Progress Report on atomic data calculation at INFLPR

V. Stancalie, G. Buica, V. Pais, and collaborators

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Collaborators:

- ITM-TF AMNSD, ISIP (many labs.);
- QUB (P.G. Burke, V. M. Burke, M .P .Scott, A. Hibbert, C. Ramsbottom);
- LIXAM (A. Klisnick);
- IAEA-CRP (inertial fusion-many labs.);

Theoretical models and numerical methods:

- RMATX II for electron excitation of Co IV ions (*ab-initio* non-perturbative approach) (ICAMDATA2007)
- R-matrix Floquet theory and code for DR (POP2005 *a*,*b*, NIMB 2009, LPB 2009)
- (TDSE) Multiphoton ionization of Ca atoms by linearly and circularly polarized laser field using *ab initio* non-perturbative method, above threshold ionization(ATI), (PRA 2006)

Multiphoton Ionization of *Ca* by Linearly and Circularly Polarized Laser Fields

- We theoretically study the ionization of the ***Ca*** atom by the third harmonic of a Ti:Sapphire laser pulse,

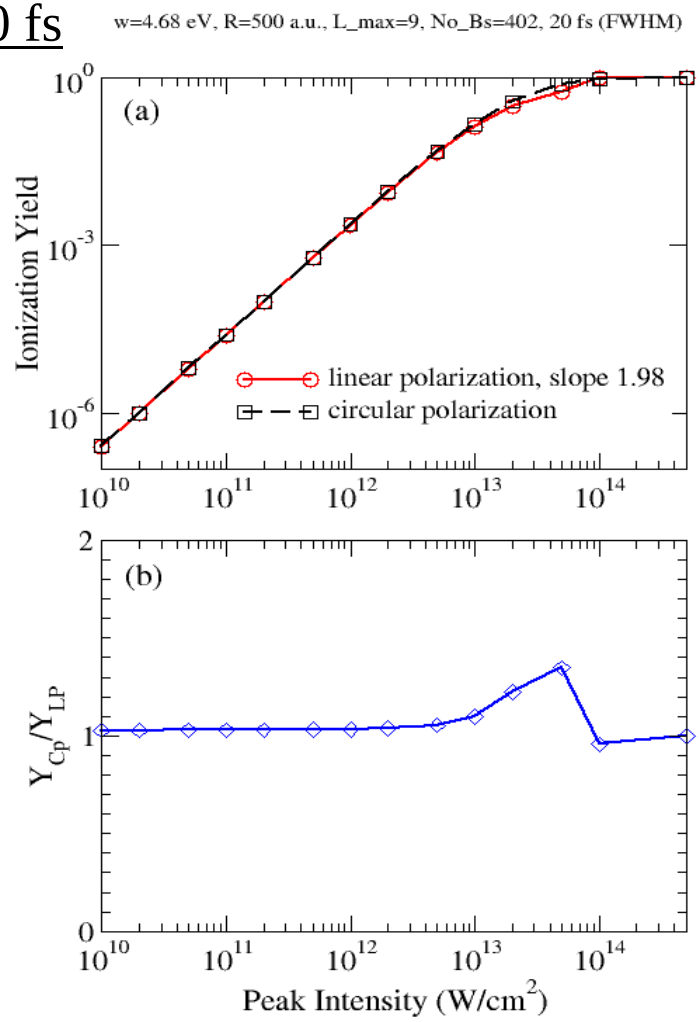
- The ***Ca*** atom (Z=20) is treated as a *two-active*-electron system: the ionic core (the nucleus and the 18 inner-shell electrons $1s^2 2s^2 2p^6 3s^2 3p^6$) and two valence electrons $4s^2$

- The time-dependent Schrödinger equation is numerically integrated on a **basis** of discretized atomic states .

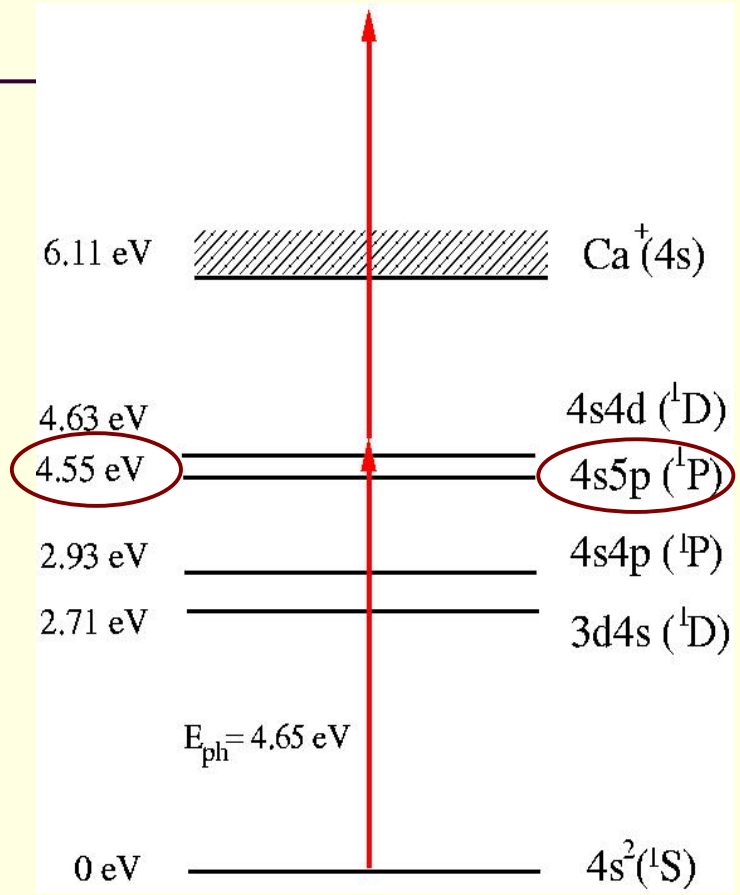
Motivation:

- to provide ab-initio data for multiphoton ionization of ***Ca*** by ***linearly*** **(LP)** and ***circularly polarized*** (**CP**) laser pulses,
- to determine the origin of the **substructures** appearing in the photoelectron energy spectrum (PES) of ***Ca***.

2-photon ionization of ***Ca*** by ***LP*** and ***CP*** laser pulses: λ = 267 nm (E_{ph} = 4.65 eV), τ = 20 fs



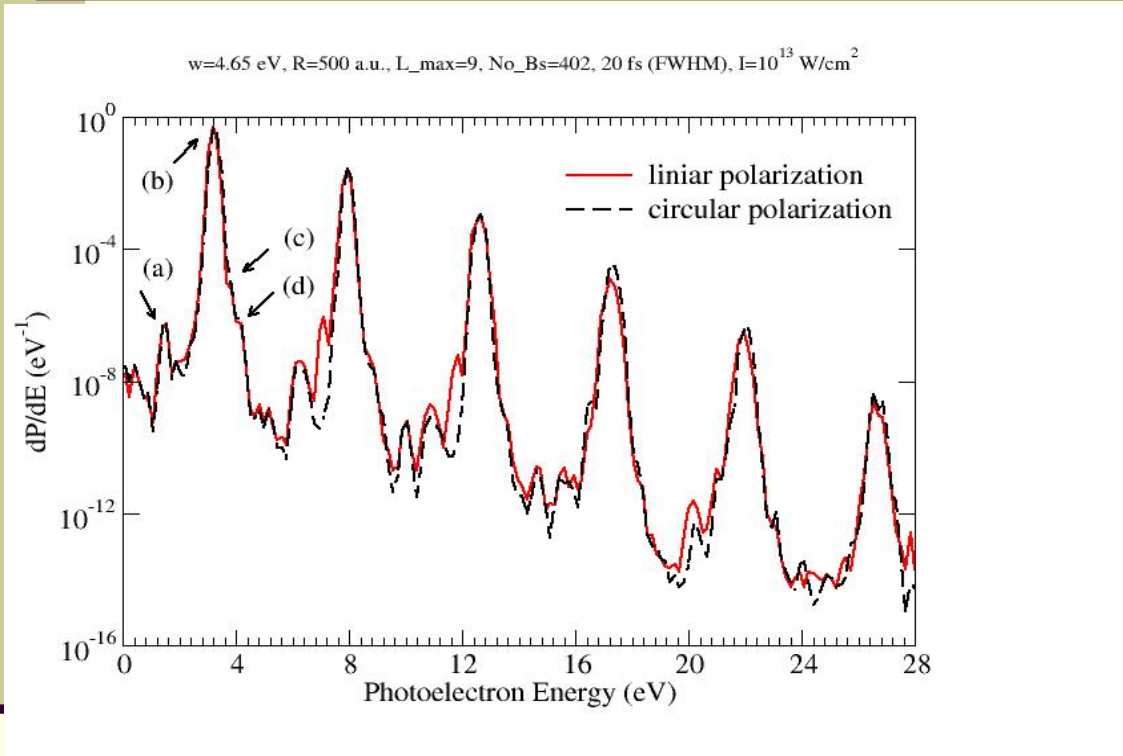
LOPT: Ionization rate = $I^N \sigma^{(N)}$, slope ~ N



*(a) Two-photon ionization yield as a function of the peak intensity by **LP** (solid) and **CP** (dashed) laser pulses.*

*(b) The ratio of the ionization yield by the **CP**, Y_{CP} to that by the **LP** light, Y_{LP}*

Photoelectron energy spectra of ***Ca*** by ***LP*** and ***CP*** laser pulses: λ = 267 nm (E_{ph} = 4.65 eV), τ = 20 fs, I = 1 x 10^{13} W/cm^2



- *The ATI substructures (a),(b),(c),(d) are equally spaced by the photon energy* E_{ph} *= 4.65 eV !*
- *The substructures are due to the real excitation of some bound states* ***4snp^{1}P,n***=*4,5,6,...etc by the laser pulse.*

Concluding remarks (I)

- We studied the multiphoton ionization of ***Ca*** by ***LP*** and ***CP*** laser pulses: Ionization yield and PES.
- We clarified the correct origin of the PES *substructures* by the third harmonic of a Ti-Sapphire laser pulse.
- The ***Ca*** atom has a ***dense*** level structure!
- The ATI *substructures* are due to the real excitation of some bound states ***4snp 1P***, ***n***=*4,5,6,...etc* by the laser pulse.

Resonant single photon ionization in Li-like ions (RMF)

- $X^{Z+}[1s^2 2s(^2S^e)] + e^-$
- $\downarrow\uparrow$
- $X^{(Z-1)**}[1s^2 2pn'l](^1P^0)$

$h\nu$ ↓ ↑

$X^{(Z-1)*}[1s^2 2sn'l(^1S^0)]$

$$2E_{1,2} = E_a + E_g - \omega - i(\Gamma_a + I\gamma)/2 \pm \Omega$$

$$\Omega = \{[d - i(\Gamma_a - I\gamma)/2]^2 + \Gamma_a I\gamma[q - i]^2\}^{1/2}$$

Real part of E as function of frequency

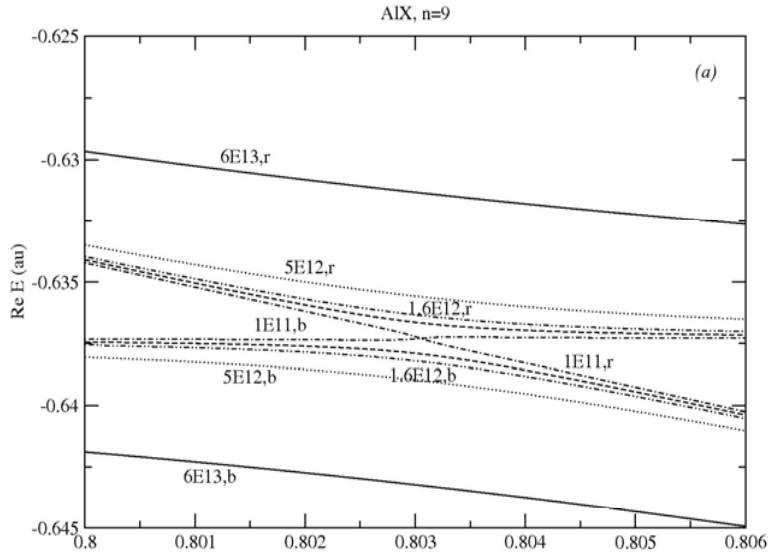


Fig. 3 *(a)*

Imaginary part of E as function of frequency

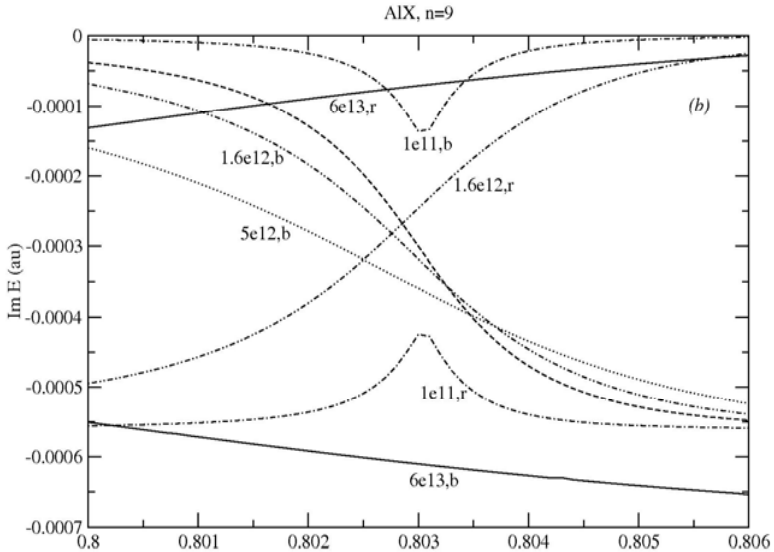
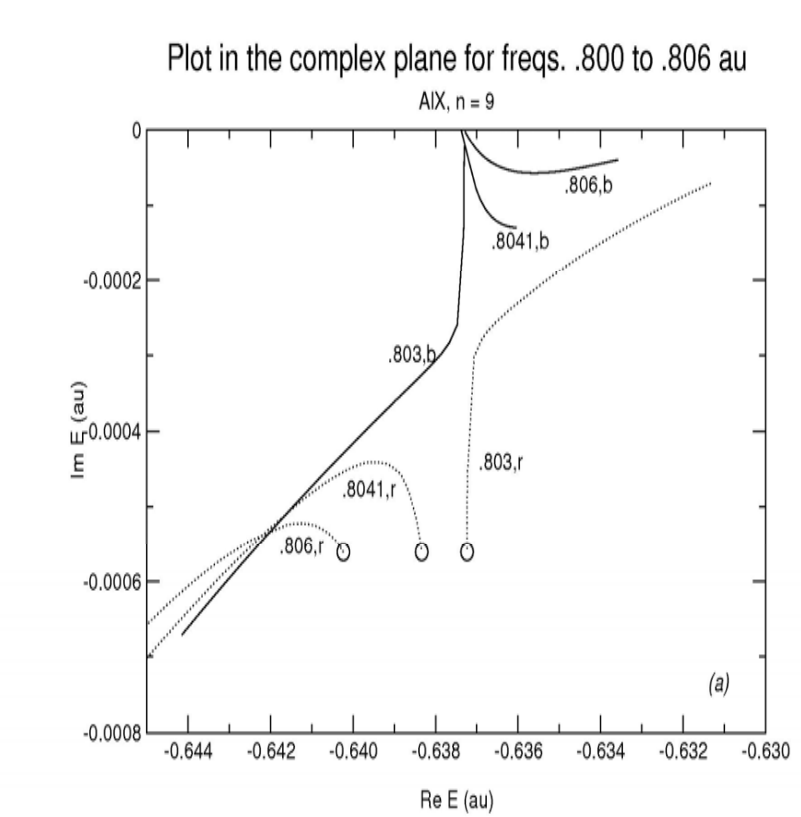
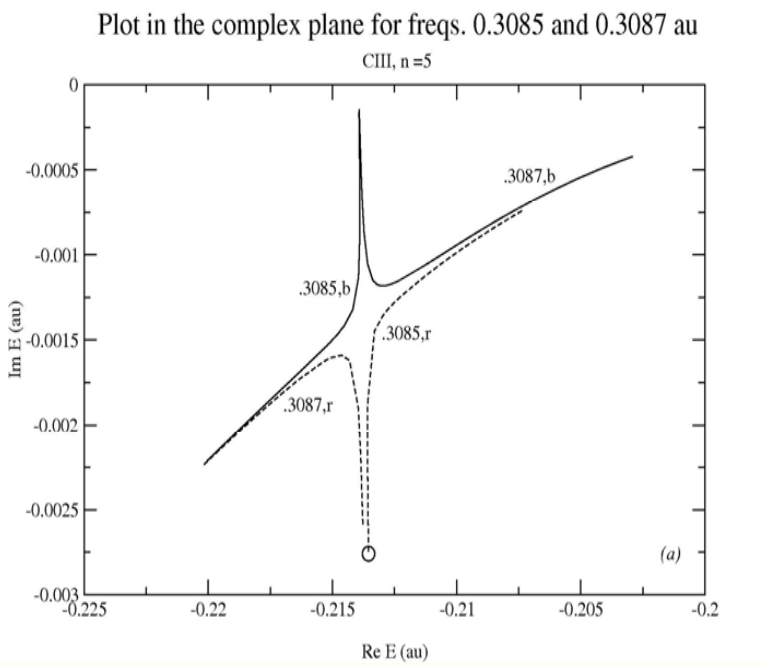


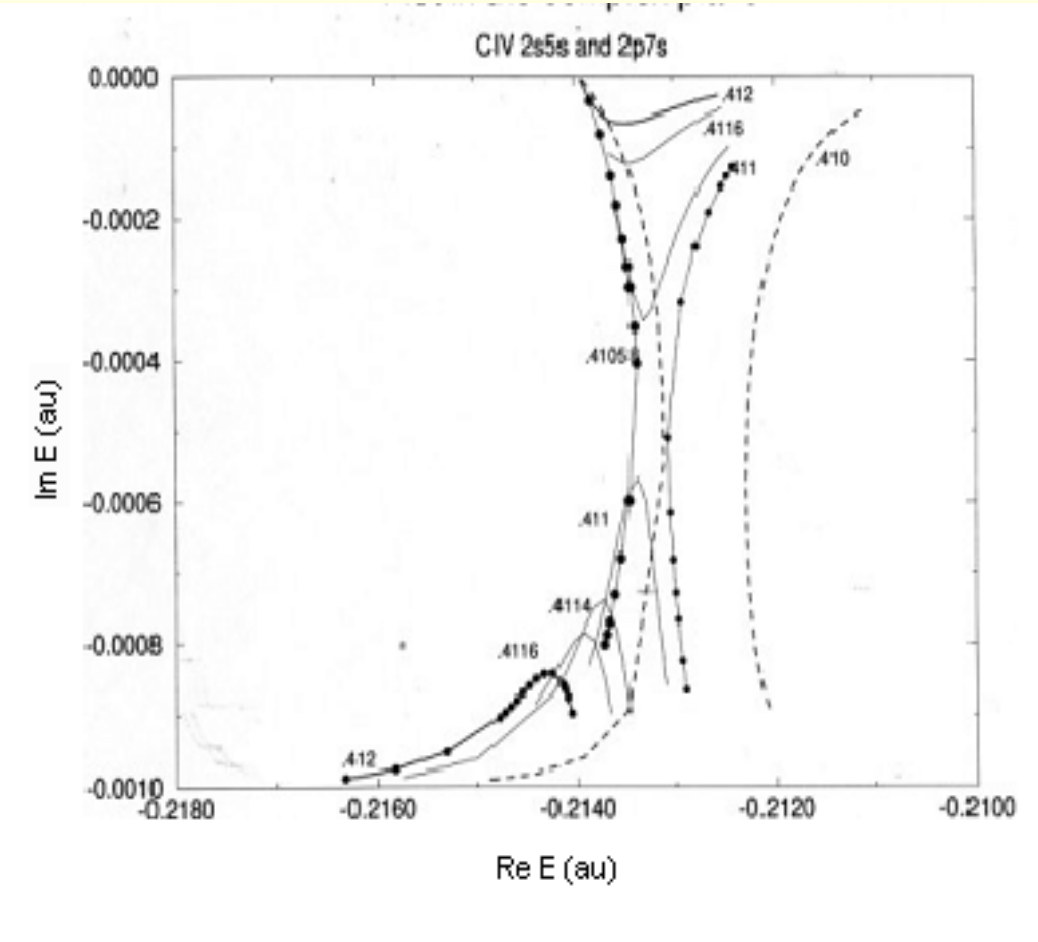
Fig. 3 *(b)*

The resulting complex energies: **LIDS structures: $\Delta n = 0$: $1s^2 2sns$-$1s^2 2pns$**





$\Delta n = 2$ transitions in CIV: $1s^2 2s5s \rightarrow 1s^2 2p7s$



	E_b(au)		E_a(au)
n	This work	OP	
5	-.21394	-.21518	.09496
6	-.13801	-.13849	.15984
7	-.10091	-.10106	.19794
8	-.07656	-.07664	.22221
9	-.06001	-.060059	.23861
10	-.04828	-.0483	.25021
11	-.03967	-.03967	.25872
12	-.03317	-.03315	.26514

Scaling with the effective quantum number:

n	I_{LIDS}(W/cm^2)	$n^{*3}Ei(LIDS)$
5	$5.5\ 10^{11}$	0.17
6	$1.9\ 10^{11}$	0.15
7	$0.9\ 10^{11}$	0.15
8	$0.4\ 10^{11}$	0.15
9	$0.25\ 10^{11}$	0.15
10	$0.2\ 10^{11}$	0.15
11	$0.04\ 10^{11}$	0.14
12	$0.07\ 10^{11}$	0.16

n	I_{LIDS}(W/cm^2)	$n^{*\,3}E_{i(\mathrm{LIDS})}$
9	$3.5\ 10^{11}$	0.195
10	$9.0\ 10^{11}$	0.197
11	$4.8\ 10^{10}$	0.198

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

Electron excitation of Co^{3+}($1s^2 2s^2 2p^6 3s^2 3p^6 3d^6 ({}^5D^e)$)

$$e^- + Co^{3+}(3p^6 3d^6\,{}^5D) \rightarrow Co^{2+*}(3p^5 3d^8, 3p^5 3d^7 4s, 3p^5 3d^7 4p)$$

$$\downarrow$$

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

Target models

A) $3p^6 3d^6$, $3p^6 3d^5 4s$, $3p^6 3d^5 4p$ (136 LS-coupled states) (3 confs.)
B) A +$3p^4 3d^8$, $3p^4 3d^7 4s$, $3p^4 3d^7 4p$(136 LS-coupled states)(6confs.)
C) B + $3p^5 3d^7$,$3p^6 3d^4 4s^2$, $3p^6 3d^4 4s4p$ (184-LS coupled states) (9confs.)

- $3p^6 3d^6$, $3p^6 3d^5 4s$, $3p^6 3d^5 4p$, $3p^6 3d^5 4d$
- $3p^6 3d^6$, $3d^5 4s$, $3d^5 4p$, $3p^5 3d^7$
- $3p^6 3d^6$, $3d^5 4s$, $3d^5 4p$, $3d^4 4s4p$
- $3p^6 3d^6$, $3d^5 4s$, $3d^5 4p$, $3d^4 4s^2$
- $3p^6 3d^6$, $3d^5 4s$, $3d^5 4p$, $3d^4 4p^2$

Summary of optimizations

- In all of the models, the *1s, 2s, 2p, 3s, 3p, 3d* radial functions have been taken from the Hartree-Fock ground state $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^6\ {}^5D$, given in the tables of Clementi and Roetti (1974).
- Using the non-relativistic Schrodinger Hamiltonian, we have established the wave functions by optimizing further three orbitals on various L = 2, 3 and 4 states.
- the *4s* function was obtained by optimizing a 4s orbital on the $3d^5(^6S)\ 4s\ ^7S$ state; hence this function will be a 'real' 4s orbital.
- The same process has been adopted to obtain 'real' function for *4p* orbital, which has been optimized on $3d^5(^6S)\ 4p\ ^7P^0$
- The '*correcting*' 4d orbital has been introduced by optimizing *4d* on $^7D^0$.

C_{jnl} , I_{jnl} , ξ_{jnl} { 1s, 2s, 2p, 3s, 3p, 3d, 4s, 4p, 4d}

$$P_{nl}(r) = \sum_j C_{jnl} r^{I_{jnl}} \exp(-\xi_{jnl} r)$$

2.

Table1. Summary of Co IV target models.

Label	Number of configs.	Configurations
1	3	$3d^6$, $3d^5 4s$, $3d^5 4p$
2	4	$3d^6$, $3d^5 4s$, $3d^5 4p$, $3p^5 3d^7$
3	4	$3d^6$, $3d^5 4s$, $3d^5 4p$, $3d^4 4s4p$
4	4	$3d^6$, $3d^5 4s$,$3d^5 4p$, $3d^4 4s^2$
5	6	$3d^6$, $3d^5 4s$, $3d^5 4p$, $3p^4 3d^8$, $3p^4 3d^7 4s$, $3p^4 3d^7 4p$
6	9	$3d^6$, $3d^5 4s$, $3d^5 4p$, $3p^4 3d^8$, $3p^4 3d^7 4s$, $3p^4 3d^7 4p$, $3p^5 3d^7$, $3p^5 3d^6 4s$, $3p^5 3d^6 4p$

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.

	Singlets	Triplets	Quintets	Septets
L	$S = 0$	$S = 1$	$S = 2$	$S = 3$
		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 $3d^6$, $3d^5 4s$, $3d^5 4p$ 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

Concluding remarks (II):

1. The target state energy levels for all 136 LS levels of calculation A has been obtained;
2. The levels for the states formed by the first 3 configurations overlap each other in energy but the $4s^2$ states all lie higher. However, the $4s^2$, 4s4p and $3p^5 3d^7$ levels overlap each other
3. The 4d states are lying, as expected, between the 4p and $4s^2$ states but overlapping both;
4. Agreement between theory and experiment is reasonably good, the energy differences of low-lying levels usually agreeing to within 15% of each other. An exception to this is the theoretical energy level for the second state which differs from the exp. value by 20%;
5. Theoretical values for the 22^{nd}, 44^{th}, 51^{st}, levels are in the wrong order.

Concluding remarks (III)

1. The target state energy levels for all 136 LS levels of **calculation B** has been obtained:
2. The addition of the extra CI functions arising from the inclusion of the electronic configuration $3p^5 3d^7$ did not effect the energy levels of even parity target states, and made very little difference (less than 0.001 Ryd) to the energy levels of the odd parity states.
3. Agreement between theory and experiment for the second state was improved to 10%;
4. Theoretical values are in good position;
5. The target states energy levels for all 136 LS levels of **calculation C** has been obtained:
6. More than 22 LS levels lie in the Co IV continuum, and experimental data are unavailable.

Thank you!