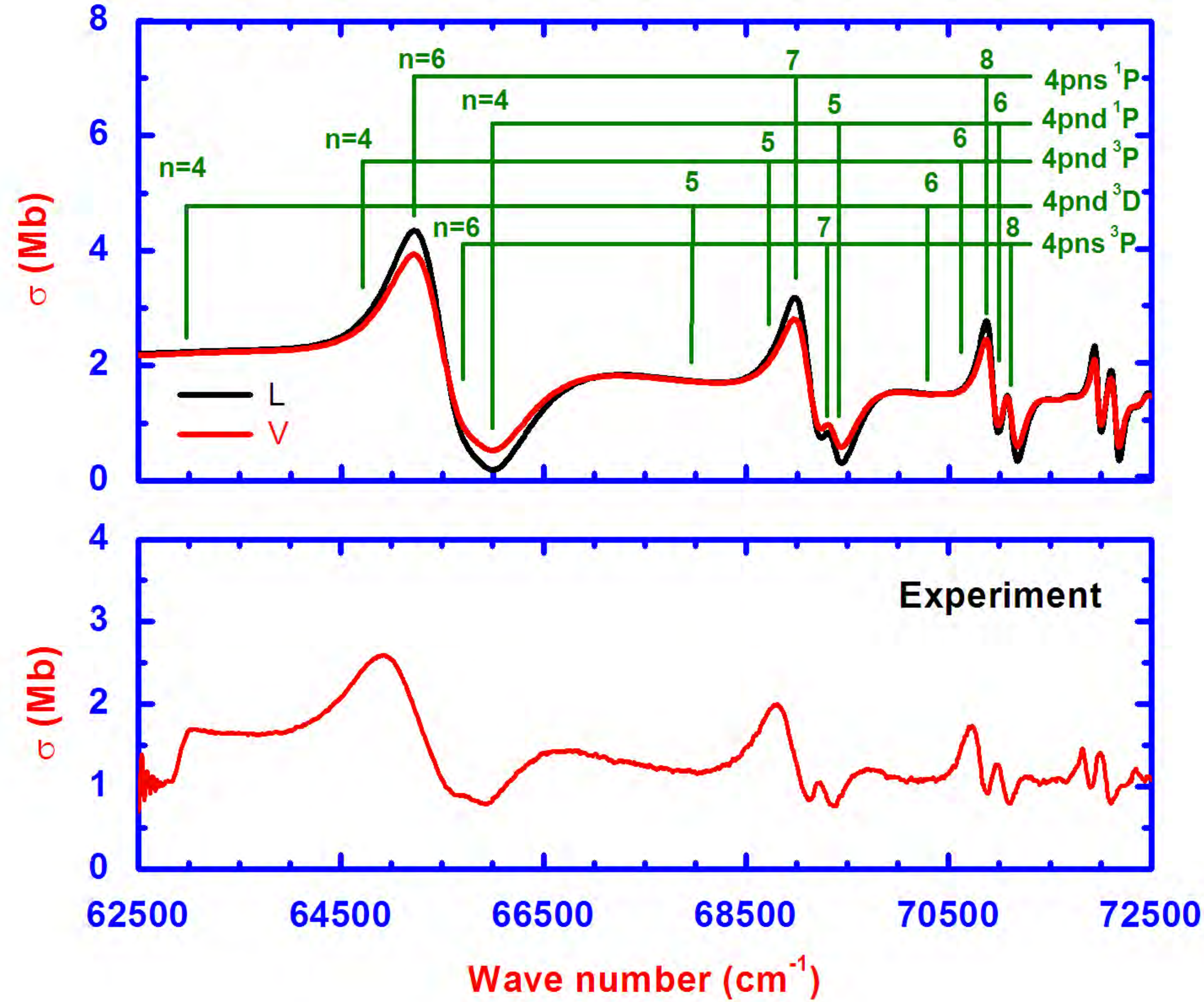
12
9
6
3
0
σ (Mb)
3d7p3P
3d7p1P
3d6f
3d8p3D
3d8p3P
3d8p1P
3d7f
9
6
3
0
σ (Mb)
Experiment
58900
59400
59900
60400
60900
Wave number (cm-1)

Ca doubly excited $^{1,3}L^{o}_{J=1}$ resonances



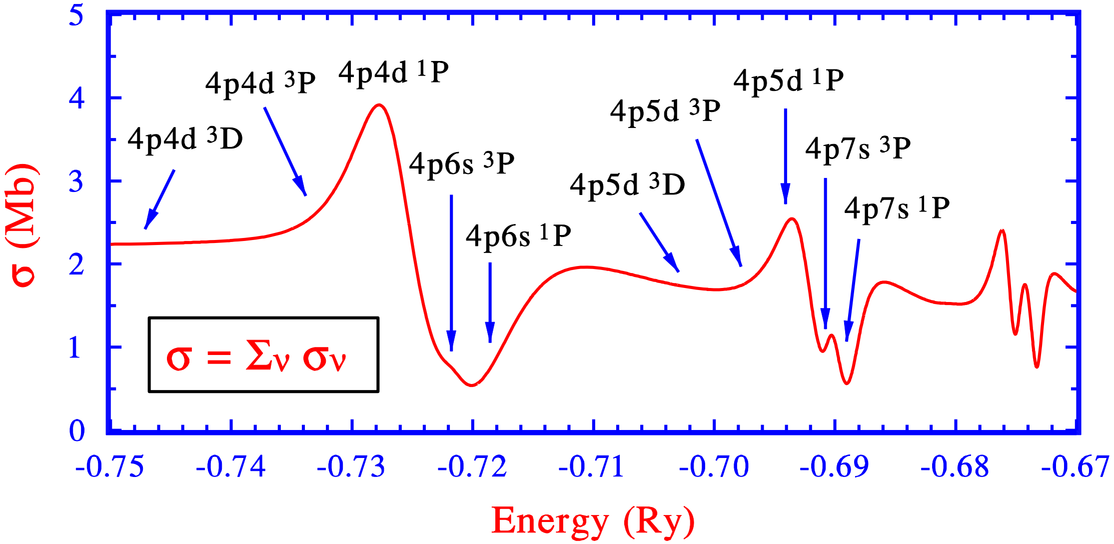
Open chs (8): 4sεp $^{1,3}P$, 3dεp $^{1,3}P$ & ^{3}D, 3dεf $^{1,3}P$ & ^{3}D

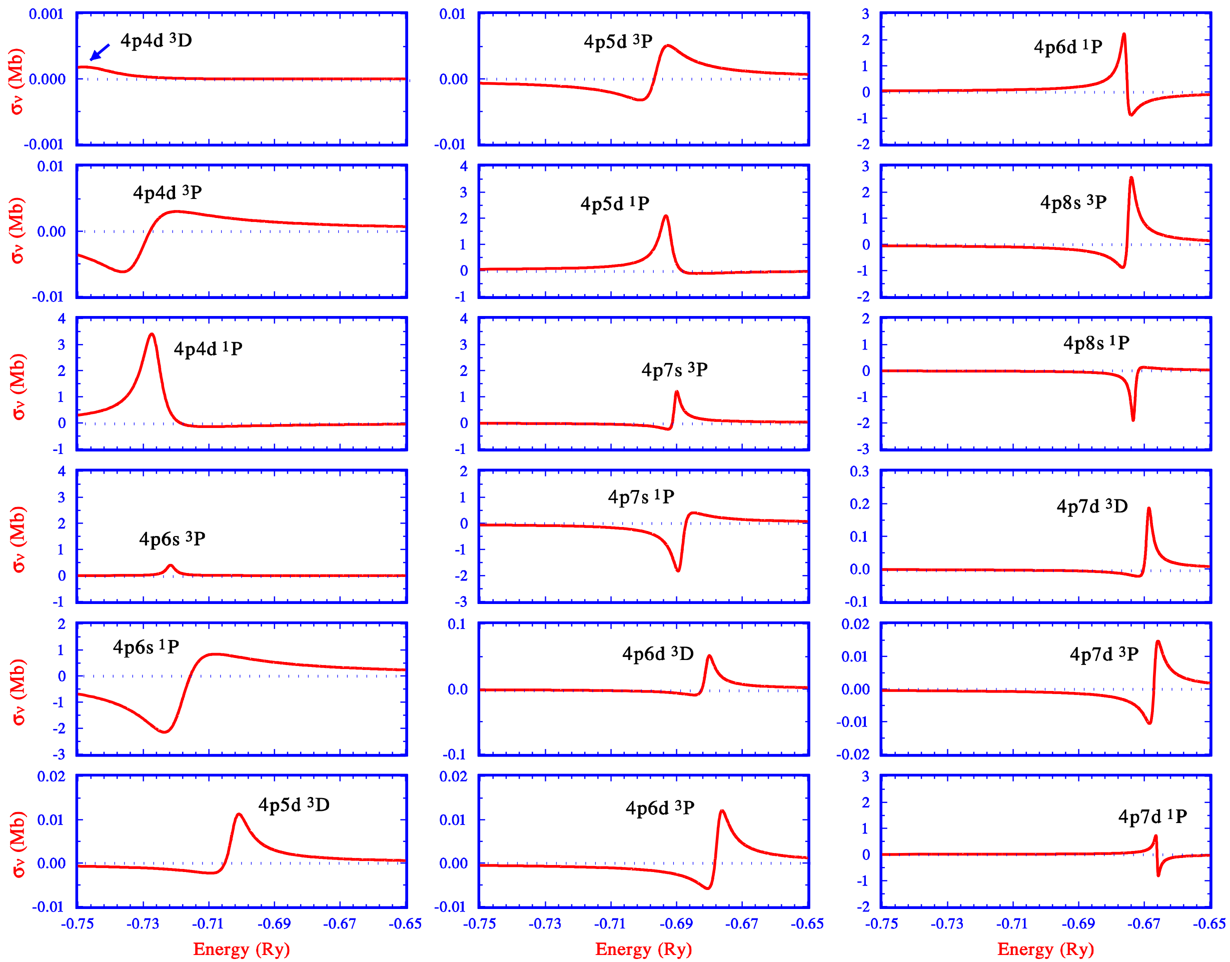
Closed chs (5): 4pns $^{1,3}P$, 4pnd $^{1,3}P$ & ^{3}D



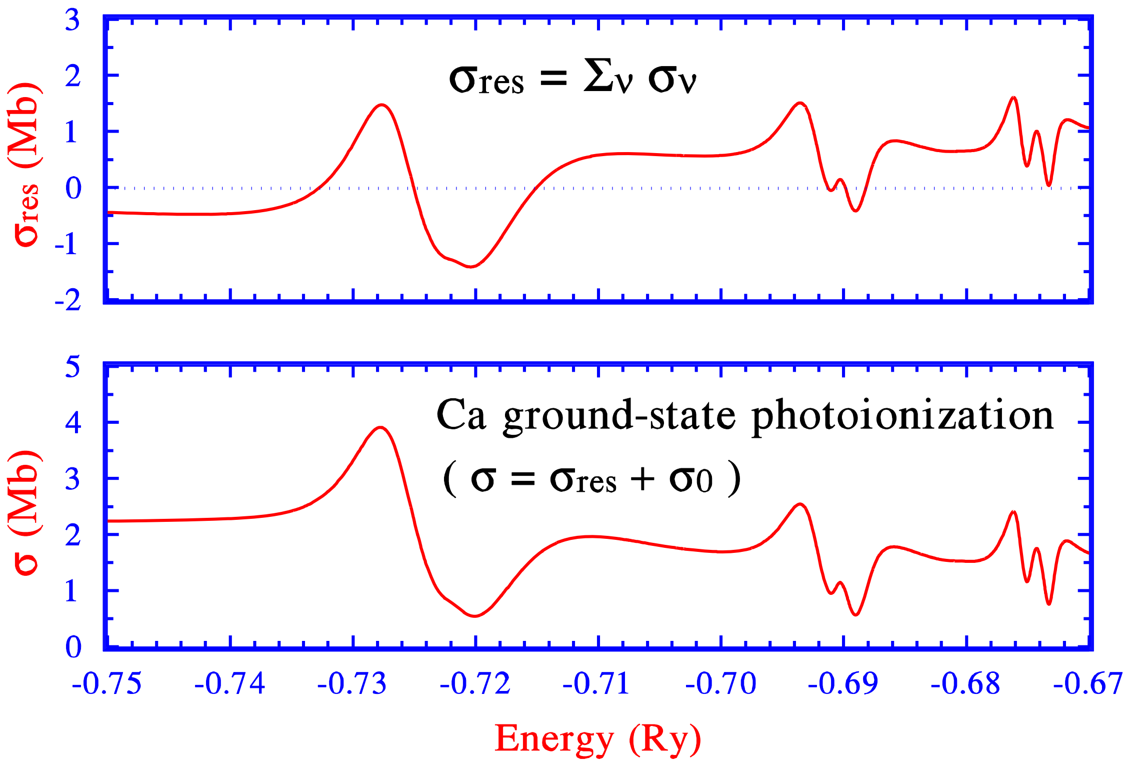
8
6
4
2
0
σ (Mb)
n=4
n=4
n=6
n=4
n=6
7
8
5
6
5
6
5
6
7
8
4pns ¹P
4pnd ¹P
4pnd ³P
4pnd ³D
4pns ³P
L
V
4
3
2
1
0
σ (Mb)
Experiment
62500
64500
66500
68500
70500
72500
Wave number (cm⁻¹)

Ca ground-state photoionization



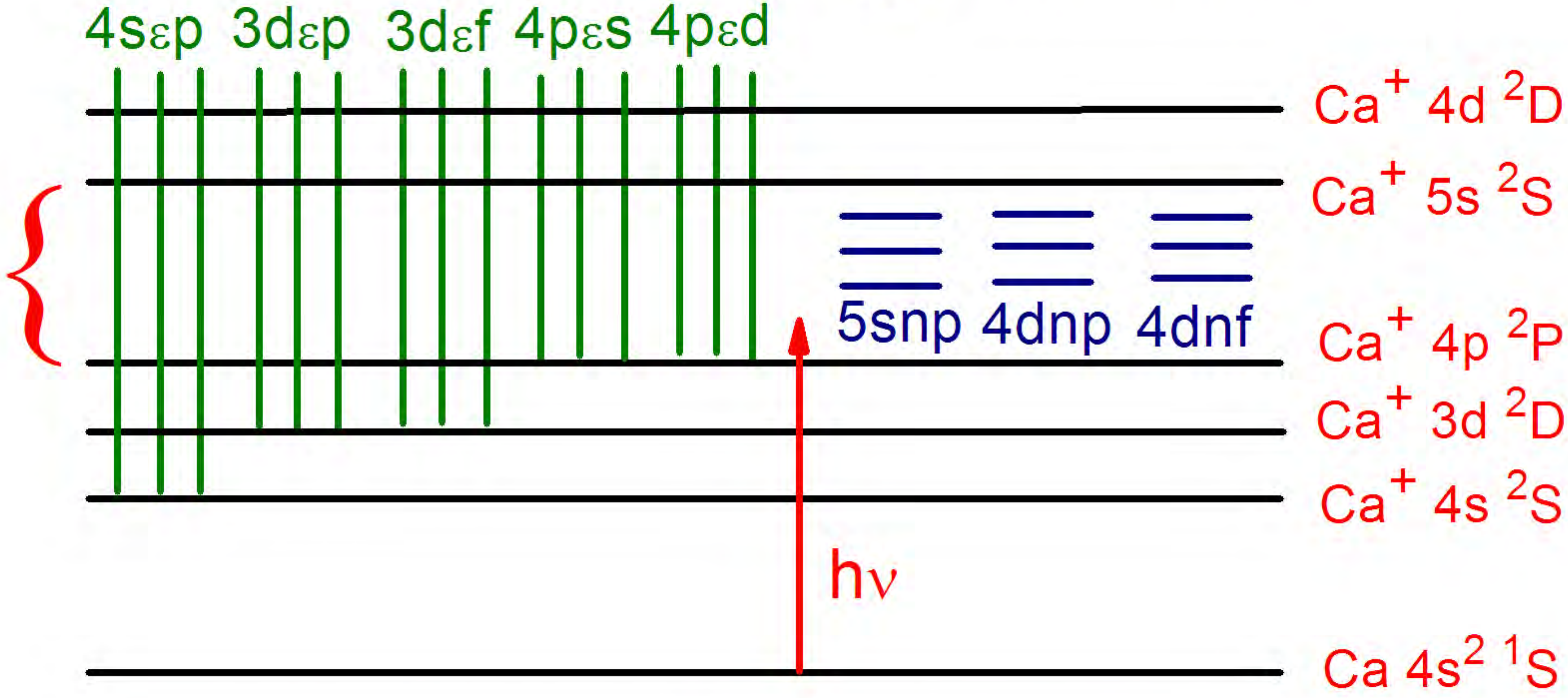


4p4d ³D
4p5d ³P
4p6d ¹P
4p4d ³P
4p5d ¹P
4p8s ³P
4p4d ¹P
4p7s ³P
4p8s ¹P
4p6s ³P
4p7s ¹P
4p7d ³D
4p6s ¹P
4p6d ³D
4p7d ³P
4p5d ³D
4p6d ³P
4p7d ¹P
σv (Mb)
Energy (Ry)
-0.75
-0.73
-0.71
-0.69
-0.67
-0.65



σres = Σν σν
σres (Mb)
Ca ground-state photoionization
(σ = σres + σ0)
σ (Mb)
Energy (Ry)

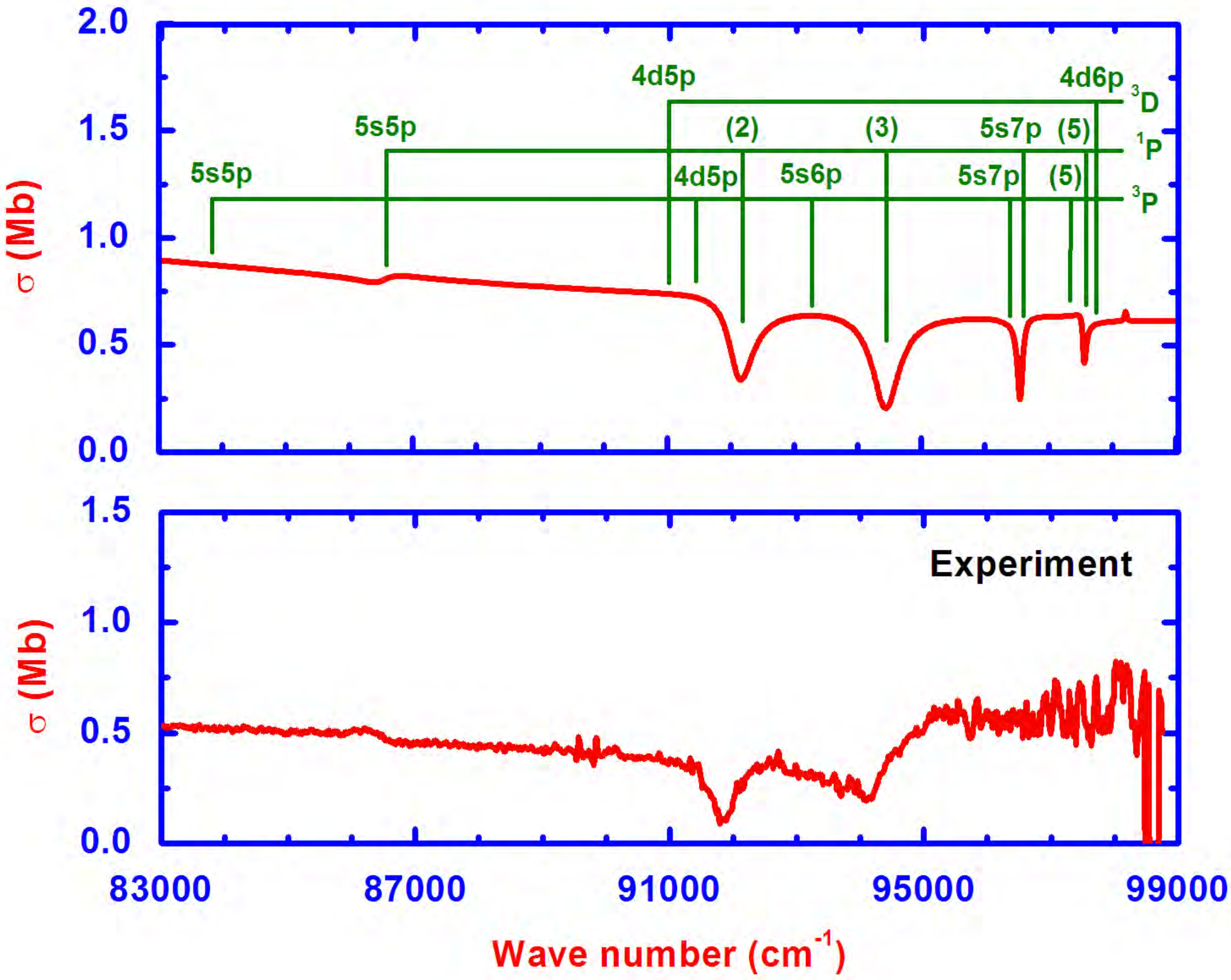
Ca doubly excited $^{1,3}L^{o}_{J=1}$ resonances



Open chs (13): 4sεp ^{1,3}P, 3dεp ^{1,3}P & ^{3}D, 3dεf ^{1,3}P & ^{3}D

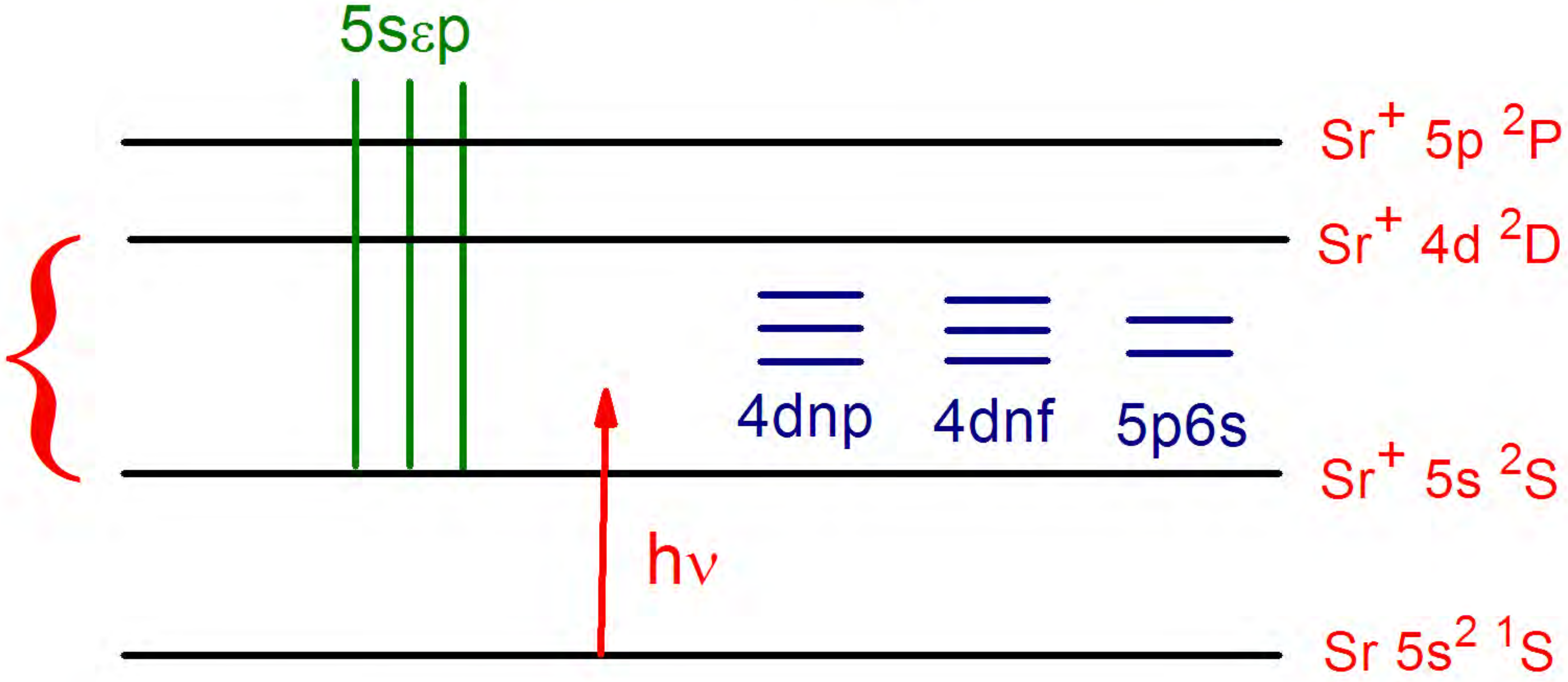
4pεs ^{1,3}P, 4pεd ^{1,3}P & ^{3}D,

Closed chs (8): 5snp ^{1,3}P, 4dnp ^{1,3}P & ^{3}D, 4dnf ^{1,3}P & ^{3}D



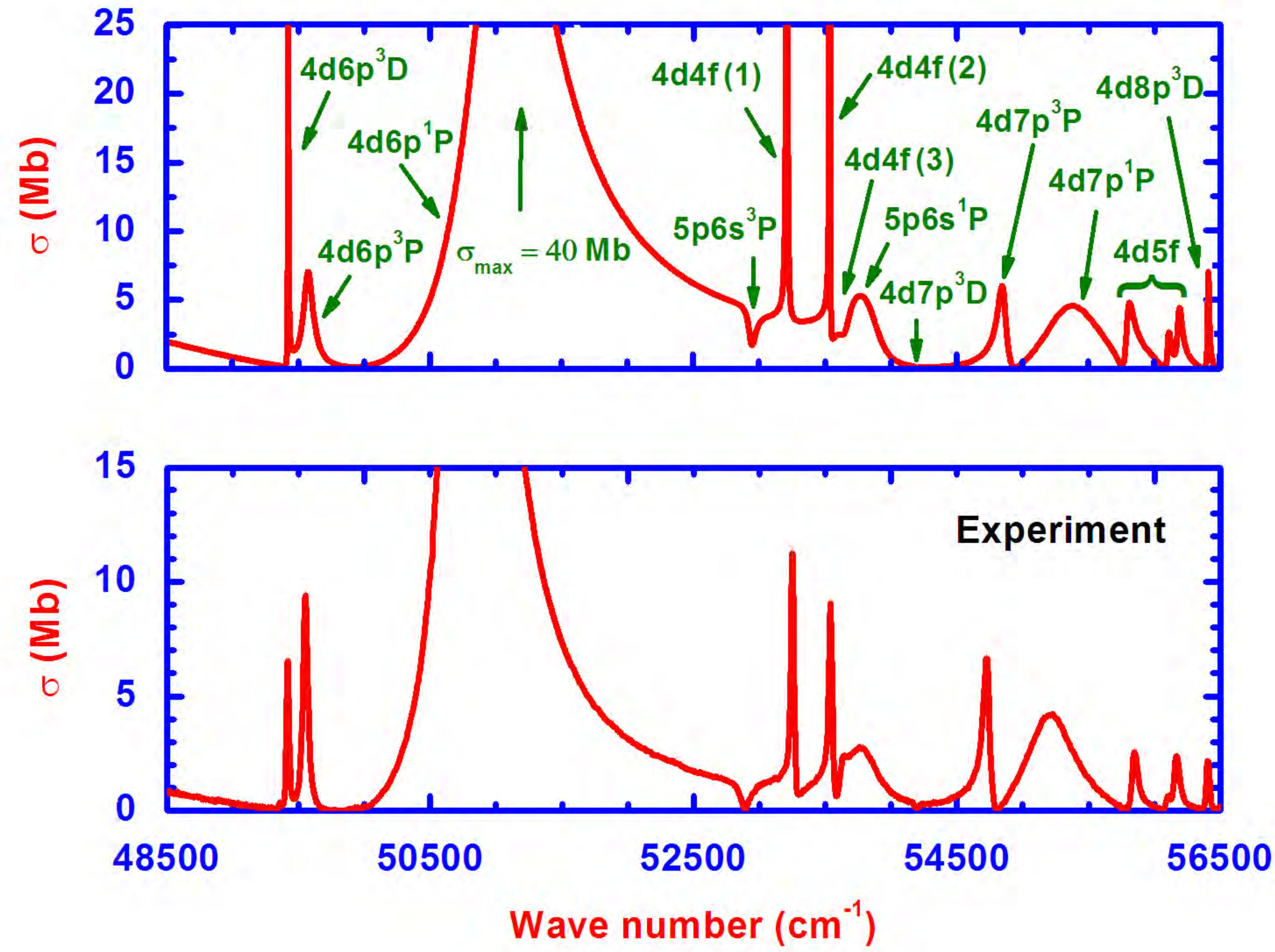
2.0
1.5
1.0
0.5
0.0
σ (Mb)
4d5p
5s5p
5s5p
(2)
(3)
5s7p
(5)
4d6p
³D
¹P
4d5p
5s6p
5s7p
(5)
³P
1.5
1.0
0.5
0.0
σ (Mb)
Experiment
83000
87000
91000
95000
99000
Wave number (cm⁻¹)

Sr doubly excited $^{1,3}L^{o}_{J=1}$ resonances

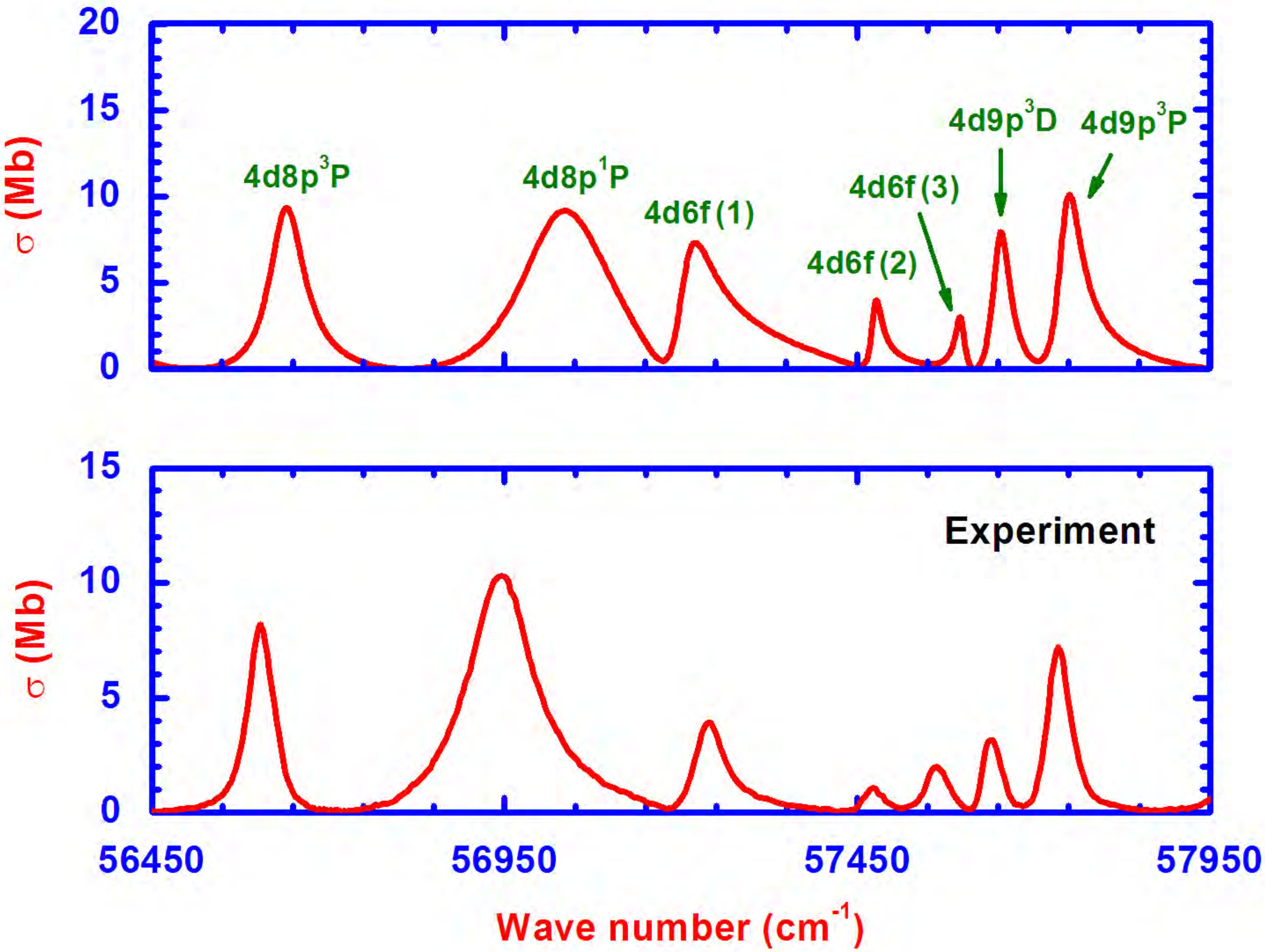


Open chs (2): 5sεp $^{1,3}P$

Closed chs (8): 5p6s $^{1,3}P$, 4dnp $^{1,3}P$ & ^{3}D, 4dnf $^{1,3}P$ & ^{3}D

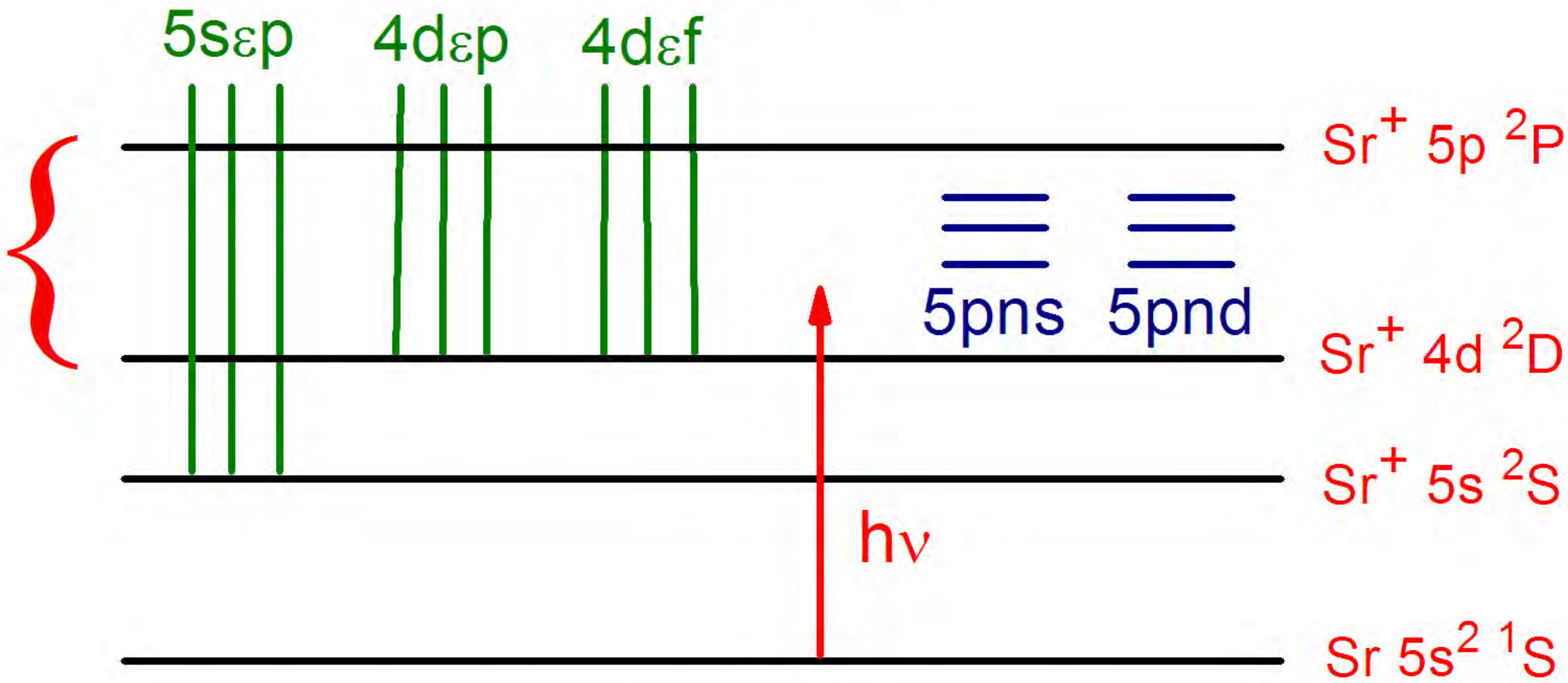


4d6p³D
4d6p¹P
4d6p³P
σmax = 40 Mb
4d4f (1)
4d4f (2)
4d4f (3)
5p6s³P
5p6s¹P
4d7p³D
4d7p³P
4d7p¹P
4d8p³D
4d5f
σ (Mb)
Experiment
Wave number (cm⁻¹)
48500
50500
52500
54500
56500



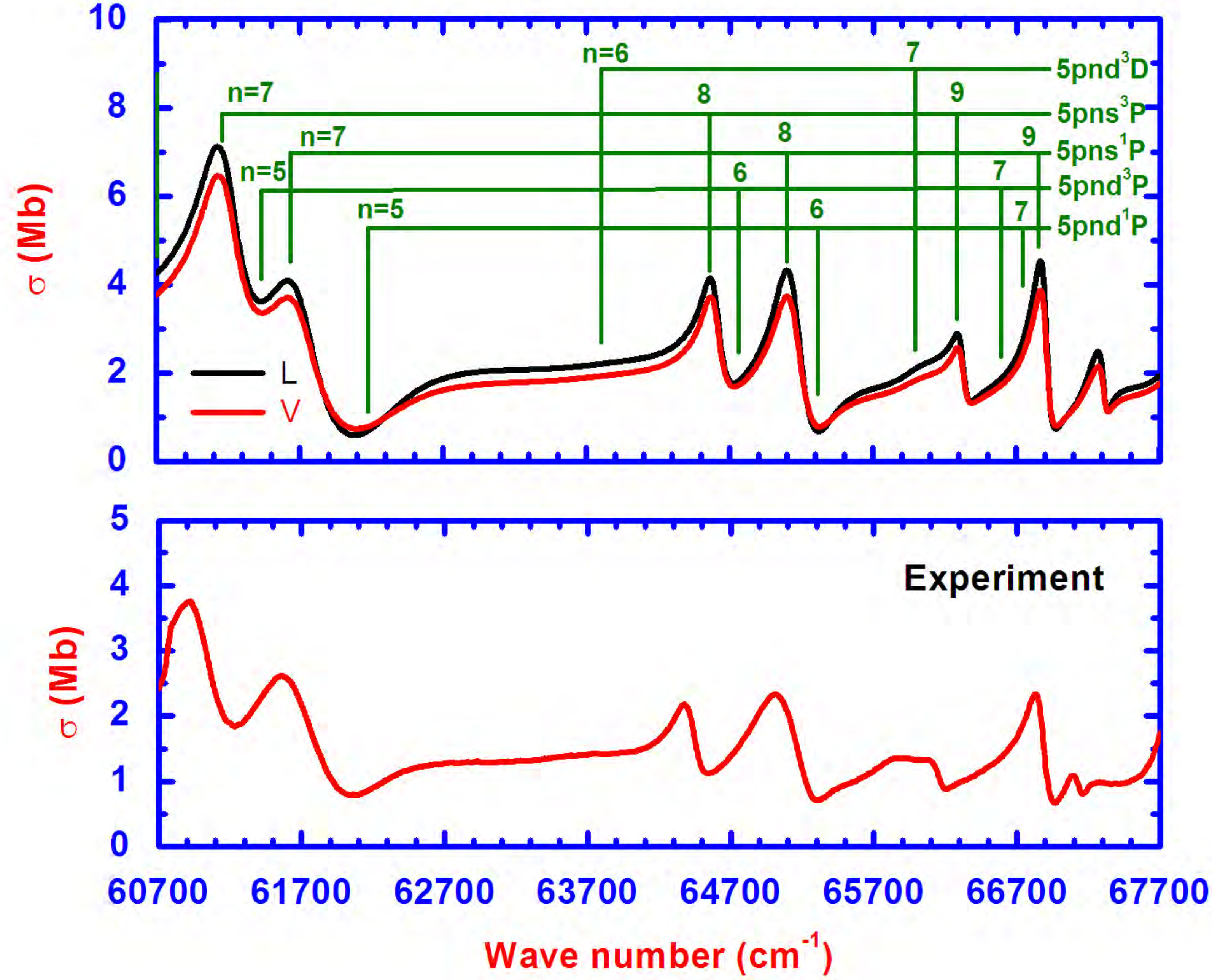
20
15
10
5
0
σ (Mb)
4d8p3P
4d8p1P
4d6f (1)
4d6f (2)
4d6f (3)
4d9p3D
4d9p3P
15
10
5
0
σ (Mb)
Experiment
56450
56950
57450
57950
Wave number (cm-1)

Sr doubly excited $^{1,3}L^{o}_{J=1}$ resonances

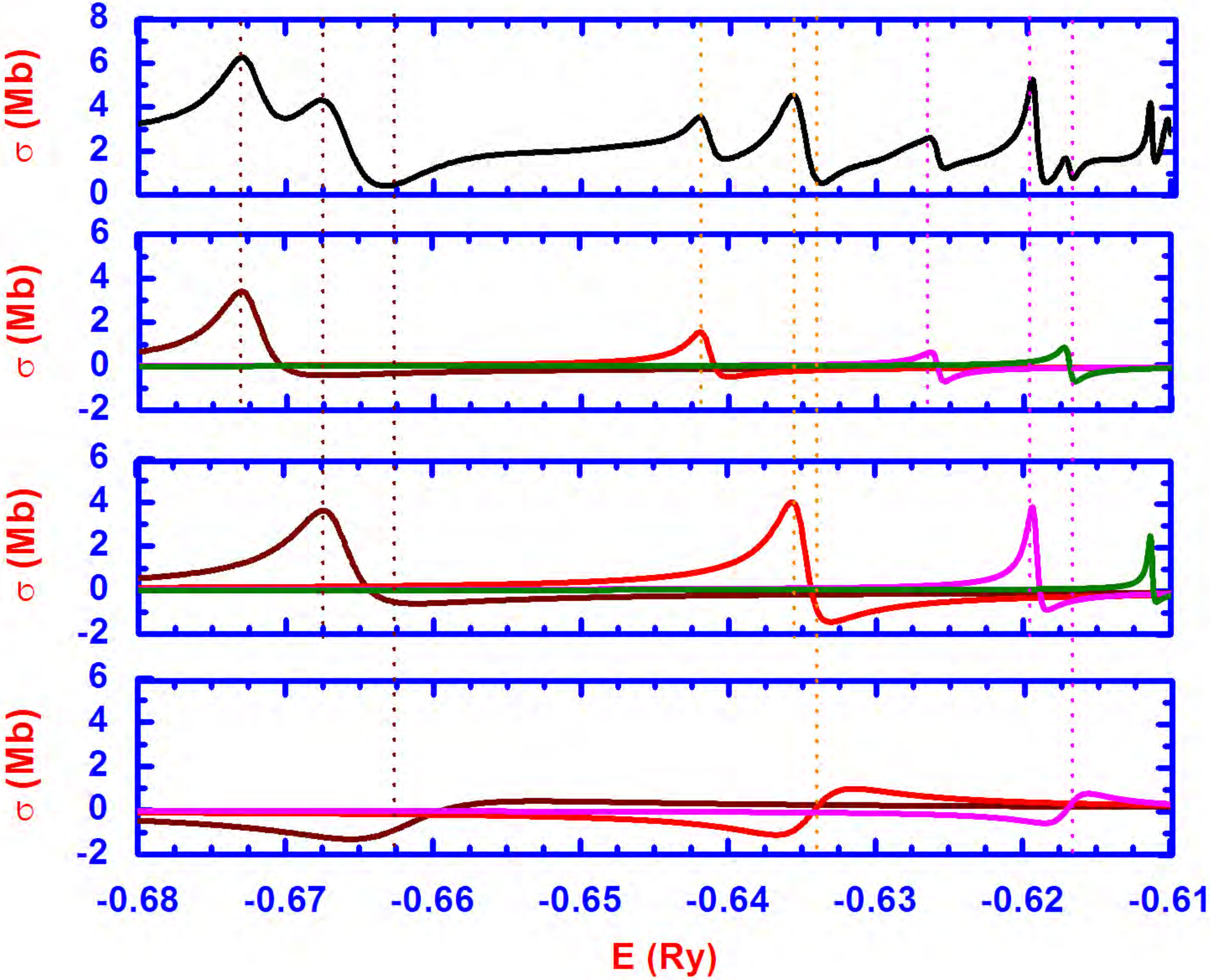


Open chs (8): 5sεp $^{1,3}P$, 4dεp $^{1,3}P$ & ^{3}D, 4dεf $^{1,3}P$ & ^{3}D

Closed chs (5): 5pns $^{1,3}P$, 5pnd $^{1,3}P$ & ^{3}D

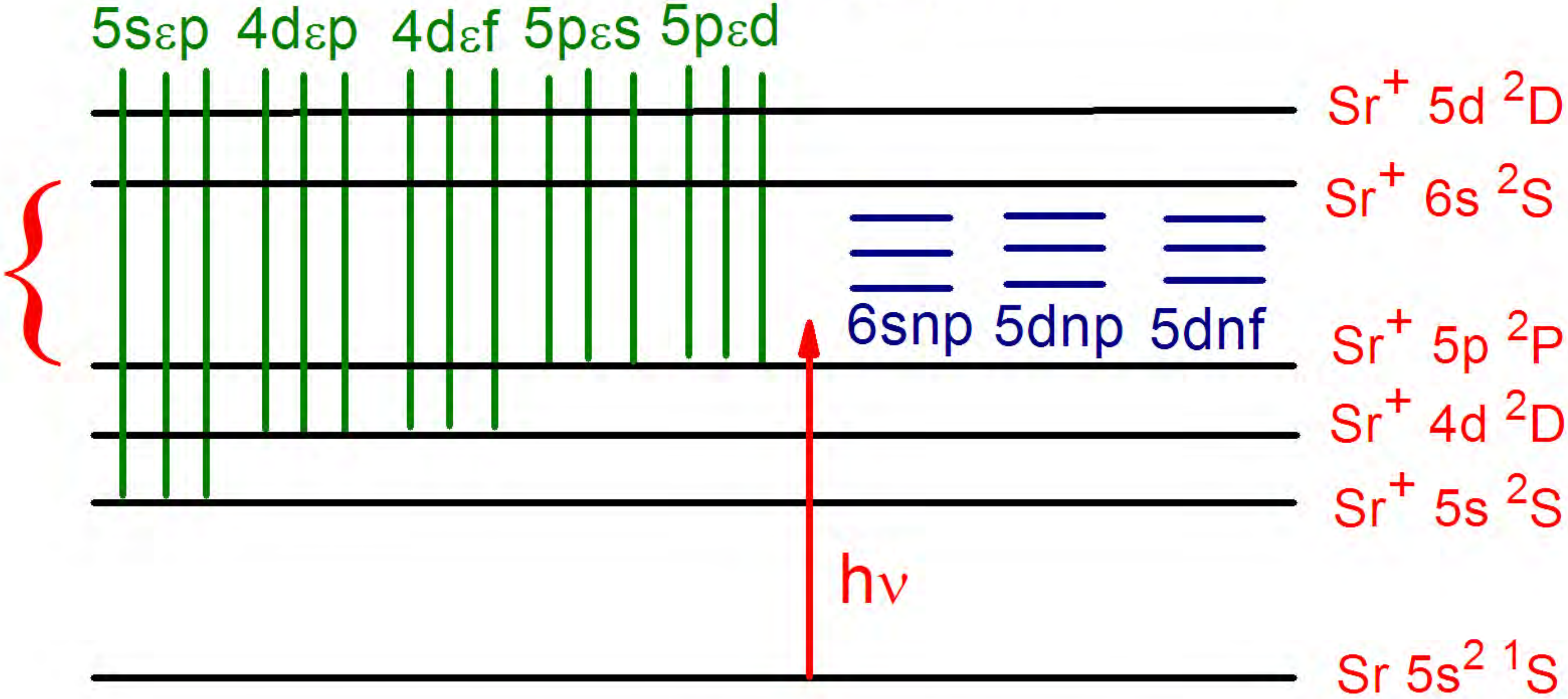


n=6
7
5pnd^{3}D
n=7
8
9
5pns^{3}P
n=7
8
9
5pns^{1}P
n=5
6
7
5pnd^{3}P
n=5
6
7
5pnd^{1}P
L
V
σ (Mb)
Experiment
σ (Mb)
Wave number (cm^{-1})



σ (Mb)
σ (Mb)
σ (Mb)
σ (Mb)
8
6
4
2
0
-2
-0.68
-0.67
-0.66
-0.65
-0.64
-0.63
-0.62
-0.61
E (Ry)

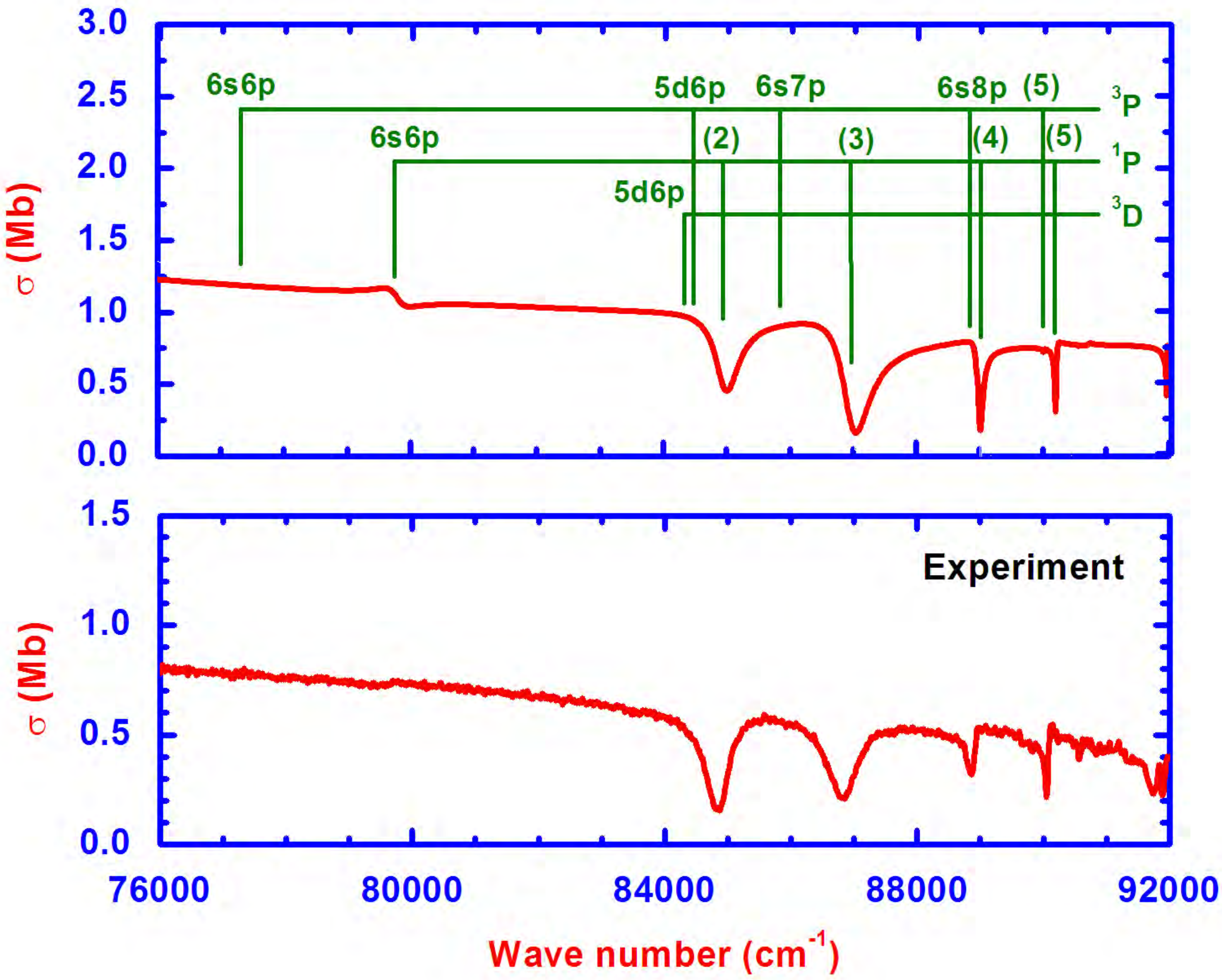
Sr doubly excited $^{1,3}L^{o}_{J=1}$ resonances



Open chs (13): 5sεp $^{1,3}P$, 4dεp $^{1,3}P$ & ^{3}D, 4dεf $^{1,3}P$ & ^{3}D

5pεs $^{1,3}P$, 5pεd $^{1,3}P$ & ^{3}D,

Closed chs (8): 6snp $^{1,3}P$, 5dnp $^{1,3}P$ & ^{3}D, 5dnf $^{1,3}P$ & ^{3}D



3.0
2.5
2.0
1.5
1.0
0.5
0.0
σ (Mb)
6s6p
6s6p
5d6p
5d6p
6s7p
6s8p
(5)
(2)
(3)
(4)
(5)
3P
1P
3D
1.5
1.0
0.5
0.0
σ (Mb)
Experiment
76000
80000
84000
88000
92000
Wave number (cm-1)

Photoionization of Ca in a static electric field

[Phys. Rev. A82, 063402 (2010)]

The Hamiltonian for atoms in an external field is given by

$$H = H_{nr} + H_{so} + F \cdot (r_1 + r_2),$$

where *F* is the electric field strength.

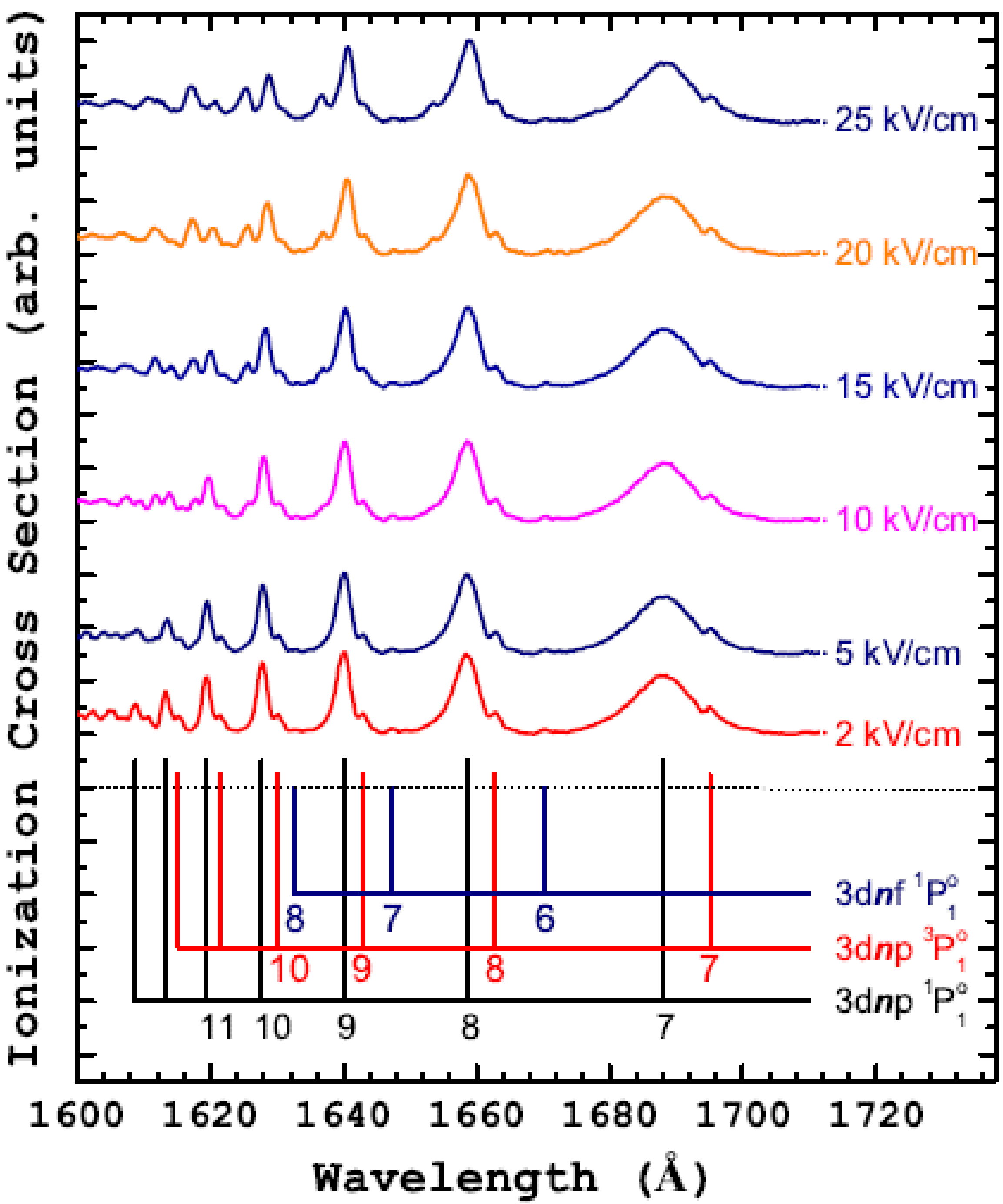
$$\mathrm{Ca\ 4s^2\ {}^1S_{J=0}} \Longrightarrow {}^{1,3}L^{o}_{J=1},\ {}^{1,3}L^{e}_{J=0},\ {}^{1,3}L^{e}_{J=2}$$

where

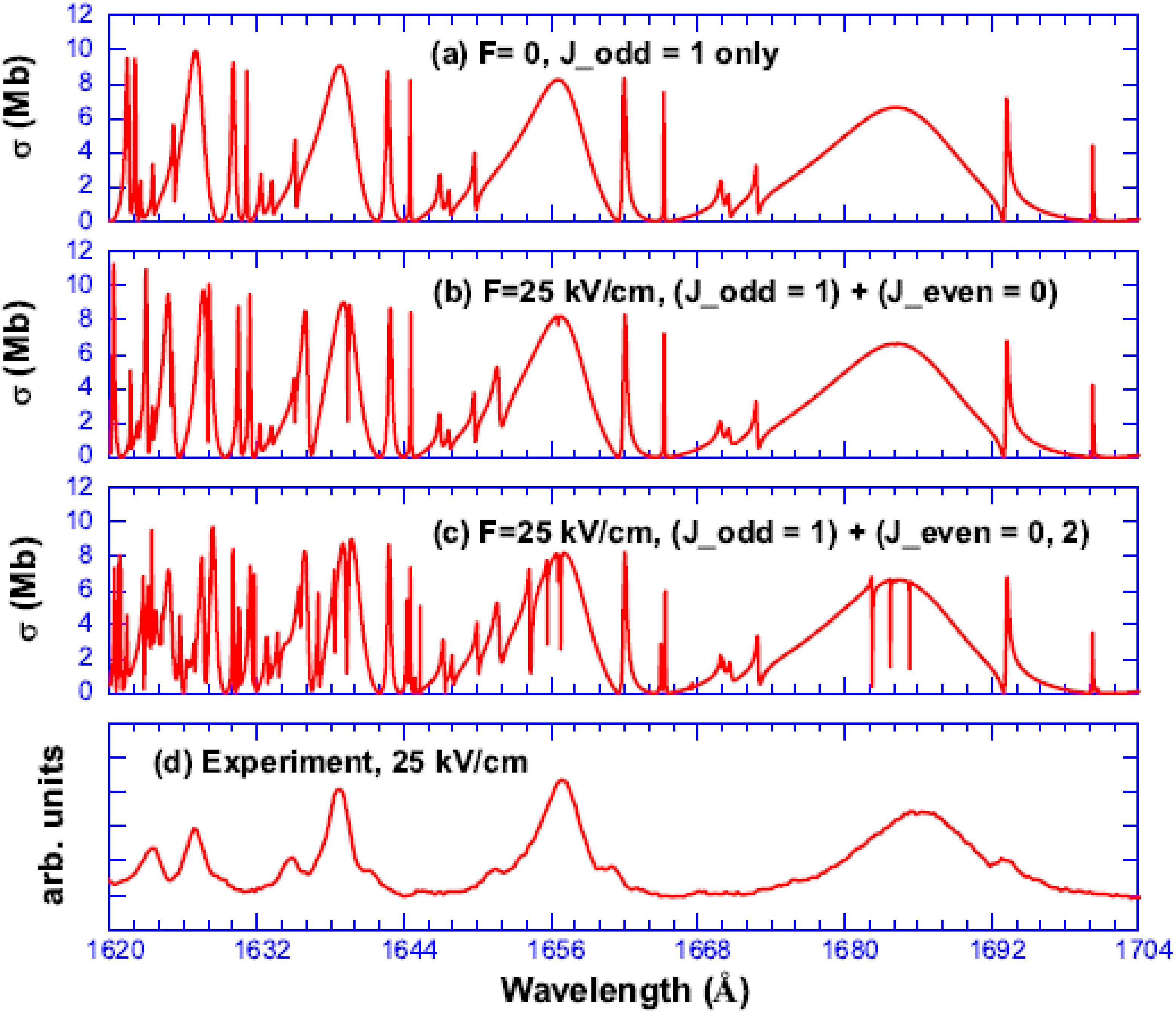
$${}^{1,3}L^{o}_{J=1} = \{\ {}^{1,3}P^{o}_{J=1},\ {}^{3}D^{o}_{J=1}\ \}$$

$${}^{1,3}L^{e}_{J=0} = \{\ {}^{1}S^{e}_{J=0},\ {}^{3}P^{e}_{J=0}\ \}$$

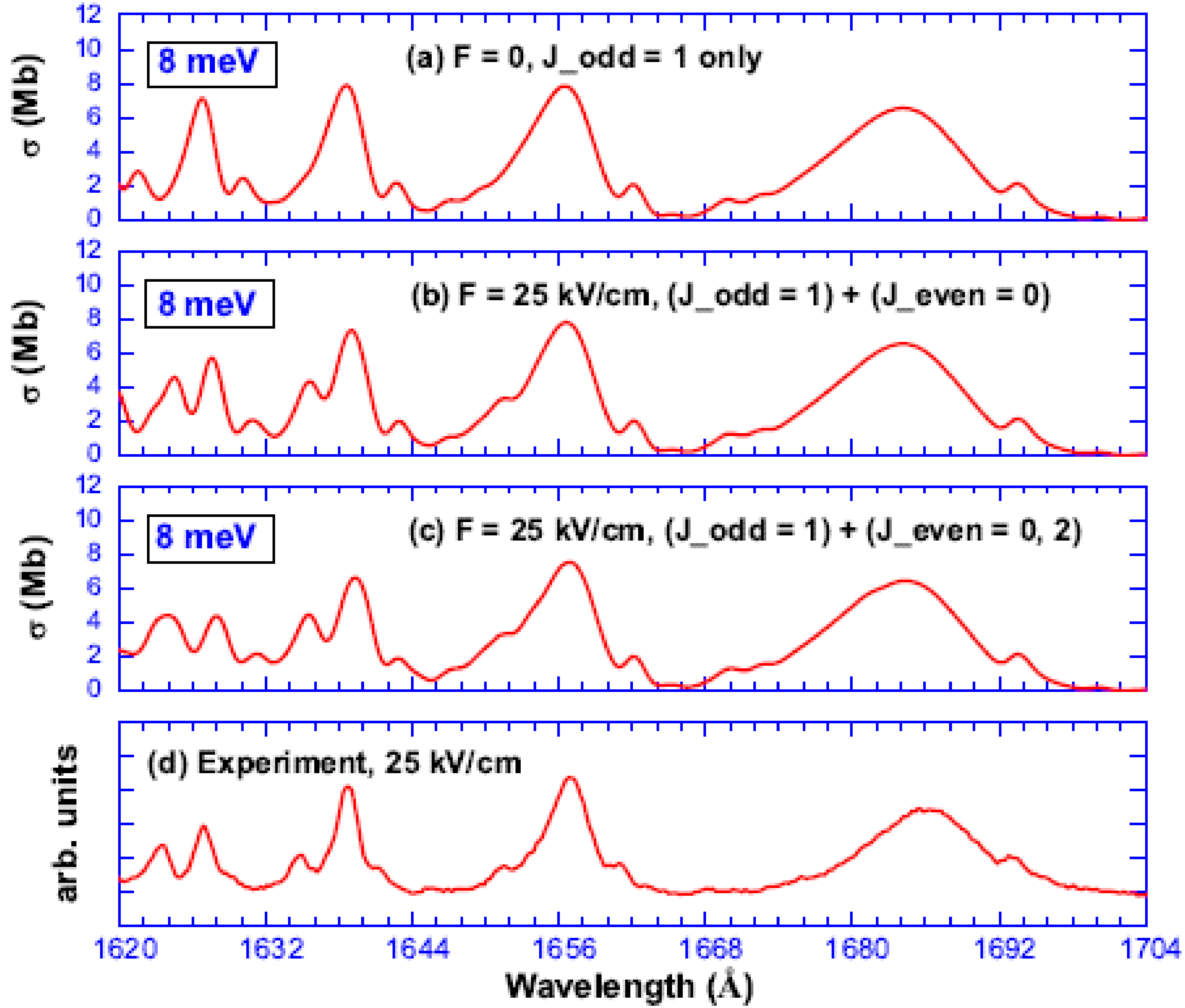
$${}^{1,3}L^{e}_{J=2} = \{\ {}^{3}P^{e}_{J=2},\ {}^{1,3}D^{e}_{J=2},\ {}^{3}F^{e}_{J=2}\ \}$$



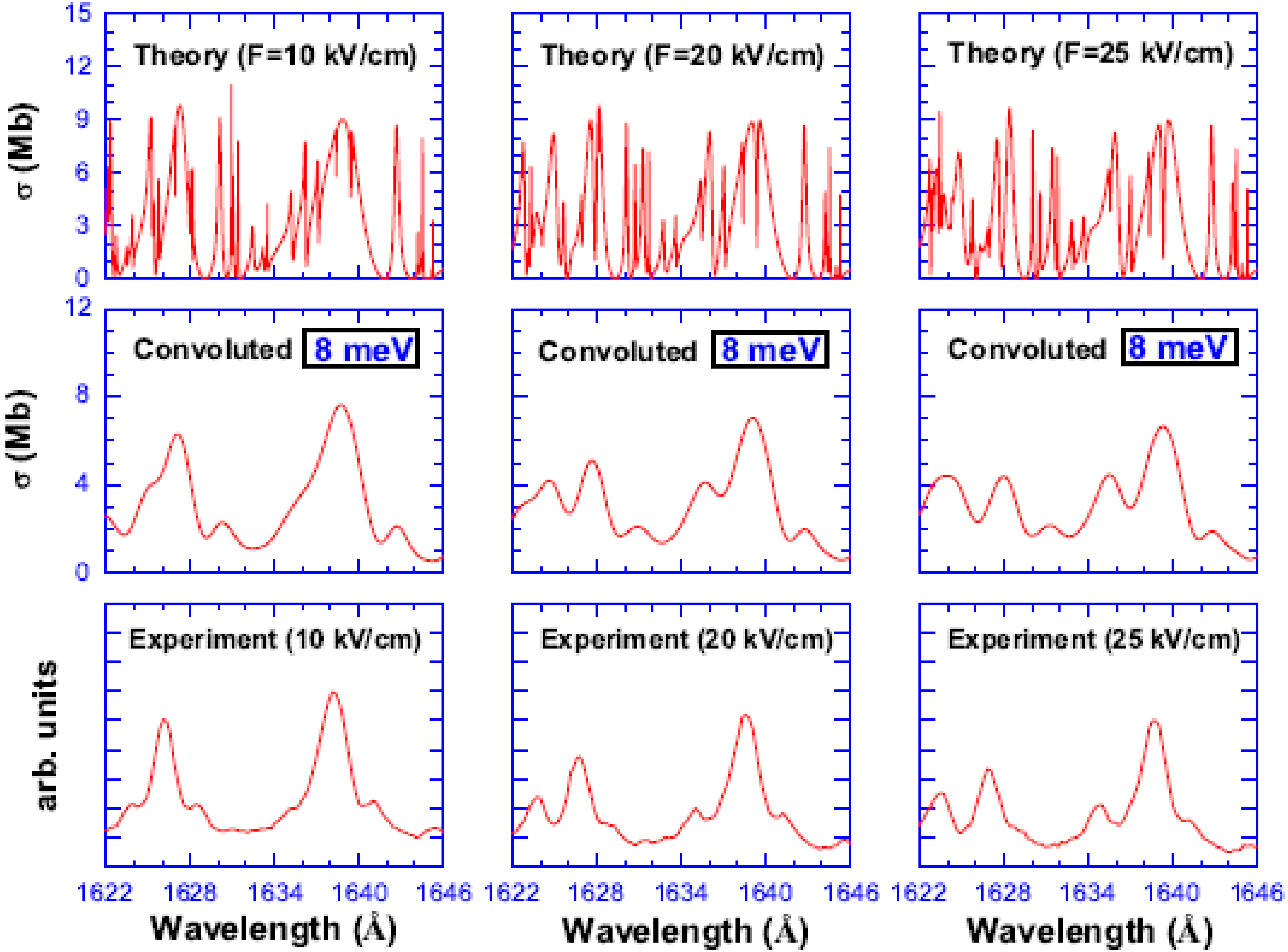
Ionization Cross Section (arb. units)
25 kV/cm
20 kV/cm
15 kV/cm
10 kV/cm
5 kV/cm
2 kV/cm
3dnf ¹P°₁
3dnp ³P°₁
3dnp ¹P°₁
8 7 6
10 9 8 7
11 10 9 8 7
1600 1620 1640 1660 1680 1700 1720
Wavelength (Å)

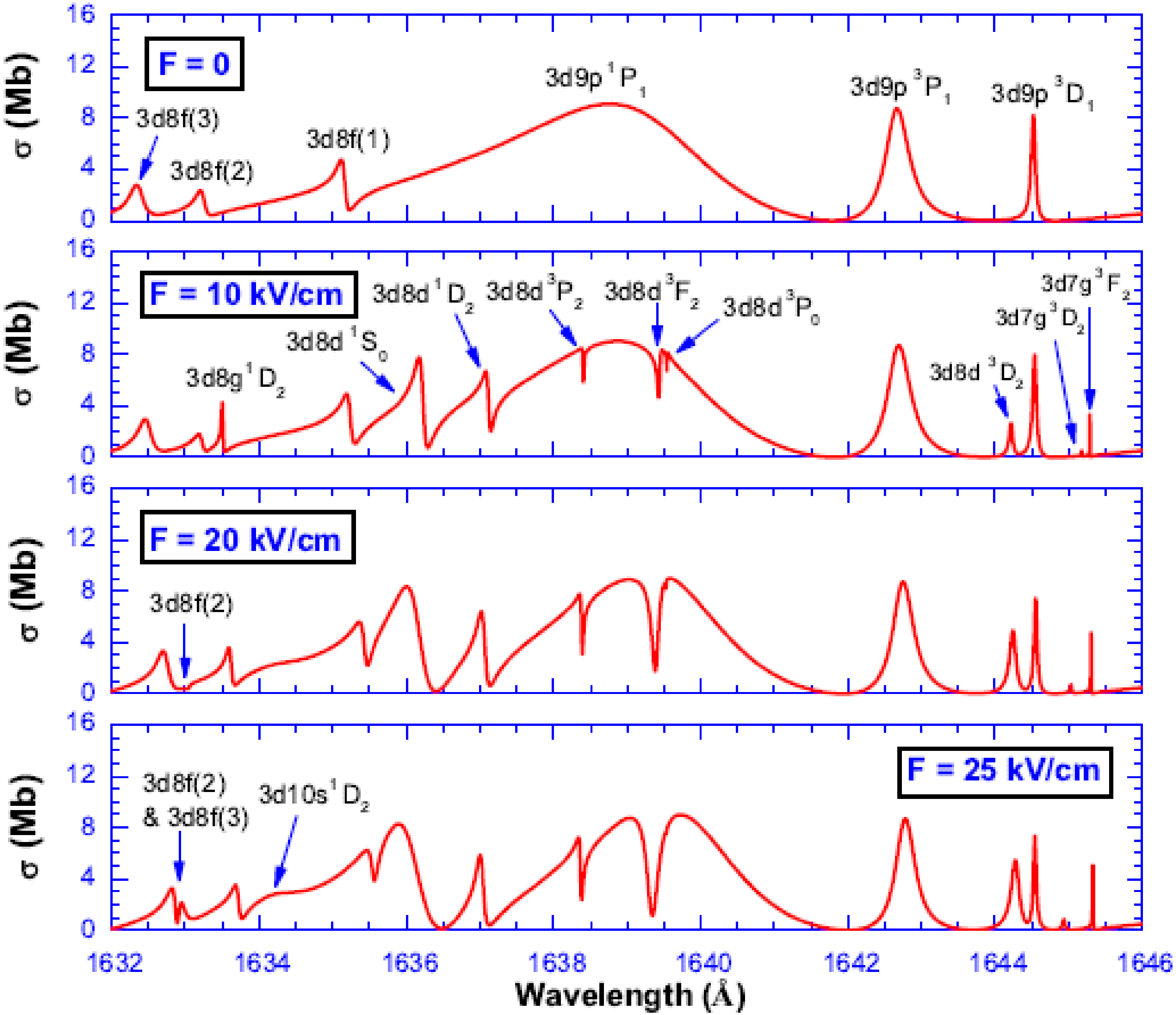


(a) F= 0, J_odd = 1 only
(b) F=25 kV/cm, (J_odd = 1) + (J_even = 0)
(c) F=25 kV/cm, (J_odd = 1) + (J_even = 0, 2)
(d) Experiment, 25 kV/cm
σ (Mb)
arb. units
0
2
4
6
8
10
12
1620
1632
1644
1656
1668
1680
1692
1704
Wavelength (Å)

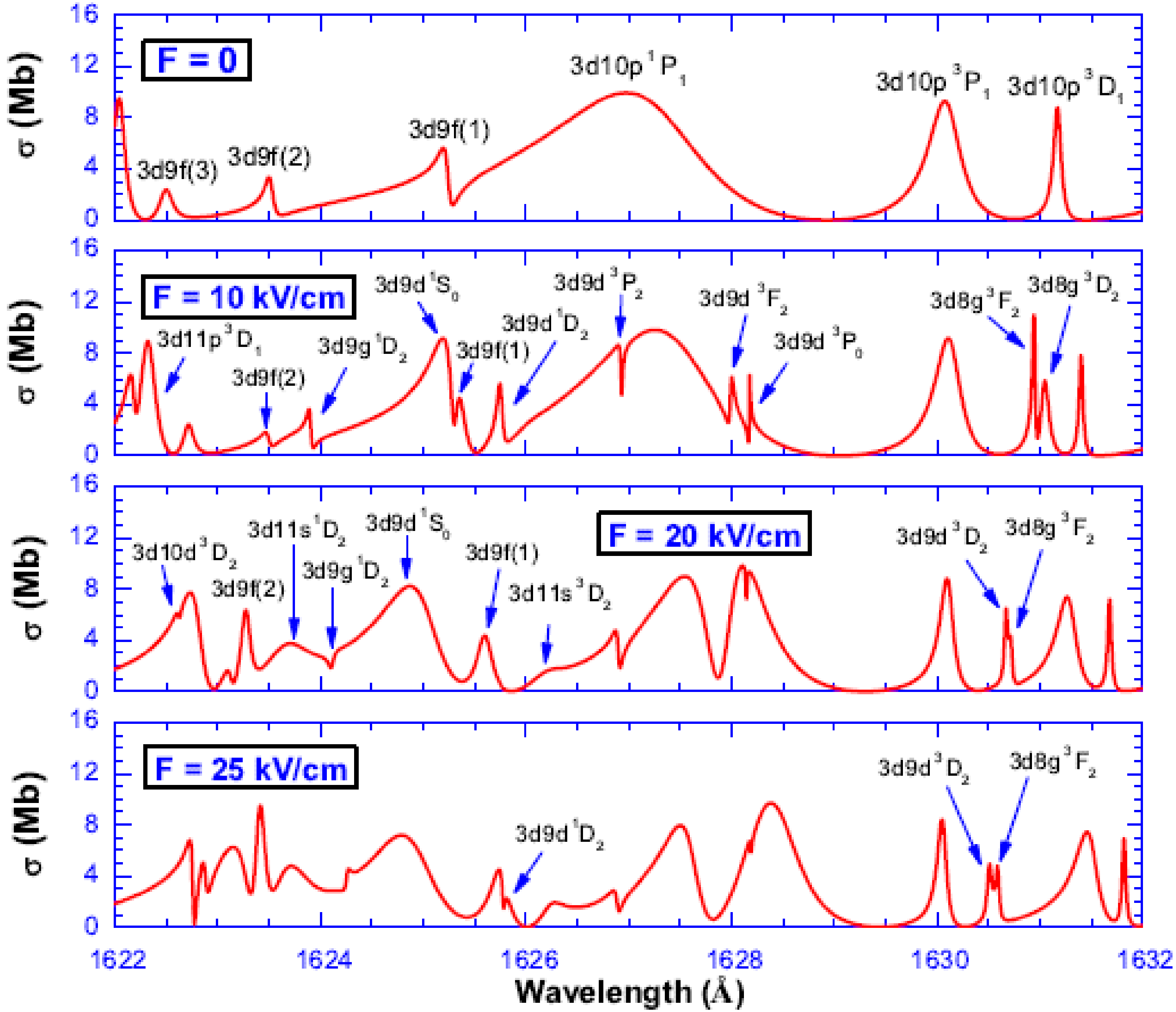


8 meV
(a) F = 0, J_odd = 1 only
8 meV
(b) F = 25 kV/cm, (J_odd = 1) + (J_even = 0)
8 meV
(c) F = 25 kV/cm, (J_odd = 1) + (J_even = 0, 2)
(d) Experiment, 25 kV/cm
σ (Mb)
arb. units
0
2
4
6
8
10
12
1620
1632
1644
1656
1668
1680
1692
1704
Wavelength (Å)

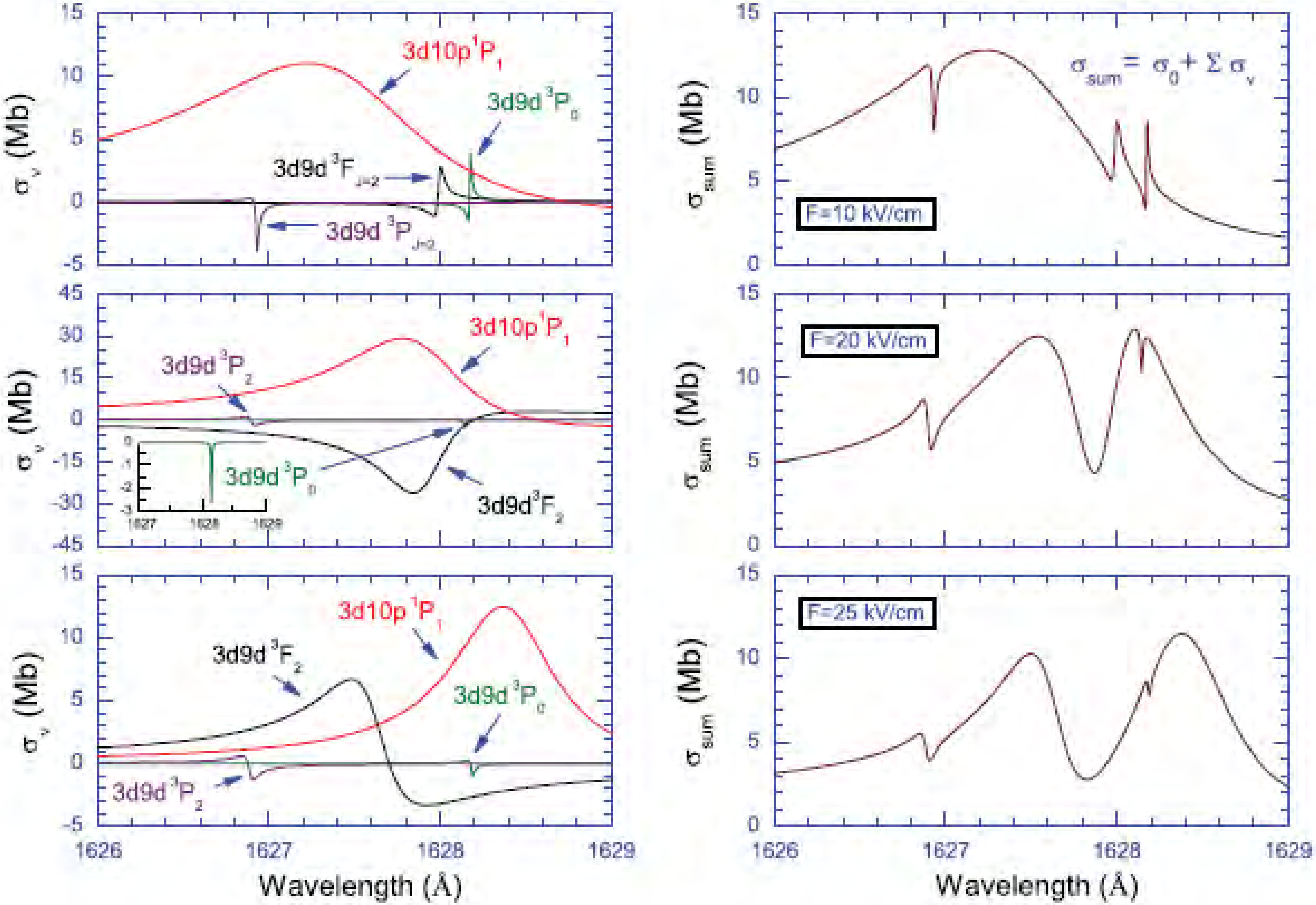

Theory (F=10 kV/cm)
Theory (F=20 kV/cm)
Theory (F=25 kV/cm)
σ (Mb)
Convoluted 8 meV
Convoluted 8 meV
Convoluted 8 meV
σ (Mb)
Experiment (10 kV/cm)
Experiment (20 kV/cm)
Experiment (25 kV/cm)
arb. units
Wavelength (Å)
Wavelength (Å)
Wavelength (Å)

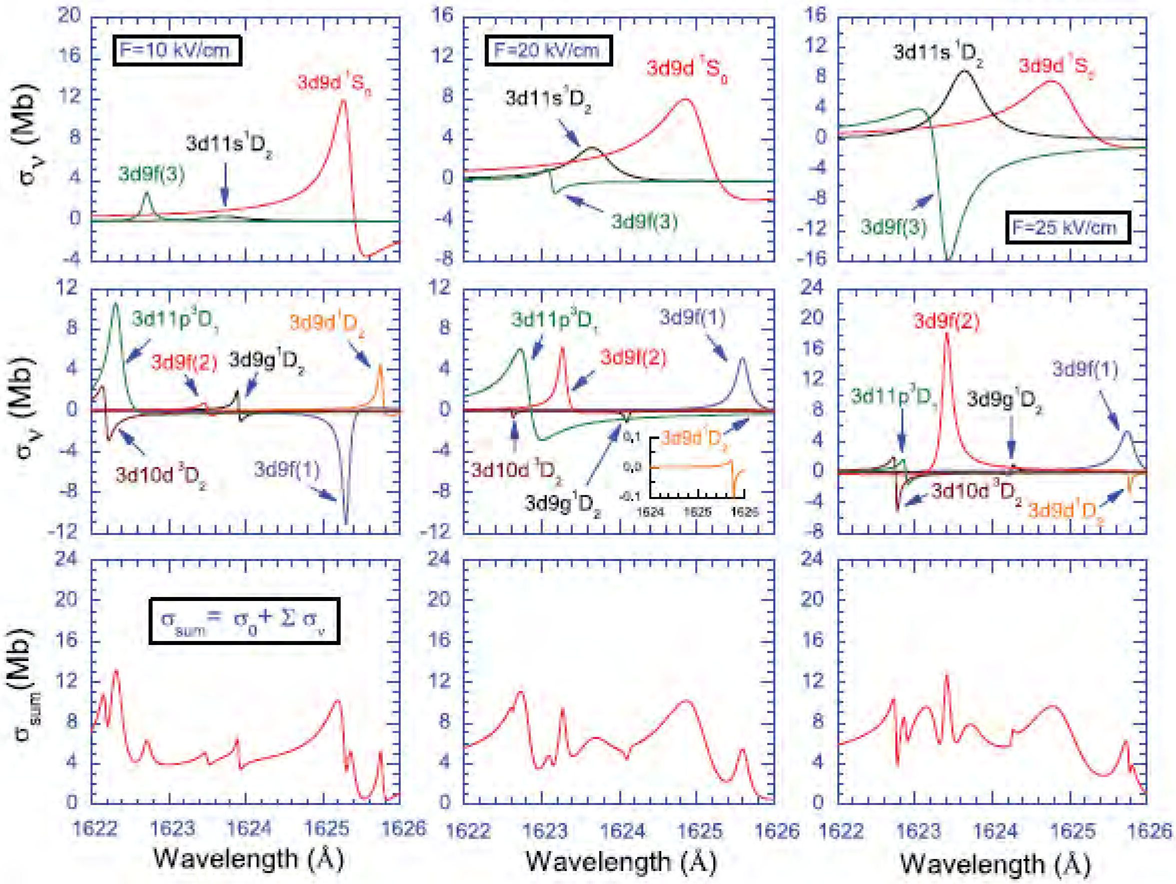


F = 0
F = 10 kV/cm
F = 20 kV/cm
F = 25 kV/cm
σ (Mb)
Wavelength (Å)
3d8f(3)
3d8f(2)
3d8f(1)
3d9p ¹P₁
3d9p ³P₁
3d9p ³D₁
3d8g ¹D₂
3d8d ¹S₀
3d8d ¹D₂
3d8d ³P₂
3d8d ³F₂
3d8d ³P₀
3d8d ³D₂
3d7g ³D₂
3d7g ³F₂
3d8f(2) & 3d8f(3)
3d10s ¹D₂

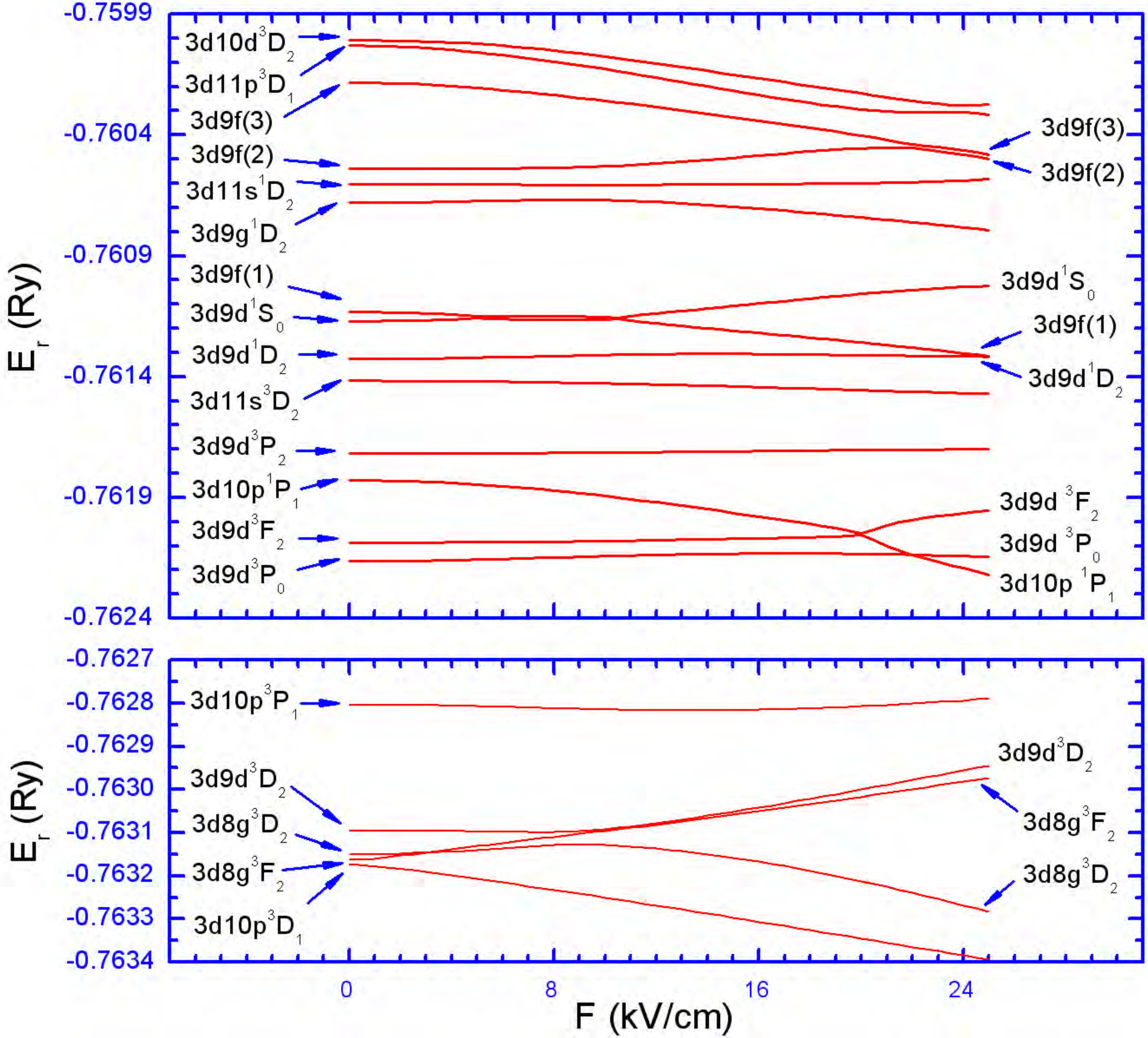


F = 0
3d10p ¹P₁
3d10p ³P₁
3d10p ³D₁
3d9f(1)
3d9f(2)
3d9f(3)
F = 10 kV/cm
3d9d ¹S₀
3d9d ³P₂
3d9d ³F₂
3d8g ³F₂
3d8g ³D₂
3d9d ¹D₂
3d11p ³D₁
3d9g ¹D₂
3d9f(1)
3d9d ³P₀
3d9f(2)
3d11s ¹D₂
3d9d ¹S₀
F = 20 kV/cm
3d10d ³D₂
3d9g ¹D₂
3d9f(1)
3d9d ³D₂
3d8g ³F₂
3d9f(2)
3d11s ³D₂
F = 25 kV/cm
3d9d ³D₂
3d8g ³F₂
3d9d ¹D₂
σ (Mb)
Wavelength (Å)

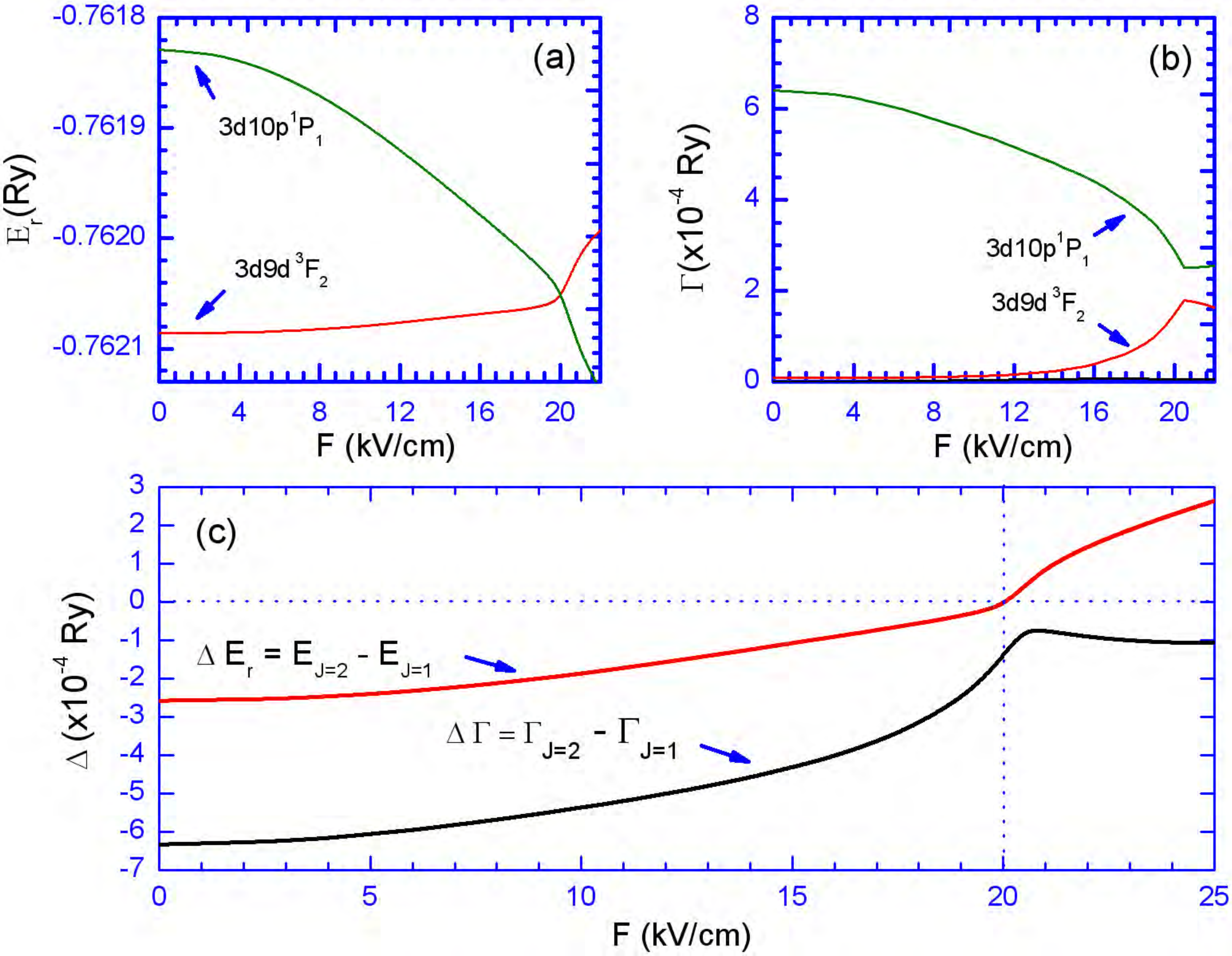

3d10p ¹P₁
3d9d ³P₀
3d9d ³F_{J=2}
3d9d ³P_{J=2}
3d9d ³P₂
3d9d ³F₂
σ_sum = σ₀ + Σ σ_v
F=10 kV/cm
F=20 kV/cm
F=25 kV/cm
σ_v (Mb)
σ_sum (Mb)
Wavelength (Å)
1626
1627
1628
1629



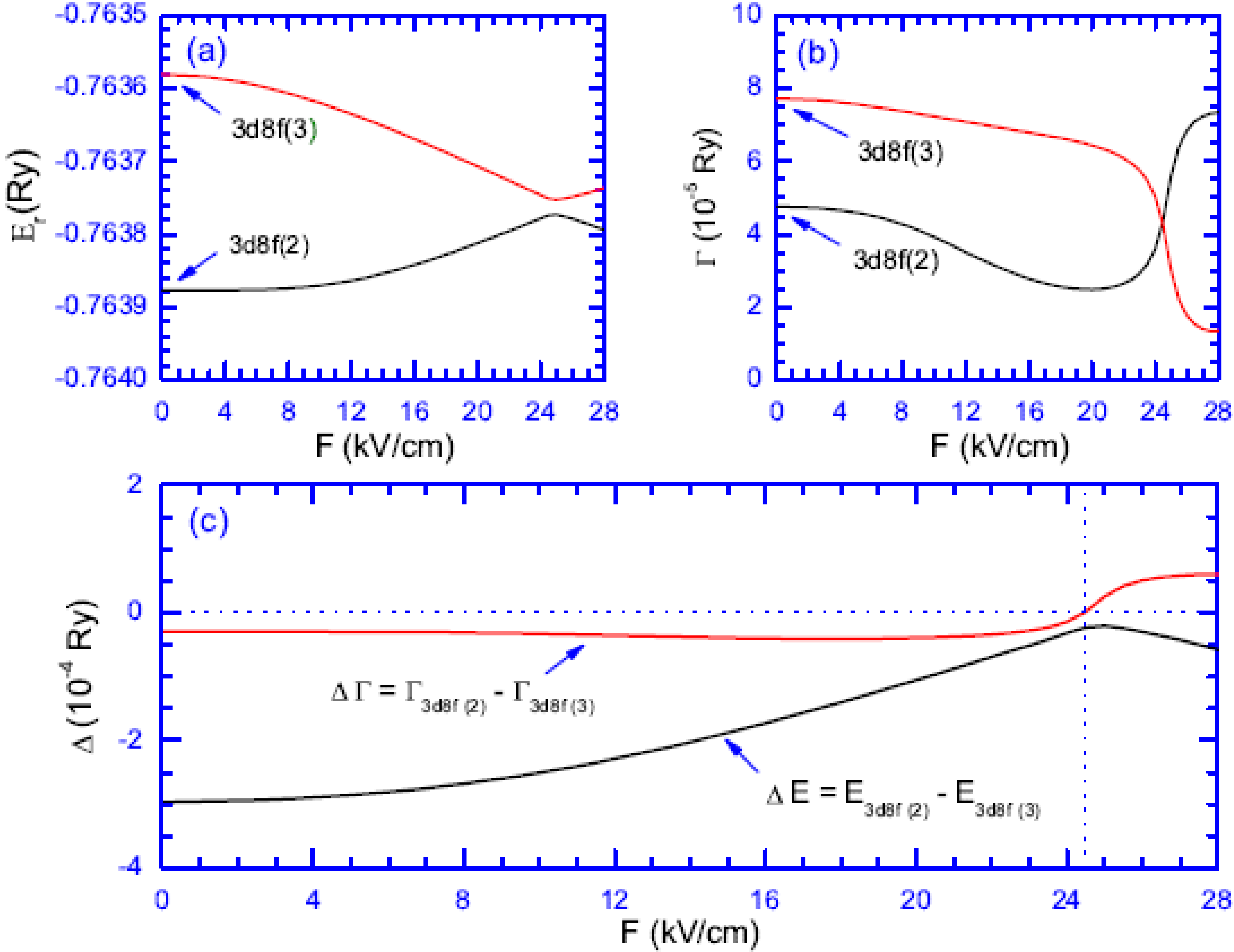
F=10 kV/cm
F=20 kV/cm
F=25 kV/cm
3d9d $^1S_0$
3d11s $^1D_2$
3d9f(3)
3d11p $^3D_1$
3d9f(2)
3d9g $^1D_2$
3d9d $^1D_2$
3d10d $^3D_2$
3d9f(1)
σ_v (Mb)
σ_{sum} (Mb)
$\sigma_{sum} = \sigma_0 + \Sigma\,\sigma_v$
Wavelength (Å)



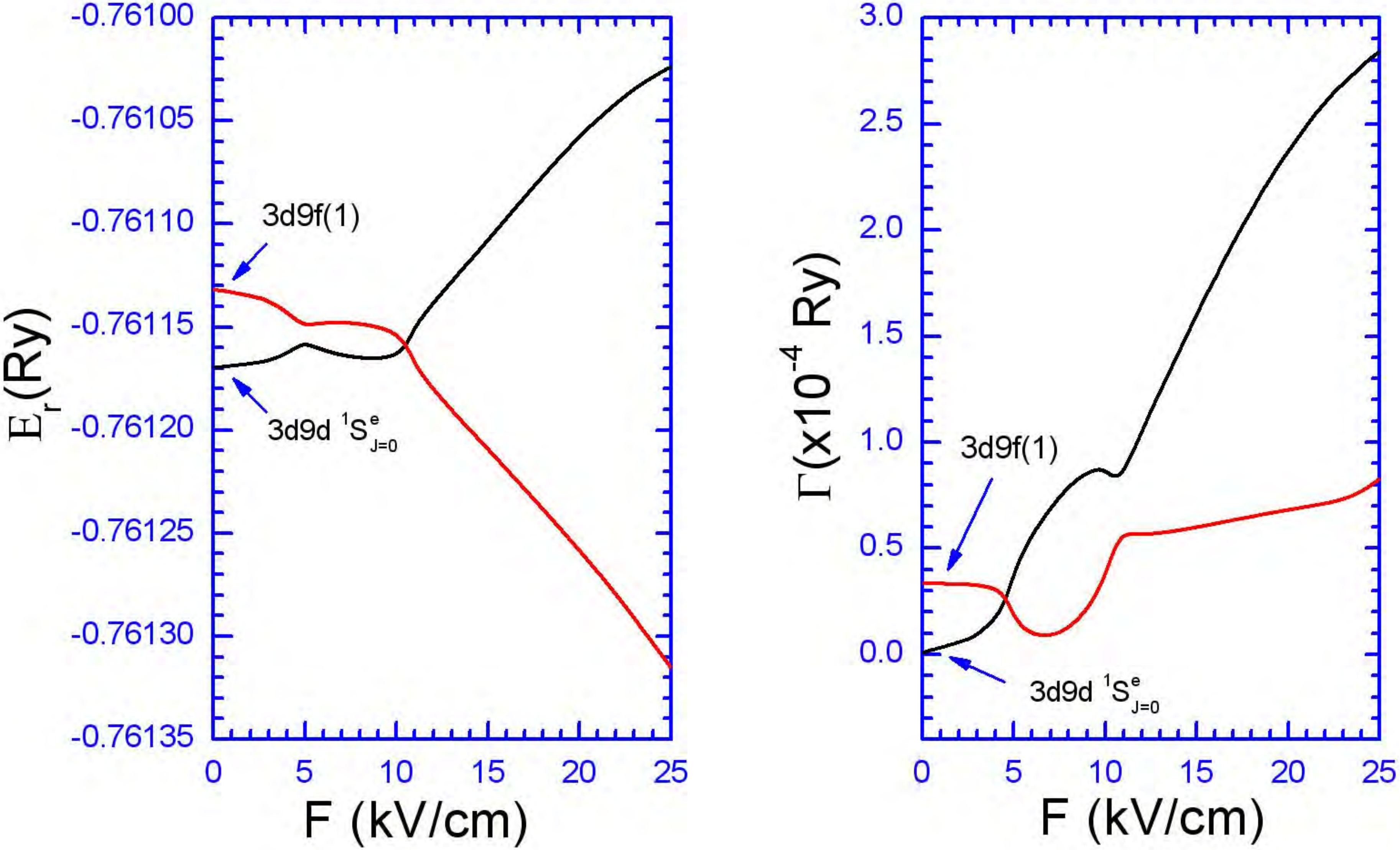
-0.7599
-0.7604
-0.7609
-0.7614
-0.7619
-0.7624
-0.7627
-0.7628
-0.7629
-0.7630
-0.7631
-0.7632
-0.7633
-0.7634
0
8
16
24
F (kV/cm)
E_r (Ry)
3d10d 3D2
3d11p 3D1
3d9f(3)
3d9f(2)
3d11s 1D2
3d9g 1D2
3d9f(1)
3d9d 1S0
3d9d 1D2
3d11s 3D2
3d9d 3P2
3d10p 1P1
3d9d 3F2
3d9d 3P0
3d10p 3P1
3d9d 3D2
3d8g 3D2
3d8g 3F2
3d10p 3D1



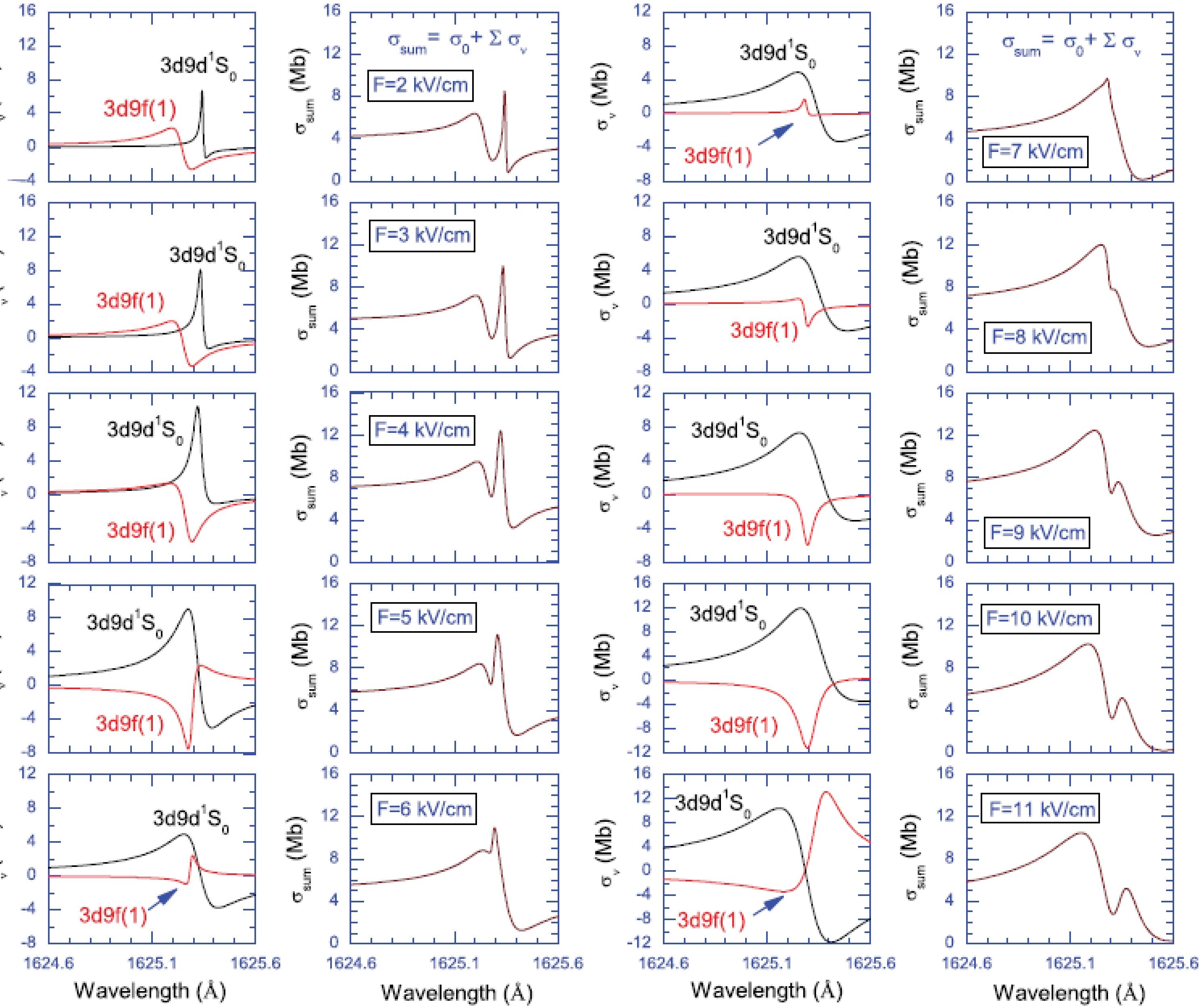
(a)
3d10p $^1P_1$
3d9d $^3F_2$
E_r(Ry)
-0.7618
-0.7619
-0.7620
-0.7621
0
4
8
12
16
20
F (kV/cm)
(b)
Γ(x10^{-4} Ry)
8
6
4
2
0
3d10p $^1P_1$
3d9d $^3F_2$
0
4
8
12
16
20
F (kV/cm)
(c)
Δ(x10^{-4} Ry)
$\Delta E_r = E_{J=2} - E_{J=1}$
$\Delta \Gamma = \Gamma_{J=2} - \Gamma_{J=1}$
3
2
1
0
-1
-2
-3
-4
-5
-6
-7
0
5
10
15
20
25
F (kV/cm)



(a)
-0.7635
-0.7636
-0.7637
-0.7638
-0.7639
-0.7640
E_r (Ry)
3d8f(3)
3d8f(2)
0
4
8
12
16
20
24
28
F (kV/cm)
(b)
10
8
6
4
2
0
Γ (10^{-5} Ry)
3d8f(3)
3d8f(2)
F (kV/cm)
(c)
2
0
-2
-4
Δ (10^{-4} Ry)
$\Delta\Gamma = \Gamma_{3d8f(2)} - \Gamma_{3d8f(3)}$
$\Delta E = E_{3d8f(2)} - E_{3d8f(3)}$
F (kV/cm)

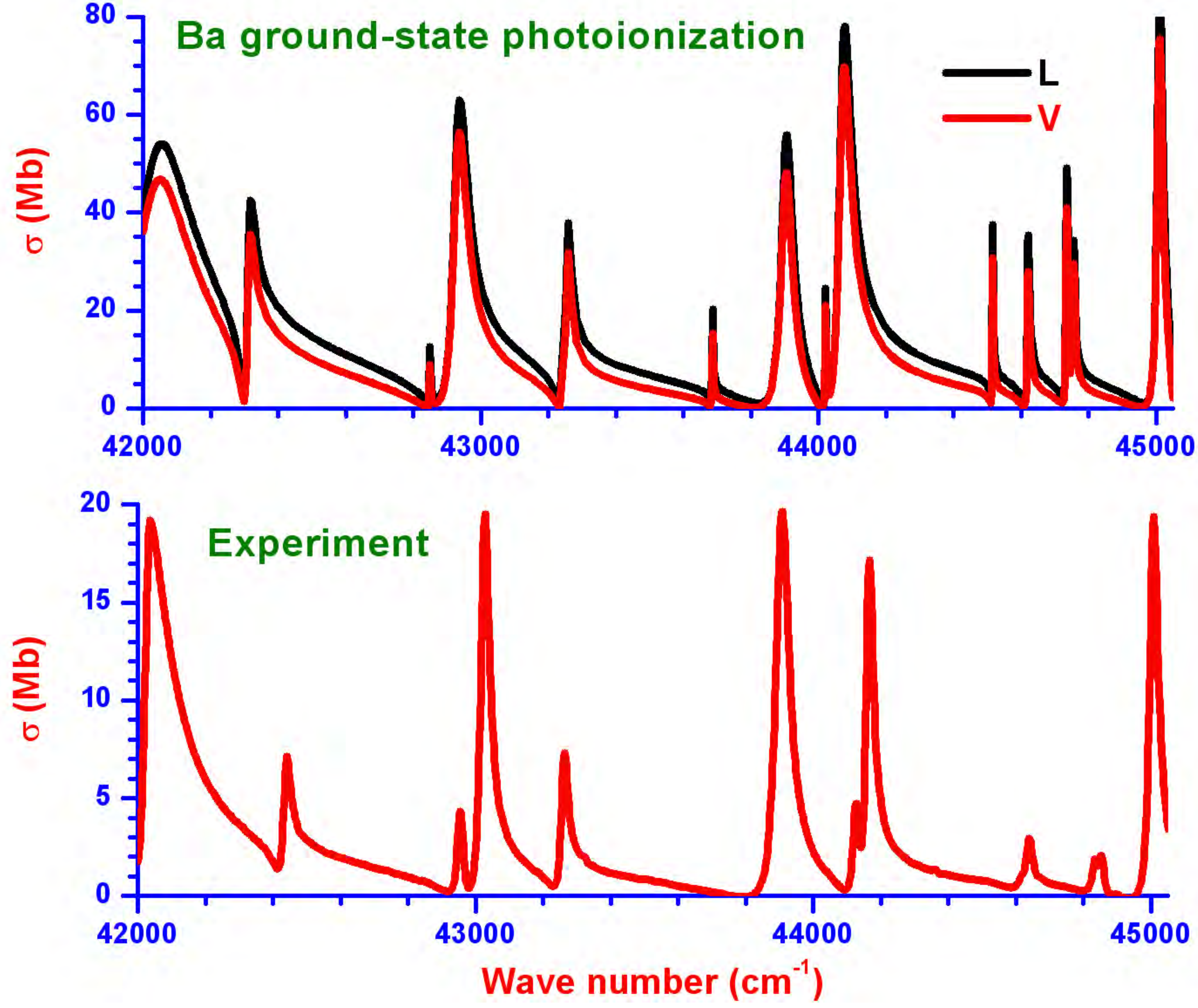


-0.76100
-0.76105
-0.76110
-0.76115
-0.76120
-0.76125
-0.76130
-0.76135
E_r(Ry)
3d9f(1)
3d9d $^1S^e_{J=0}$
0
5
10
15
20
25
F (kV/cm)
3.0
2.5
2.0
1.5
1.0
0.5
0.0
Γ(x10^{-4} Ry)
3d9f(1)
3d9d $^1S^e_{J=0}$
0
5
10
15
20
25
F (kV/cm)



σ_v (Mb)
3d9d¹S₀
3d9f(1)
σ_sum (Mb)
σ_sum = σ₀ + Σ σ_v
F=2 kV/cm
F=3 kV/cm
F=4 kV/cm
F=5 kV/cm
F=6 kV/cm
F=7 kV/cm
F=8 kV/cm
F=9 kV/cm
F=10 kV/cm
F=11 kV/cm
1624.6
1625.1
1625.6
Wavelength (Å)
Wavelength (Å)
Wavelength (Å)
Wavelength (Å)

Photoionization calculation for Ba



Two - state approximation (complex)

$$\begin{vmatrix} E - E_a(F) & V_{ab}(F) \\ V_{ba}(F) & E - E_b(F) \end{vmatrix} = 0 \longrightarrow E_{1,2}(F)$$

Where V_{ab} is the matrix element of spin-orbit interaction

$$E_1(F) - E_2(F) = \delta E(F) - i\,\delta\Gamma(F) = A^{1/2}, \quad A = (E_a - E_b)^2 + C,$$

Where $C = 4\,V_{ab}(F)\,V_{ba}(F) = C_R + i\,C_i$

Crossing near a field strength $F = F_0$:

If crossing in *energy*, $\delta E(F_0) = 0$, *$A < 0$* and *real.*

If crossing in *width*, $\delta\Gamma(F_0) = 0$, *$A > 0$* and *real.*

Near crossing (as F approaches F_0)

$$E_a(F) - E_b(F) \longrightarrow [(E_a(F_0) - E_b(F_0)] + a\,(F - F_0),$$
$$= \Delta E - i\,(\Delta\Gamma / 2) + (a_R + i a_i)\,(F - F_0).$$

Where a_R is the rate of change in energy and a_i in width

Near crossing in *energy*, ΔE --> *0* and $a_R >> a_i$.

$$E_a(F) - E_b(F) \longrightarrow -\,i\,(\Delta\Gamma / 2) + a_R(F - F_0).$$

Near crossing in *width*, $\Delta\Gamma$ --> *0* and $a_i >> a_R$.

$$E_a(F) - E_b(F) \longrightarrow \Delta E + i\,a_i\,(F - F_0).$$

$$A = (E_a - E_b)^2 + (c_R + i\, c_i)$$

Near crossing in *energy*, (A < 0 and real)

$$E_a(F) - E_b(F) \longrightarrow - i\,(\Delta\Gamma / 2) + a_R(F - F_0).$$

$$A = - (\Delta\Gamma/2)^2 + a_R^2\,(F - F_0)^2 - i\, a_R(\Delta\Gamma)(F - F_0) + (c_R + i\, c_i)$$

$$a_R(F - F_0) = c_i / \Delta\Gamma, \longrightarrow A = - (\Delta\Gamma/2)^2 + c_R + (c_i / \Delta\Gamma)^2$$

$$E_1(F) - E_2(F) = - i\, \delta\Gamma = A^{1/2}$$

$\longrightarrow$ **Slow varying $\delta\Gamma = - (- A)^{1/2}$**

$\longrightarrow$ **No sign change !**

$$A = (E_a - E_b)^2 + (c_R + i\, c_i)$$

Near crossing in *width*, (A > 0 and real)

$$E_a(F) - E_b(F) \longrightarrow \Delta E + i\, a_i(F - F_0).$$

$$A = (\Delta E)^2 - a_i^2 (F - F_0)^2 + i\, 2a_i(\Delta E)(F - F_0) + (c_R + i\, c_i)$$

$$a_i(F - F_0) = -(c_i / 2\Delta E), \longrightarrow A = (\Delta E)^2 + c_R - (c_i / 2\Delta E)^2$$

$$E_1(F) - E_2(F) = \delta E = A^{1/2}$$

→ **Slow varying $\delta E = A^{1/2}$**

→ **No sign change !**