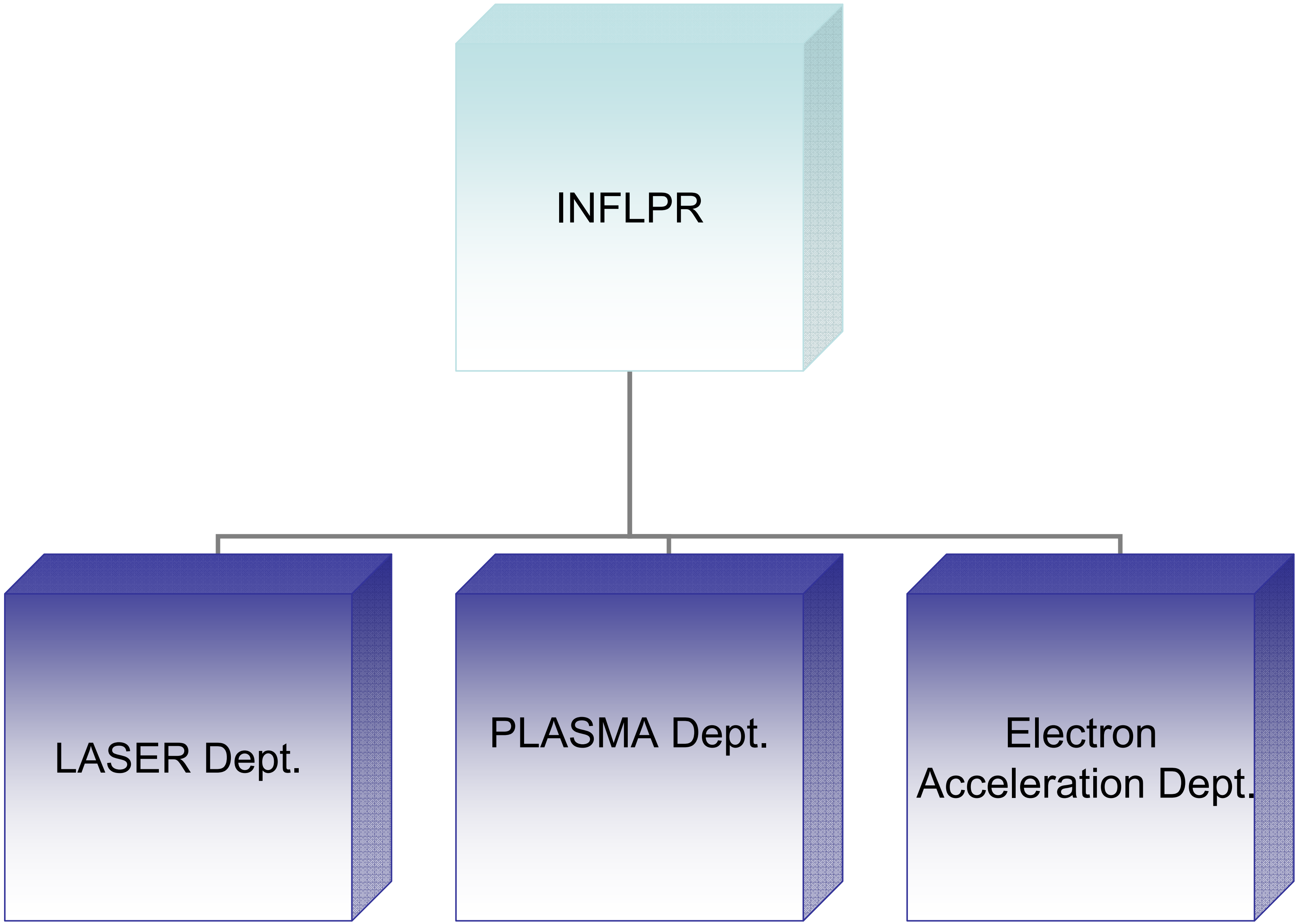
Fundamental research at INFLPR

V. Stancalie
Laser Department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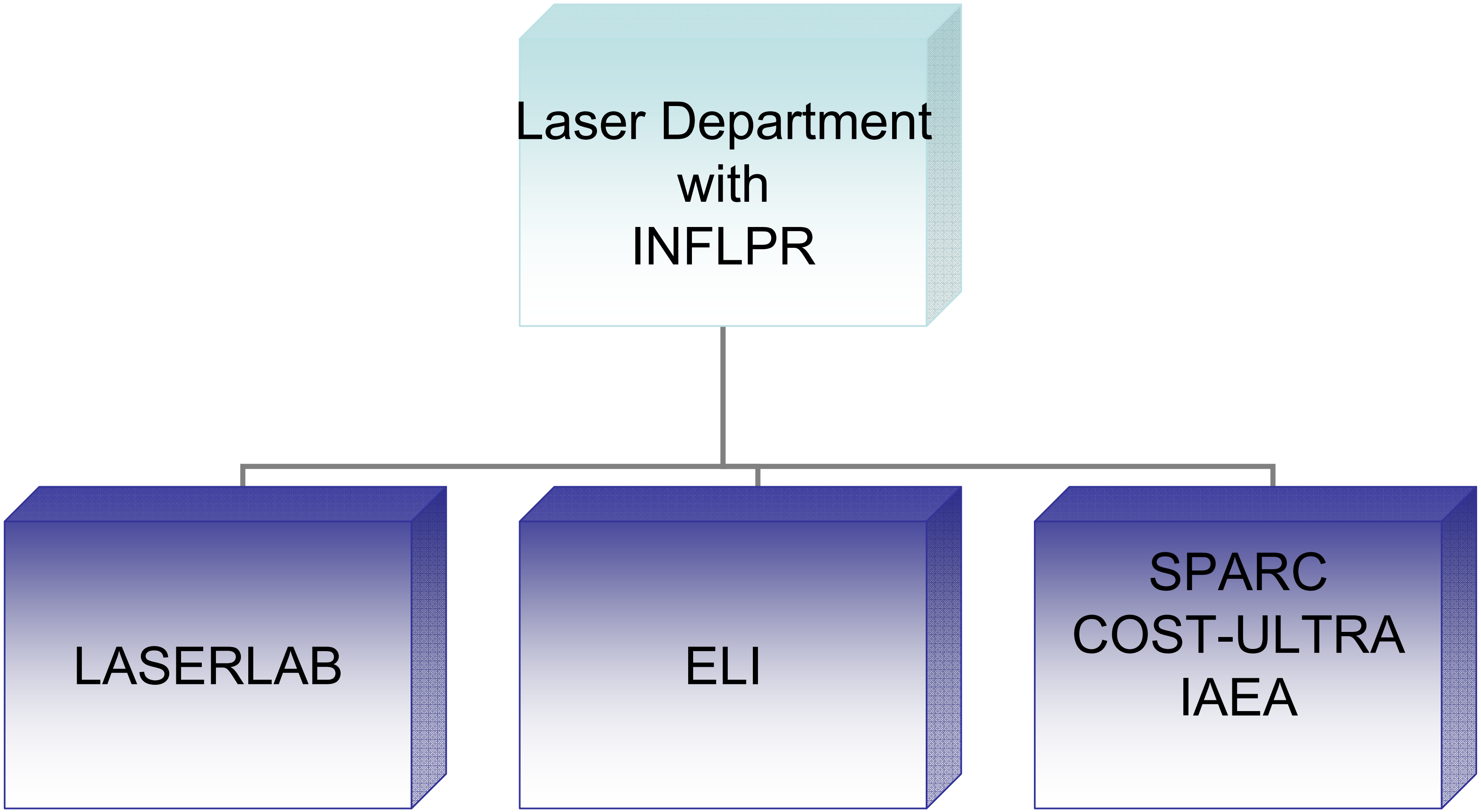
LASER Dept.
PLASMA Dept.
Electron Acceleration Dept.


Laser Department
with
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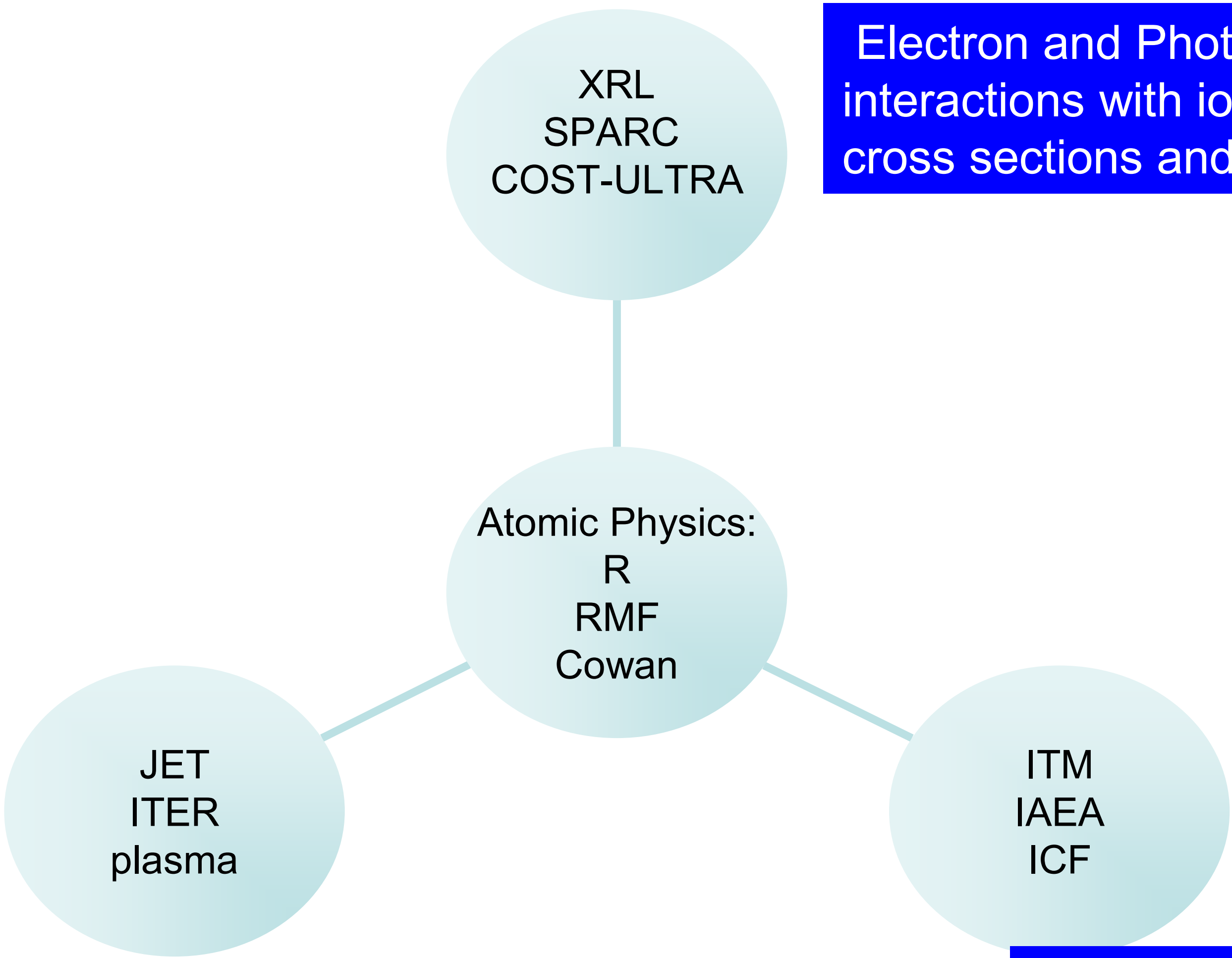


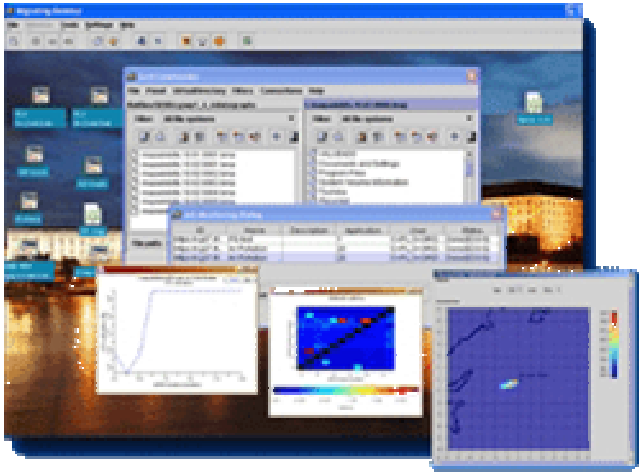
Electron and Photon interactions with ions, cross sections and rates

Fast particle
Induced transitions

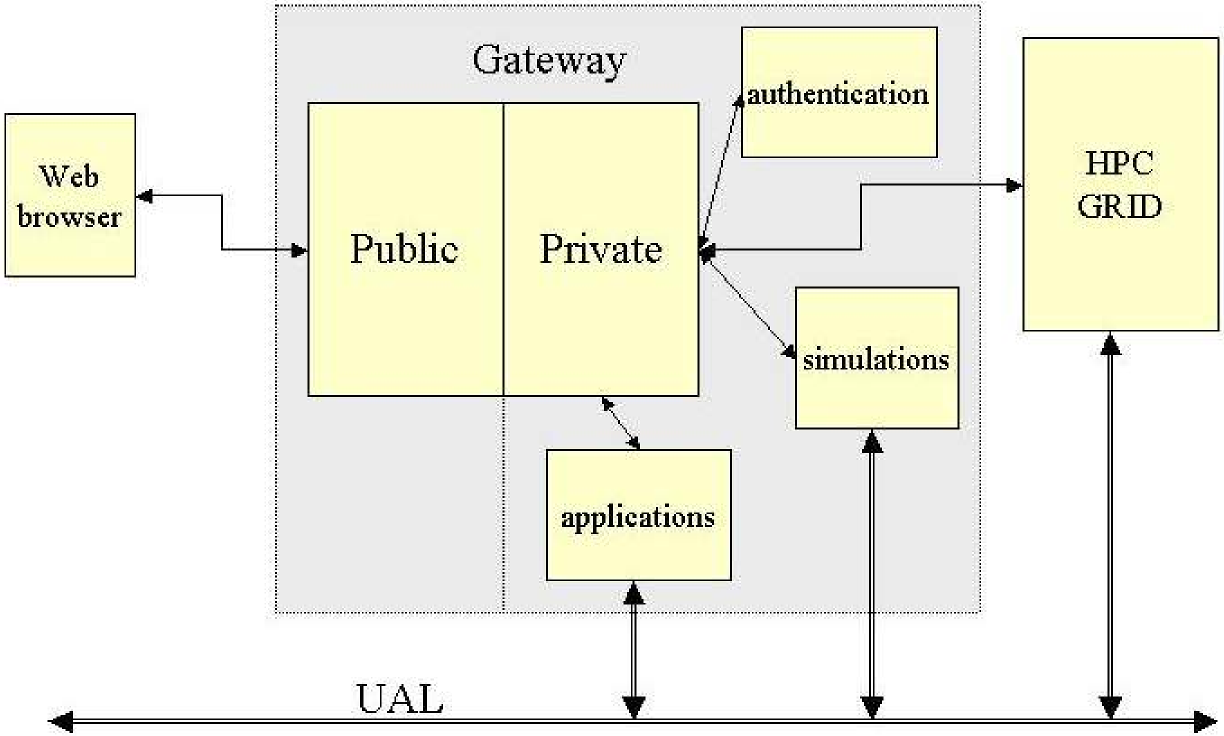
Atomic data, collision strengths:
Ba-like, Ca-like, Zn-like W ion ;
Fe-peak elements: ***Co, Ni***
Provision of jointly used tools for theory **and modeling:**
Generic flux surface, TM Portal

Integrating Applications

- Web based tools, web services
- Command line tools
- Graphical tools (SCILAB)
  - – XWindow Protocol
  - – VNC
  - – Migrating Desktop Project



Portal Architecture



Portal Architecture

Atomic data production

- R-matrix for Li-like and Be-like ions
- R-matrix Floquet for LIDS and DR
- R-matrix for Fe-peak elements: Co 3+
- Cowan's suite codes for W ions
- Local codes for ion-impact excitation

Study on the Laser induced or assisted phenomena

- *(LIDS) Laser-induced degenerate states model for* nonperturbative treatment of dielectronic recombination of Li-like into Be-like ions (*POP2005,POP2005, AIP Conf Ser.2006*);
- *(LICS) Laser-induced continuum structures* in Potassium, the modification of the photoelectron angular distribution(*PRA2005*);
- *Free-free transitions in laser-assisted* electron-Hydrogen scattering in a laser field within the second order perturbation theory, elastic and inelastic scattering, polarization effects due to the laser field, circular dichroism (*JPB 2001*);
- *Multiphoton ionization* of the Magnesium atom by linearly and circularly polarized laser field using *ab-initio* nonperturbative method, above-threshold ionization (ATI), coherent phase control(*PRA,2006*).

Double poles in the S matrix in laser assisted electron-atom scattering

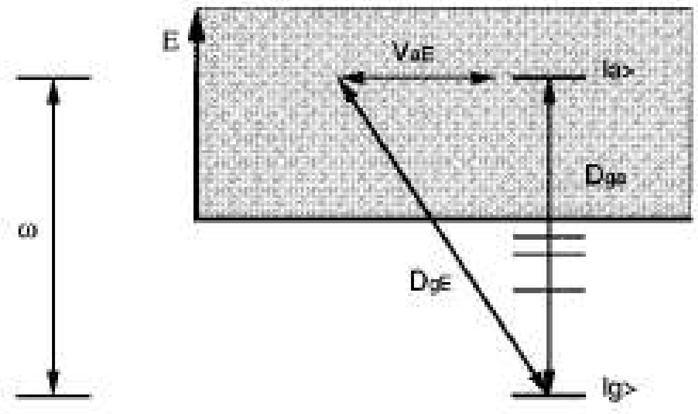


Diagram illustrating the first double-resonant process considered. The electron energy is chosen to be at an electron-atom scattering resonance corresponding to an autoionizing state of the (N+1)-electron system. The laser of angular frequency ω resonantly couples the autoionizing state and the ground state (or some excited bound state) of the (N+1)-electron atom.

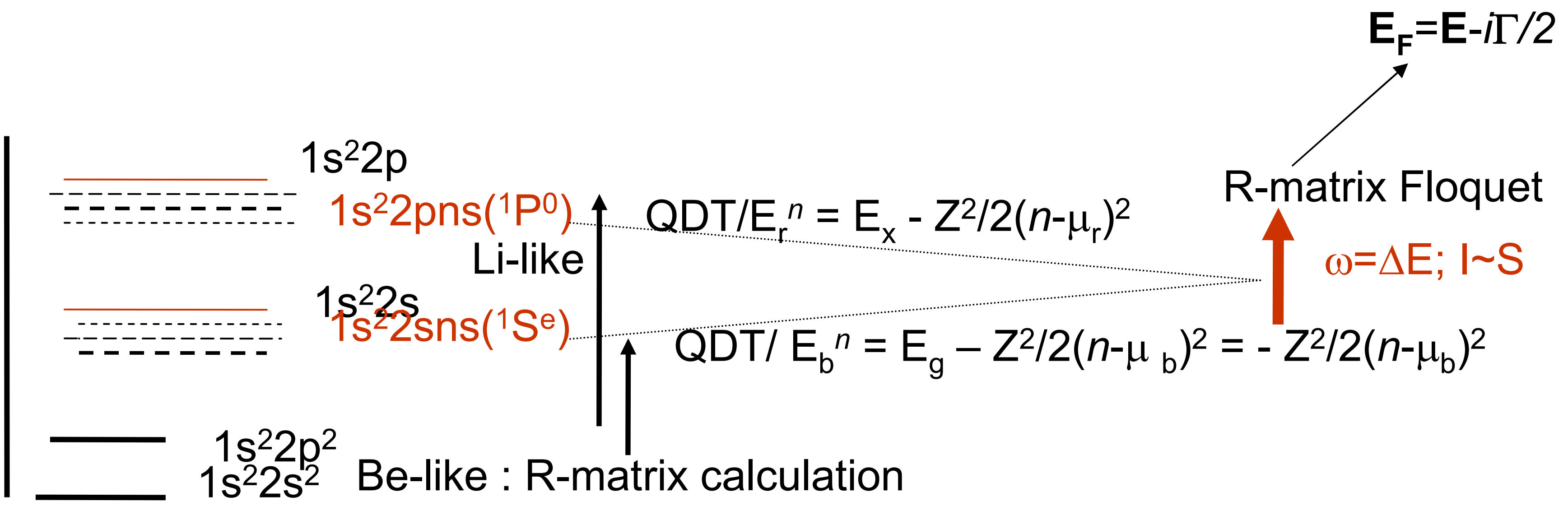
QDT & RMF

- *Basic process of interest*

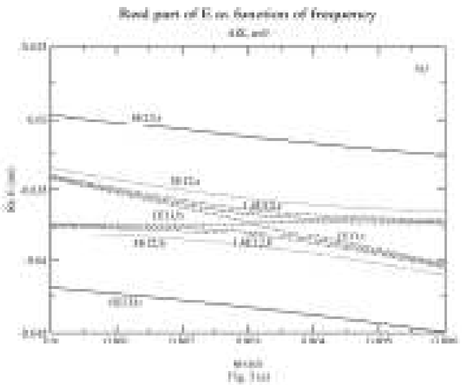
$$X^{Z+}[1s^2 2s(^2S^e)] + e^- \longrightarrow X^{**}[1s^2 2pns](^1P^0)$$

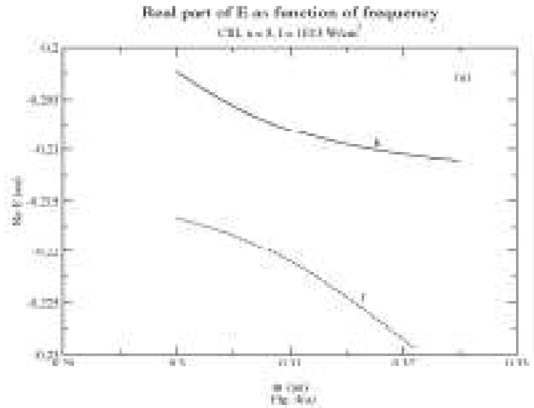
$$\downarrow$$

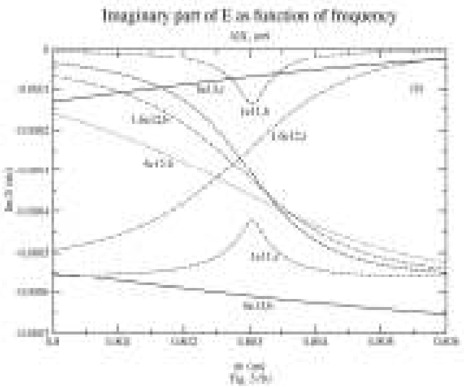
$$X^{Z+1}[1s^2 2sns](^1S^e) + h\nu$$

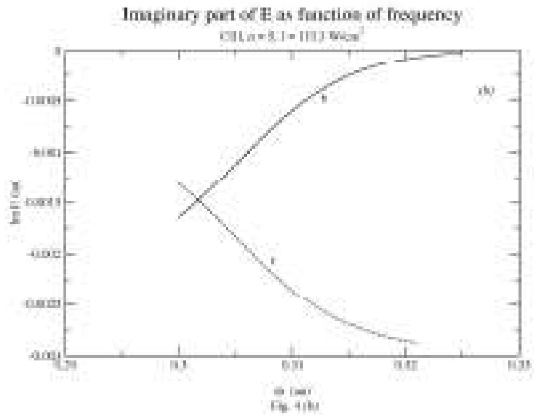


The motion of the complex energies in the complex plane as function of the field intensity for different frequencies and atomic parameters; the critical region where a crossing (or a avoiding crossing) of trajectories occurs

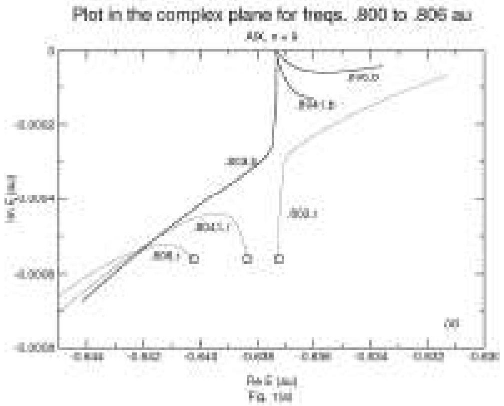


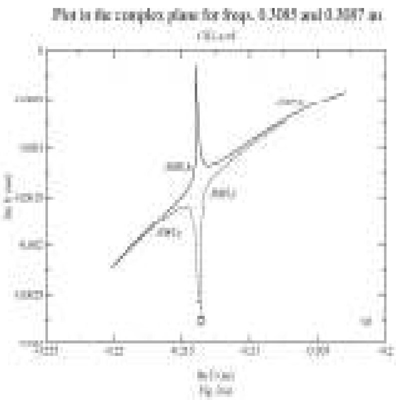


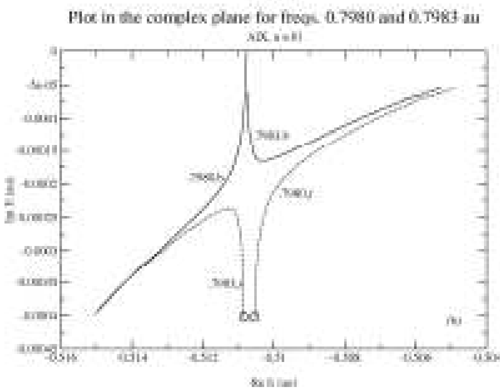


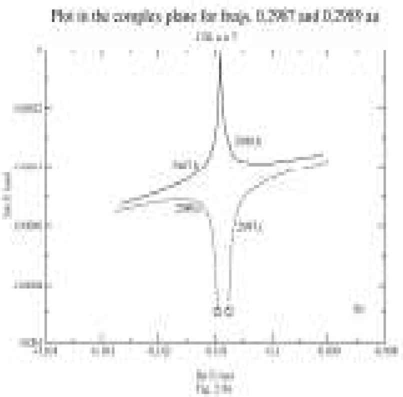


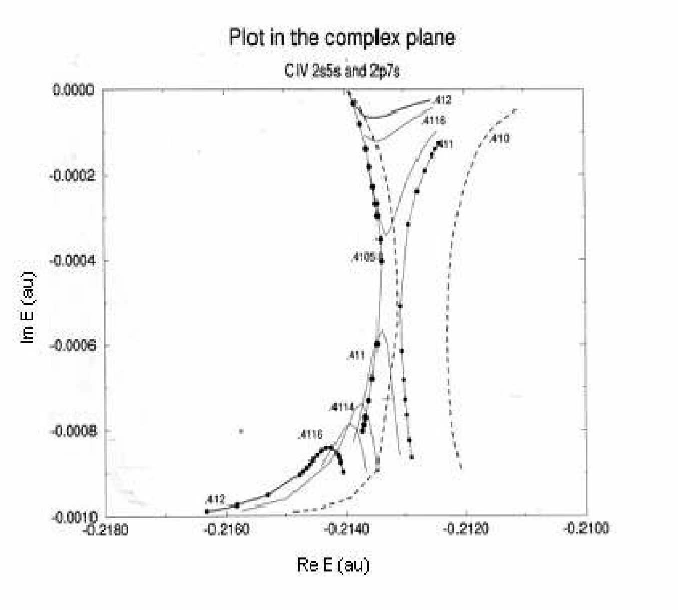
LIDS for DR: electron-collision and radiative processes are included in a consistent way











Consequences of the one-photon LIDS

- trapping” of population at some non zero field intensity;
- The rate of ionisation of the ‘ground’ excited Rydberg state will first increase with intensity and then exhibit a typical “stabilisation”, namely, a decrease of the ionisation rate with increasing intensity >>> Population transfer from the excited to autoionizing state

The 2-state model indicates that at degeneracy there are two points corresponding to :

$$\delta^{\pm} = \Gamma_a[q \pm \sqrt{q^2+1}; \qquad I^{\pm} = (\delta^{\pm})^2 / \gamma_a \Gamma_a$$

If we take q>0, then the trapping frequency is given by:

$$\omega^T(I) = E_a - E_g + \frac{1}{2} q[\Gamma_g - \Gamma_a]$$

At this trapping frequency, the poles in the S matrix in laser-assisted electron-scattering are :

$$z_1^T(I,\omega^T(I)) = E_a + \frac{1}{2} q\Gamma_g - \frac{i}{2}[\Gamma_a + \Gamma_g],$$

$$z_2^T(I,\omega^T(I)) = E_a - \frac{1}{2} q\Gamma_a$$

$$T(E,I,\omega^T)=\frac{1}{2\pi}\frac{\Gamma_a+\Gamma_g}{[E-E_a-q\frac{1}{2}\Gamma_g+i\frac{1}{2}[\Gamma_a+\Gamma_g]}$$

$$\sigma(E,I,\omega^T)=\frac{2\pi g}{E}\frac{\frac{1}{4}[\Gamma_a+\Gamma_g]}{[E-E_a-q\Gamma_g/2]^2+\frac{1}{4}[\Gamma_a+\Gamma_g]^2}$$

$$\Gamma^{r,n}=I/\omega_{LIDS} \qquad \to\Gamma^{r,n(CIV)}/\Gamma^{r,n(AlXI)}=11/4$$

$$\Gamma^{a,n(CIV)}/\Gamma^{a,n(ALXI)}=(11/4)^{1/3}$$

$$B^{n,CIV}=\Gamma^{r,n}/\Gamma^{LIDS}=0.986/n^3, \quad B^{n,ALXI}=\Gamma^{r,n}/\Gamma^{LIDS}=0.306/n^3$$

$$B^{ALXI}/B^{CIV}\approx 1/3$$

$$\mu\to\mu+\frac{\Delta}{\pi}=\mu-\frac{1}{\pi}\arctan\frac{E_n-E_\varphi-F(E_n)}{\pi\left|V_{E_n}\right|^2}$$

$$V_{ac}\to V_{ac}+M_{ac}^1 I \qquad \Gamma_a=2\pi\left|V_{ac}+M_{ac}^1 I\right|^2$$

Electron collisions with Fe-peak elements: Ni^{4+}, Co^{3+} 'two-particle-one-hole' resonances

- $e^- + Ni^{4+}(3p^6 3d^6\ ^5D) \rightarrow Ni^{3+\,*}(3p^5\,3d^8,\ 3p^5\,3d^7 4s$ or $3p^5\,3d^7 4p)$

  $\downarrow$

  $Ni^{4+}(3p^6 3d^6, 3p^6 3d^5 4s$ or $3p^6 3d^5 4p) + e^-$

Co^{3+} ($1s^2 2s^2 2p^6 3s^2 3p^6 3d^6$ ^5D):

Target models:

$3p^2$-$3d^2$ two electron promotions

(A) Includes all levels in the target approximation with the electronic configurations $3p^6 3d^6$, $3p^6 3d^5 4s$ and $3p^6 3d^5 4p$

(the Hartree-Fock orbitals of the $1s^2 2s^2 2p^6 3s^2 3p^6 3d^6$ ^5D ground state configuration augmented with three spectroscopic orbitals, namely, the *4s*, *4p* and *4d*)

136 LS coupled states with a maximum of around 400 channels for any $LS\pi$ symmetry.

(B) 6-state *LS* –coupled R-matrix calculation. We included in the R-matrix expansion all 136 LS coupled states which arise from six target configuration $3d^6$, $3d^5$ 4s, $3d^5$ 4p + $3p^4$ $3d^8$, $3p^4$ $3d^7$ 4s and $3p^4$ $3d^7$ 4p looking at the effect of configuration interaction

a) *L* = 2, 3 and 4 to illustrate the role of configuration interaction, two-particle-one-hole resonances (M.P.Scott et al. 2006) and the position of the $3d^5$ 4d levels.

b) the inclusion of the $3p^2$-$3d^2$ two electron promotions in order to try and account for electron-correlation effects in the both the target and scattering wavefunctions)

(C)9-state *LS* –coupled R-matrix calculation. Starting with the 136-level model, we included in the R-matrix expansion all states which arise from nine target configuration:

$3d^6$, $3d^5 4s$, $3d^5 4p$,
$3p^4 3d^8$, $3p^4 3d^7 4s$, $3p^4 3d^7 4p$,
$3p^5 3d^7$, $3p^5 3d^6 4s$, $3p^5 3d^6 4p$

***a)* 152 *LS* coupled states which arise from four target configuration $3d^6$, $3d^5 4s$, $3d^5 4p$, $3d^4 4s^2$,**

***b)* 184 *LS* coupled states which arise from four target configuration $3d^6$, $3d^5$ 4s, $3d^5$ 4p, $3p^5$ $3d^7$ and**

***c)* 272 *LS* coupled states which arise from four target configuration $3d^6$, $3d^5 4s$, $3d^5 4p$ and $3p^6 3d^4 4s 4p$.**

2.

Table1. Summary of Co IV target models.

Label	Number of configs.	Configurations
1	3	$3d^6$, $3d^54s$, $3d^54p$
2	4	$3d^6$, $3d^54s$, $3d^54p$, $3p^53d^7$
3	4	$3d^6$, $3d^54s$, $3d^54p$, $3d^44s4p$
4	4	$3d^6$, $3d^54s$,$3d^54p$, $3d^44s^2$
5	6	$3d^6$, $3d^54s$, $3d^54p$, $3p^43d^8$, $3p^43d^74s$, $3p^43d^74p$
6	9	$3d^6$, $3d^54s$, $3d^54p$, $3p^43d^8$, $3p^43d^74s$, $3p^43d^74p$, $3p^53d^7$, $3p^53d^64s$, $3p^53d^64p$

Table 3. The number of *LS*-coupled scattering channels for even and odd parity associated with the total angular momentum value L = 2 in e^- - Co^{3+} collisions using the three-configuration model for specific spin symmetries in the present 136-state calculation.

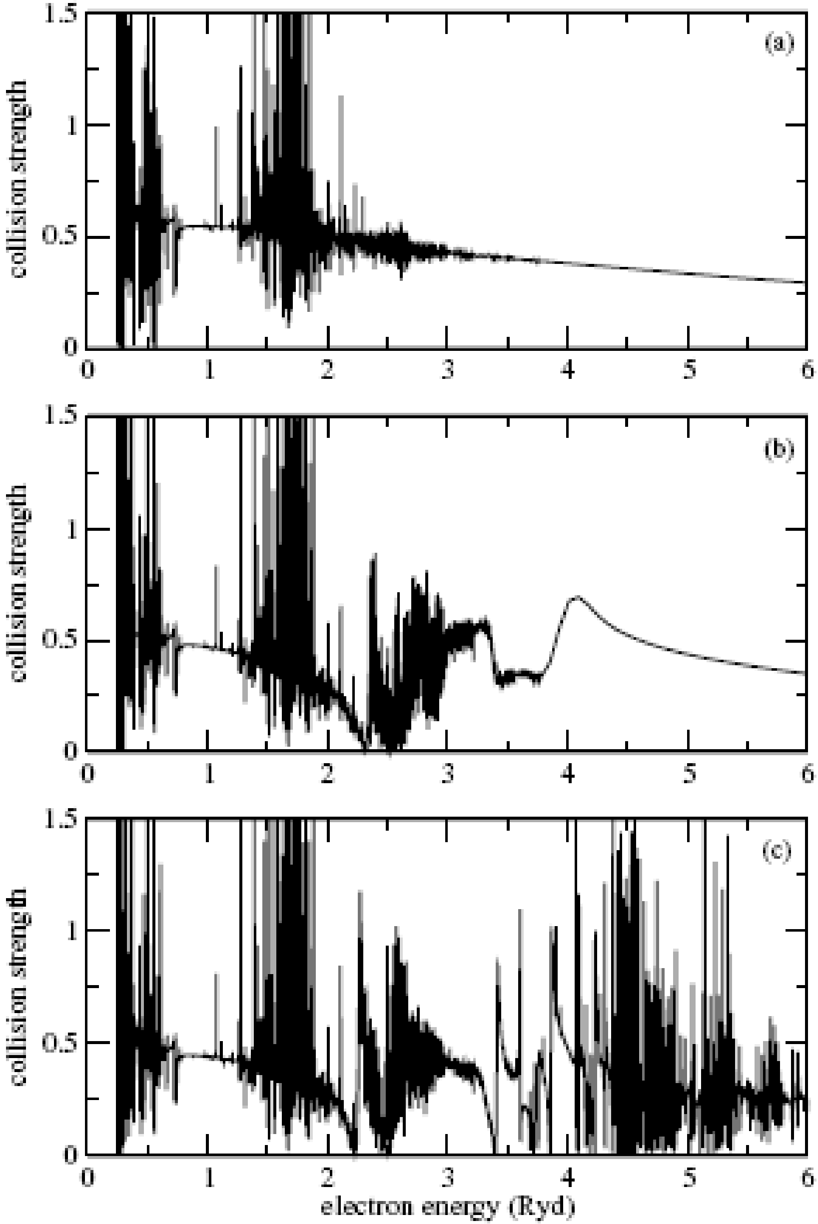
L	Singlets S =0	Triplets S = 1	Quintets S = 2	Septets S = 3
		Even parity		
2	117	147	41	3
		Odd parity		
	105	144	38	1

Table 4. Summary of the total number of coupled channels associated with the total angular momentum value L = 2 in e^- - collision of Co IV states of particular spin (S_i) belonging to $3d^6$, $3d^54s$, $3d^54p$ configurations.

S_i = 1/2		S_i = 3/2		S_i = 5/2		S_i = 7/2	
Even parity	Odd parity	Even parity	Odd parity	Even parity	Odd parity	Even parity	Odd parity
264	269	188	182	44	39	3	1

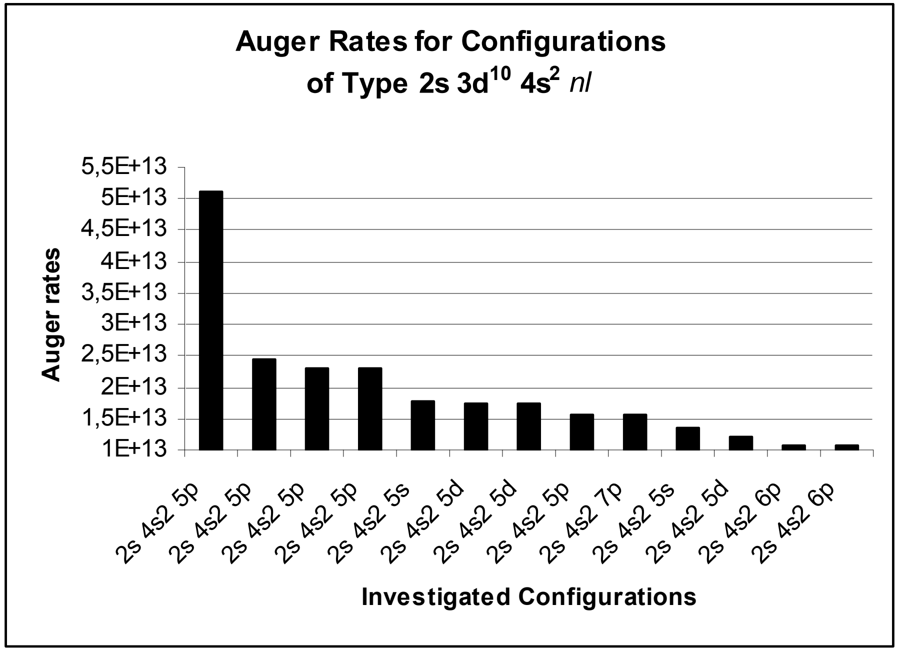
Ni^{4+} Model

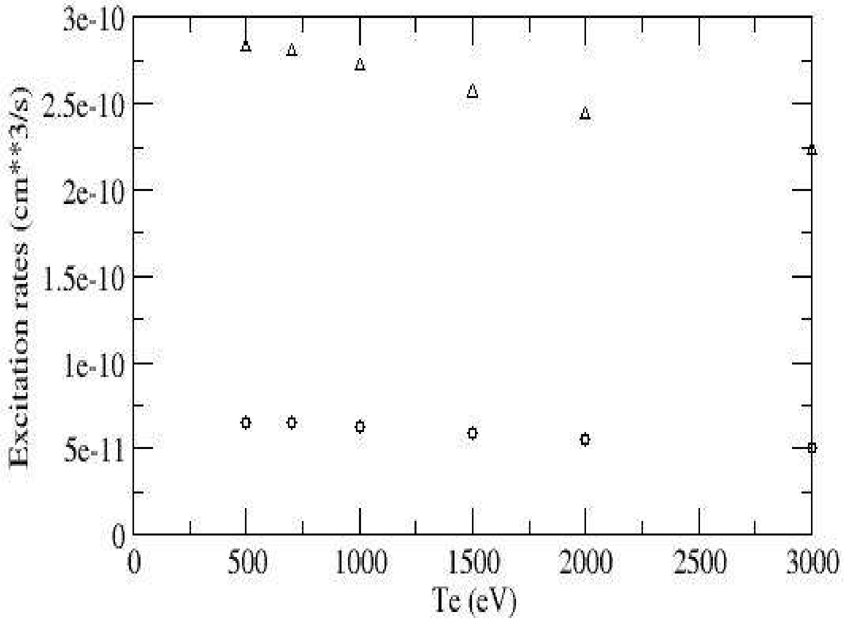
- Calculation (A) -136 LS-coupled target where the intermediate resonance states are not included;
- Calculation (B): (A)+$3p^53d^8$, $3p^53d^74s$ and $3p^53d^74p$ (136 LS-coupled states)
- Calculation (C) = (B) + $3p^5$ $3d^7$ (184 –LS coupled states)

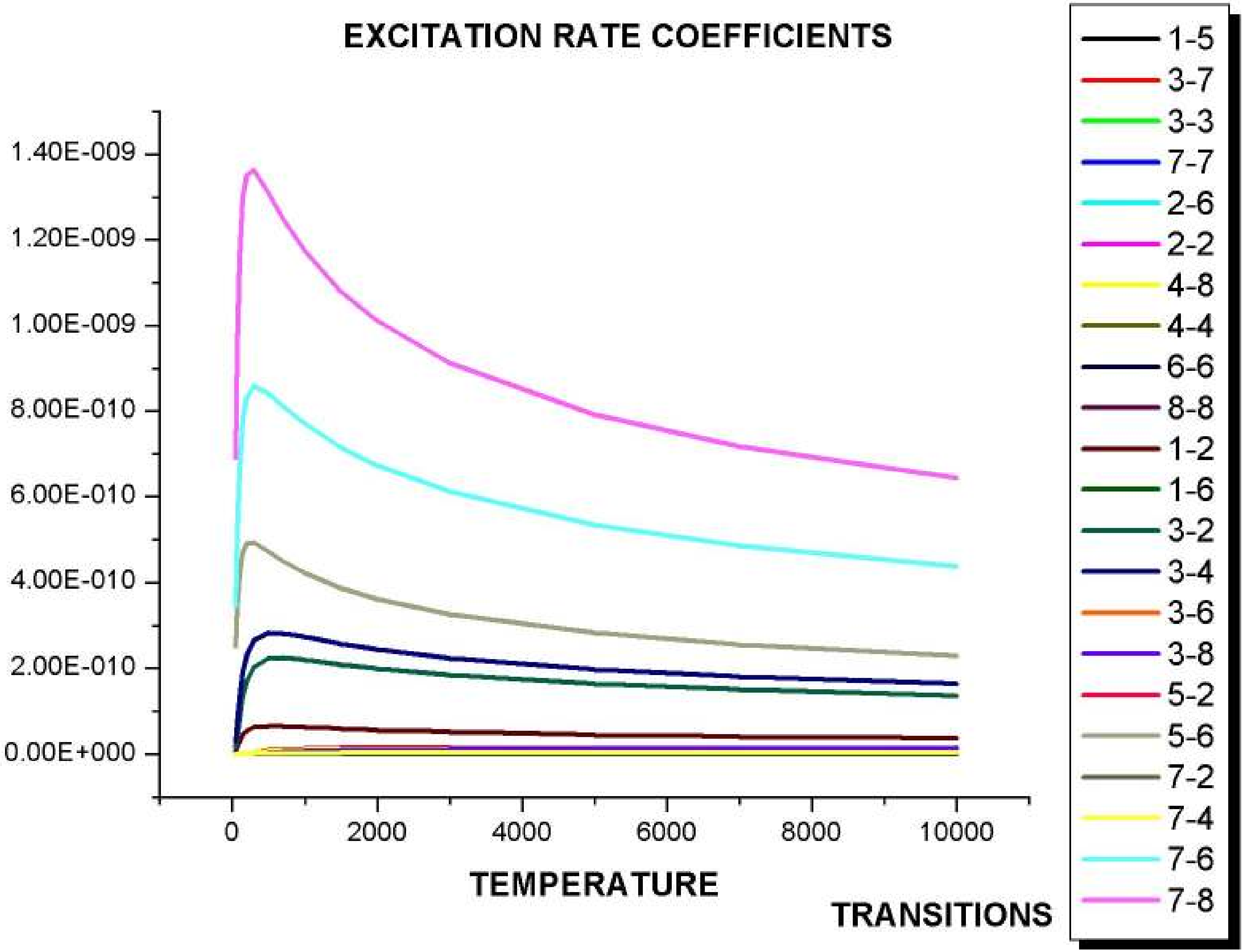


collision strength
(a)
(b)
(c)
electron energy (Ryd)

- Selected electron excitation rates, for $3d^{10}4s^2$–$3d^{10}4s4p$ (o) and $3d^{10}4s4d$-$3d^{10}4s4f$ (Δ) transition
- Position and widths of the resonant states of type $1s^2 2s 2p^6 3s^2 3p^6 3d^{10} 4s^2 nl$







electron impact excitation rates and collision strengths for transitions of type 3d104s*nl* – 3d104s*n'l'*, *n, n'*=4,5, and ΔJ=0,1.

Thank you!