Project for “Action Fédératrice Etoiles”

Laboratory astrophysics and analysis of stellar spectra

PI : Lydia Tchang-Brillet

Members of the project:

- 1. Nicole Feautrier (LERMA), Elisabetta Caffau (GEPI)
  (Atomic collisions)
- 2. Lydia Tchang-Brillet, C. Balança, N. Champion (LERMA), Coralie Neiner, Richard Monier (LESIA)
  (Vacuum UV spectroscopy)

Laboratory studies of Vacuum Ultra-Violet (VUV) emission spectra of heavy element ions

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Collaborations: Ali Meftah[2,1], Djamel Deghiche[2] et doctorants Kamel Arab[2], Anis Chikh[2] Jean-François Wyart[1,3]

1 LERMA, Observatoire de Paris-Meudon, PSL Research University; Sorbonne Universités, CNRS, Meudon, France

2 Laboratoire de Physique et Chimie Quantique, University Mouloud Mammeri in Tizi-Ouzou, Algeria

3 Laboratoire Aimé Cotton, CNRS, Université de Paris-Saclay, Orsay, France

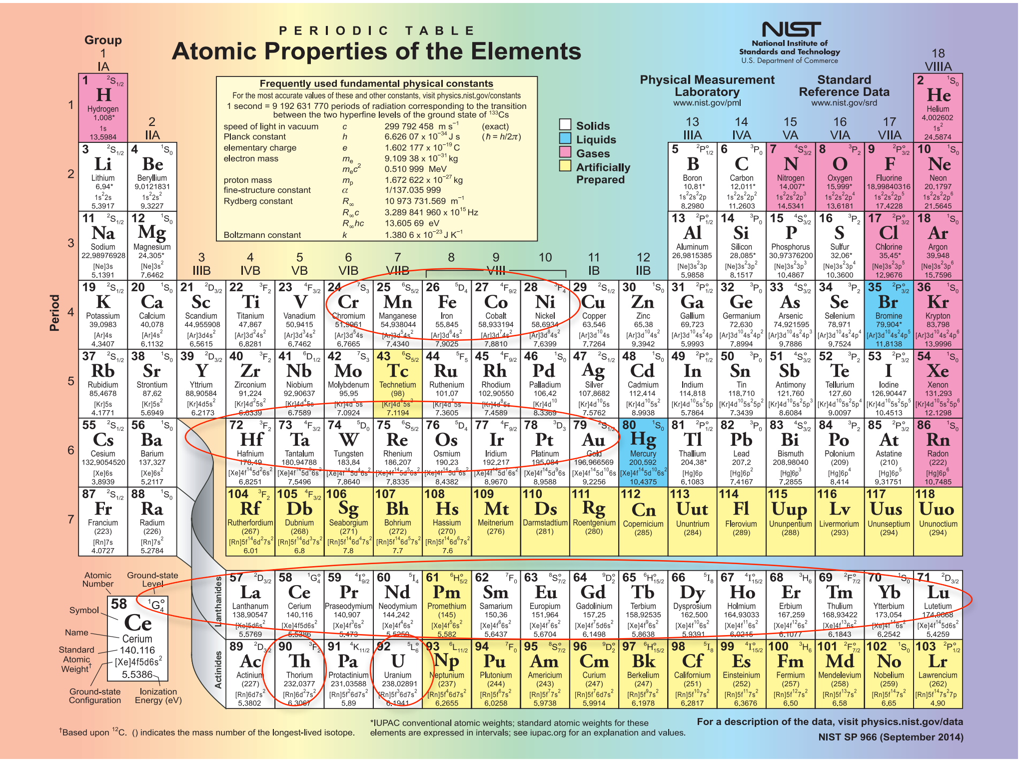
Huge amount of spectroscopic data needed for modeling astrophysical and laboratory plasmas

Since Hubble Space Telescope /STIS ⇒ high quality observational data

✧ Transition metals and lanthanides in stellar spectra
(ex: chemically peculiar stars) ⇒ Abundances

✧ Fe V and Ni V lines in
White Dwarf spectra
⇒ variation of α / gravitation

✧ r-process element ions
(lanthanides and actinides)
formed in neutron star mergers



PERIODIC TABLE
Atomic Properties of the Elements

NIST National Institute of Standards and Technology
U.S. Department of Commerce

Physical Measurement Laboratory
www.nist.gov/pml

Standard Reference Data
www.nist.gov/srd

Frequently used fundamental physical constants
For the most accurate values of these and other constants, visit physics.nist.gov/constants
1 second = 9 192 631 770 periods of radiation corresponding to the transition between the two hyperfine levels of the ground state of ^{133}Cs

speed of light in vacuum	c	299 792 458 m s^{-1}	(exact)
Planck constant	h	6.626 07 x 10^{-34} J s	($\hbar = h/2\pi$)
elementary charge	e	1.602 177 x 10^{-19} C	
electron mass	m_e	9.109 38 x 10^{-31} kg	
	m_ec^2	0.510 999 MeV	
proton mass	m_p	1.672 622 x 10^{-27} kg	
fine-structure constant	α	1/137.035 999	
Rydberg constant	R_∞	10 973 731.569 m^{-1}	
	$R_\infty c$	3.289 841 960 x 10^{15} Hz	
	$R_\infty hc$	13.605 69 eV	
Boltzmann constant	k	1.380 6 x 10^{-23} J K^{-1}	

☐ Solids
🟦 Liquids
🟥 Gases
🟨 Artificially Prepared

Period	1 IA	2 IIA	3 IIIB	4 IVB	5 VB	6 VIB	7 VIIB	8 VIII	9 VIII	10 VIII	11 IB	12 IIB	13 IIIA	14 IVA	15 VA	16 VIA	17 VIIA	18 VIIIA
1	1 H Hydrogen																	2 He Helium
2	3 Li Lithium	4 Be Beryllium											5 B Boron	6 C Carbon	7 N Nitrogen	8 O Oxygen	9 F Fluorine	10 Ne Neon
3	11 Na Sodium	12 Mg Magnesium											13 Al Aluminum	14 Si Silicon	15 P Phosphorus	16 S Sulfur	17 Cl Chlorine	18 Ar Argon
4	19 K Potassium	20 Ca Calcium	21 Sc Scandium	22 Ti Titanium	23 V Vanadium	24 Cr Chromium	25 Mn Manganese	26 Fe Iron	27 Co Cobalt	28 Ni Nickel	29 Cu Copper	30 Zn Zinc	31 Ga Gallium	32 Ge Germanium	33 As Arsenic	34 Se Selenium	35 Br Bromine	36 Kr Krypton
5	37 Rb Rubidium	38 Sr Strontium	39 Y Yttrium	40 Zr Zirconium	41 Nb Niobium	42 Mo Molybdenum	43 Tc Technetium	44 Ru Ruthenium	45 Rh Rhodium	46 Pd Palladium	47 Ag Silver	48 Cd Cadmium	49 In Indium	50 Sn Tin	51 Sb Antimony	52 Te Tellurium	53 I Iodine	54 Xe Xenon
6	55 Cs Cesium	56 Ba Barium		72 Hf Hafnium	73 Ta Tantalum	74 W Tungsten	75 Re Rhenium	76 Os Osmium	77 Ir Iridium	78 Pt Platinum	79 Au Gold	80 Hg Mercury	81 Tl Thallium	82 Pb Lead	83 Bi Bismuth	84 Po Polonium	85 At Astatine	86 Rn Radon
7	87 Fr Francium	88 Ra Radium		104 Rf Rutherfordium	105 Db Dubnium	106 Sg Seaborgium	107 Bh Bohrium	108 Hs Hassium	109 Mt Meitnerium	110 Ds Darmstadtium	111 Rg Roentgenium	112 Cn Copernicium	113 Uut Ununtrium	114 Fl Flerovium	115 Uup Ununpentium	116 Lv Livermorium	117 Uus Ununseptium	118 Uuo Ununoctium

Lanthanides	57 La Lanthanum	58 Ce Cerium	59 Pr Praseodymium	60 Nd Neodymium	61 Pm Promethium	62 Sm Samarium	63 Eu Europium	64 Gd Gadolinium	65 Tb Terbium	66 Dy Dysprosium	67 Ho Holmium	68 Er Erbium	69 Tm Thulium	70 Yb Ytterbium	71 Lu Lutetium
Actinides	89 Ac Actinium	90 Th Thorium	91 Pa Protactinium	92 U Uranium	93 Np Neptunium	94 Pu Plutonium	95 Am Americium	96 Cm Curium	97 Bk Berkelium	98 Cf Californium	99 Es Einsteinium	100 Fm Fermium	101 Md Mendelevium	102 No Nobelium	103 Lr Lawrencium

Atomic Number, Ground-state Level, Symbol, Name, Standard Atomic Weight†, Ground-state Configuration, Ionization Energy (eV): 58, $^1G^\circ_4$, Ce, Cerium, 140.116, [Xe]4f5d6s^2, 5.5386

†Based upon ^{12}C. () indicates the mass number of the longest-lived isotope.

*IUPAC conventional atomic weights; standard atomic weights for these elements are expressed in intervals; see iupac.org for an explanation and values.

For a description of the data, visit physics.nist.gov/data

NIST SP 966 (September 2014)

Lanthanide ions: IV and V spectra

$5p^6 4f^N$ and $4f^{N-1}$ nl, $5p^5 4f^N$nl open subshells

- Existing experimental data rather incomplete

- Dense and complex spectra in the Vacuum Ultra Violet (VUV) range (300-3000Å)

➔ need high resolution studies and systematic isoelectronic or isoionic approach

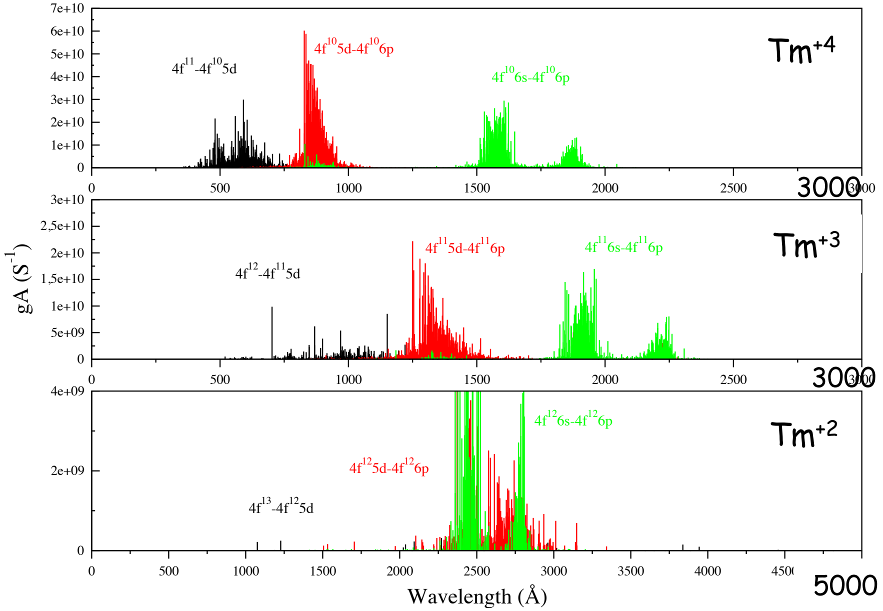
- Current works : Tm V, extension of Tm IV, high configurations of Nd IV

Also analysis of the Dy^{3+} spectrum and extension of Er^{3+}, U^{4+} spectra

Transition metal ions
Mn^{3+}, Fe^{5+}, Ni^{6+}
(coll. Ryabtsev and colleagues, Institute of Spectroscopy Troitsk, Moscow, Russia and T. Raassen, P. Uylings Amsterdam)

Spectra of some Thulium ions (Tm)

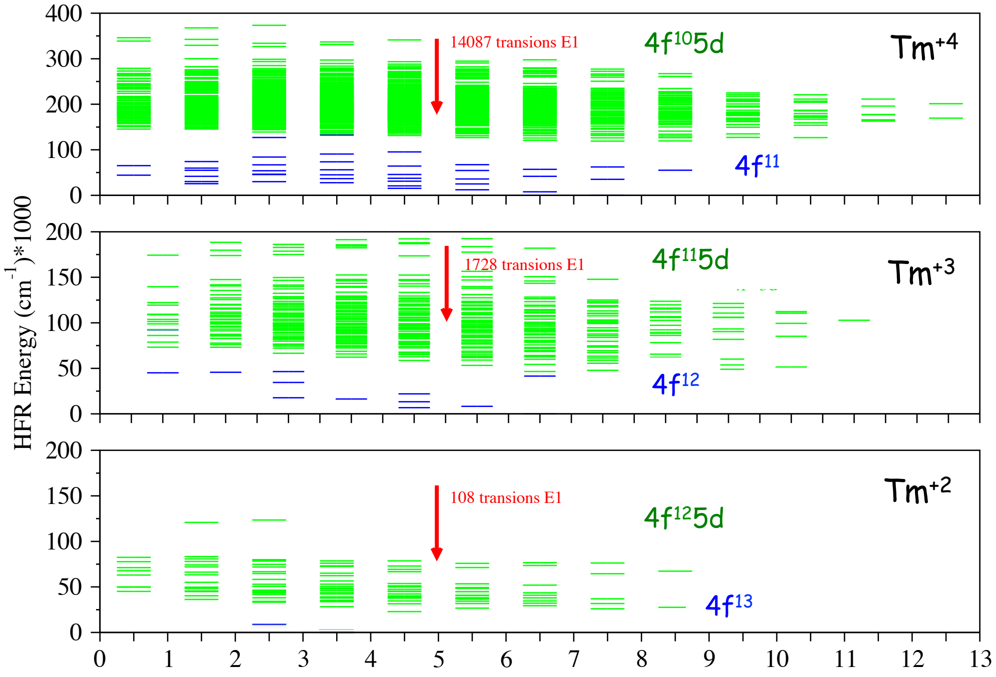
Spectrum predicted (HFR energy parameters)



λ (Å)

Predicted transition arrays

Resonance Transitions in Tm V, Tm IV and Tm III

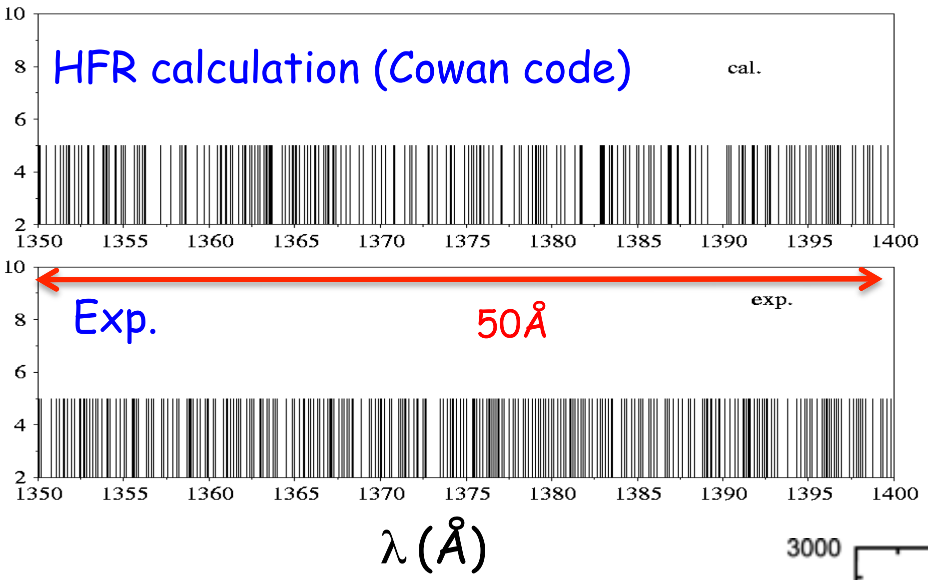


J

Energy levels

Nd IV spectrum

Direct identification $\lambda_{cal} \Leftrightarrow \lambda_{exp}$ impossible !!

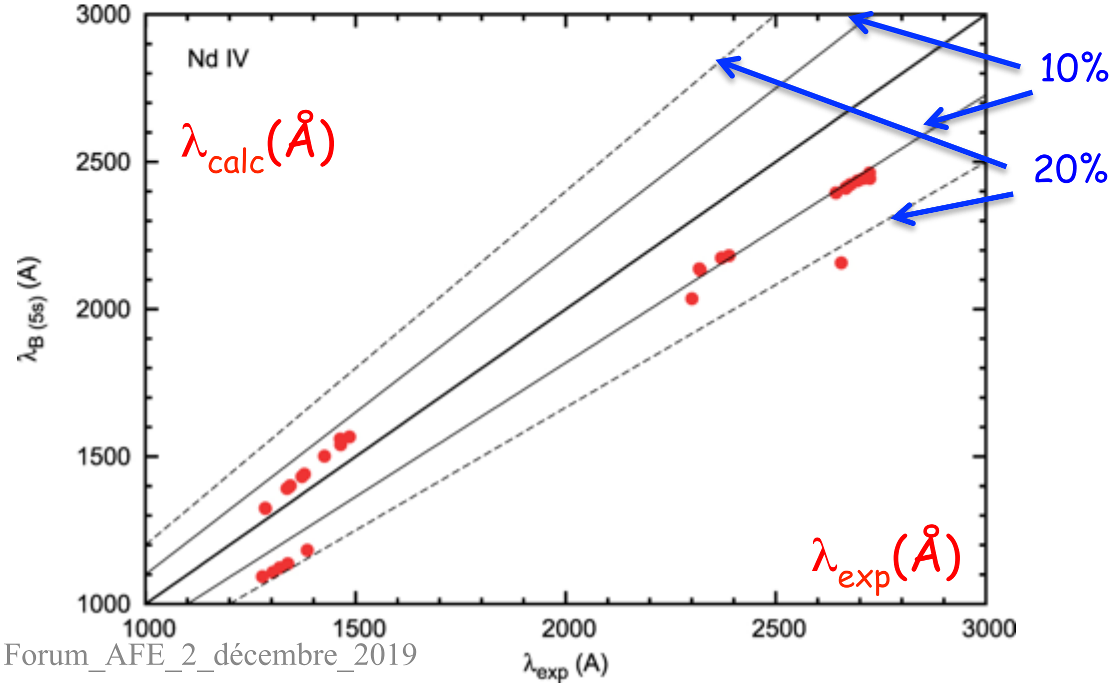


~ 180 lines ∈ (1350-1400Å)

$4f^3$ - $4f^25d$, $4f^25d$- $4f^26p$ transitions

Wyart et al J. Phys. B 2007

$\Delta\lambda_{exp}$ = ± 0.001-0.005 Å
$\Delta\lambda/\lambda \sim 10^{-6}$ at 1000Å



Multiconfiguration Dirac-Hartree-Fock calculations (GRASP2 code)
Comparison λ_{cal} and λ_{exp}

G. Gaigalas et al. ApJS 2019

High resolution VUV normal incidence 10m-spectrograph
Paris - Meudon Observatory

- Concave holographic grating focal distance 10.7 m, 3600 lines/mm, dispersion = 0.25 Å /mm first order

- Resolution ~ 150 000 (8mÅ, slit 30μm)

- One single exposure : 2 x 120Å on 18″ photographic plates
  or 2 x 100Å on 15″ image plates (IP)

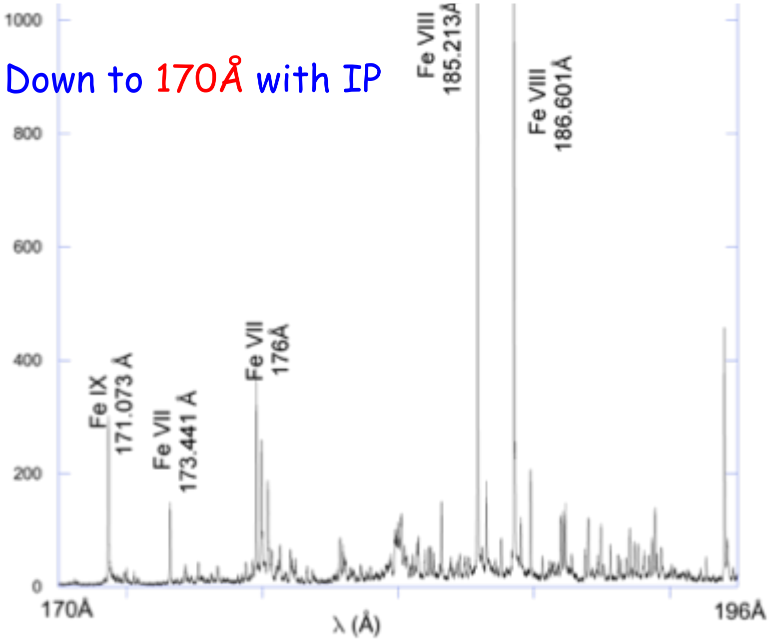
- Wavelength range : 300-3000 Å

Light sources :

High voltage vacuum sparks for moderately charged ions (2 – 7 times)

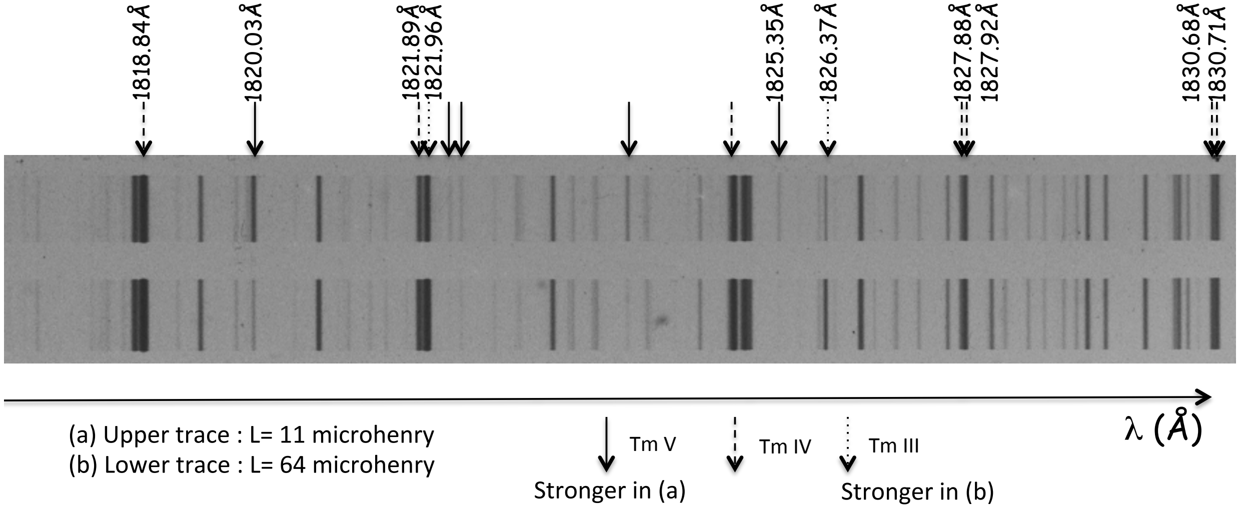
Hollow Cathode for neutral or singly charged ions

(Penning discharge for molecular spectra)



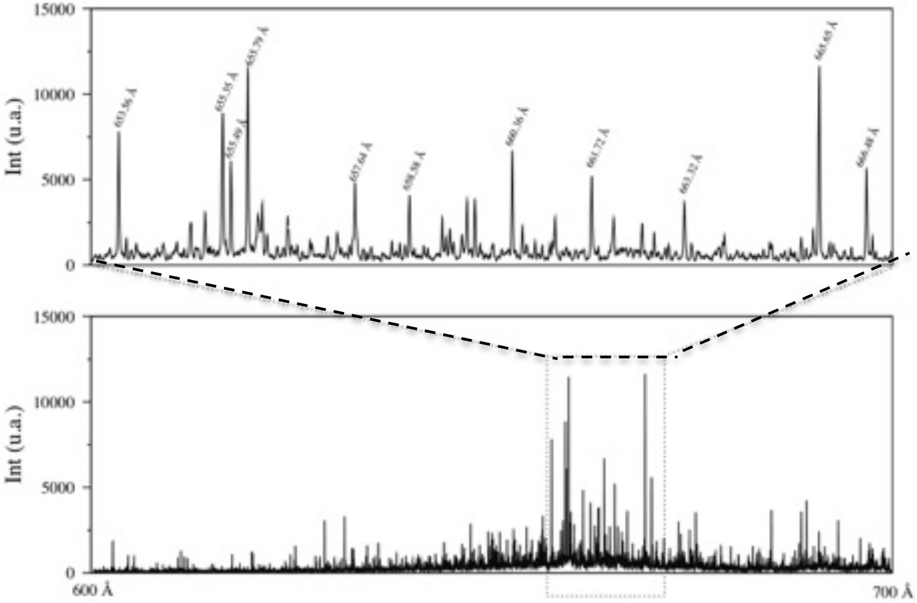
Down to 170Å with IP

Sections of thulium vacuum spark emission spectrum on image plate



(a) Upper trace : L= 11 microhenry
(b) Lower trace : L= 64 microhenry

Tm V lines (600-700Å)



Tm III, IV, V lines (1810-1830Å)

Complementarity

Image plate :
linear response in intensities
over 5 orders of magnitude

Photographic plate:
For better wavelength measurements
Δλ = ± 0.001-0.005Å

The aim of the analysis :

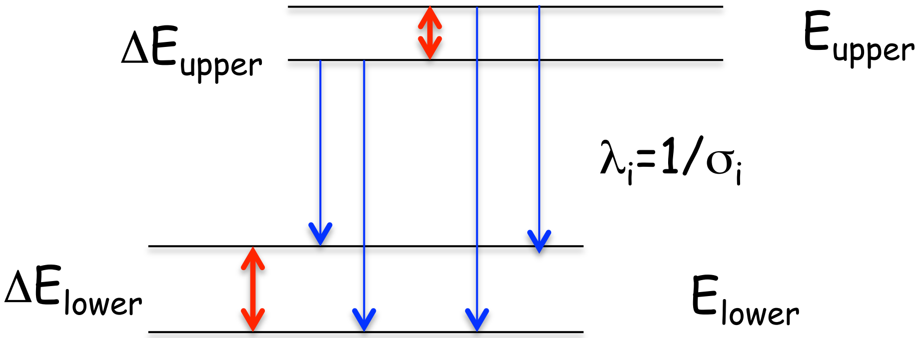
to build the experimental energy level scheme from observed line wavelengths

✧ Ritz combination principle :

$$\sigma = (\lambda)^{-1} = E_{upper} - E_{lower}\ (\mathrm{cm}^{-1})$$

\+

Selection rules



✧ Consistency : Line intensities ←→ calculated gA

⇒ assign a correct J value to each level

Theoretical Method (Racah-Slater): Parametric calculations
RCN/RCG/RCE codes by R.D. Cowan

1) Ab initio step : Relativistic Hartree-Fock (HFR) $H = H_0 + H_1$

H_0 : central field → Hartree-Fock solution

H_1 = electrostatic int. + relativistic corr. (spin-orbit)

- Diagonalization of H_1 → basis set of one or several configurations (CI)

⇒ E_{cal} and gA or log(gf)

Iterations

2) Semi-empirical step (RCE-LSQ fit)

matrix element : $H_{1ij} = \sum_{\alpha} c_{ij}^{\alpha} P_{\alpha}$ c_{ij}^{α} : angular part → Racah algebra

P_{α} : radial integral → ajustable energy parameters

Least squares fits to minimize $\Delta E = \sqrt{\sum_{i} (E_i^{exp} - E_i^{cal.})^2 / (N_l - N_p)}$ $N_l \gg N_p$

Iterative cycle (diagonalization + LSQ fit)
Key points

- Correction of ab initio configuration $E_{average}$ according to observed transition array wavelengths ⇒ improved CI effects

- Correct correspondance $E_{cal} \Leftrightarrow E_{exp}$ for levels of same J ⇒ gA

- Good initial values for parameters : HFR values x scaling factors

Initial values of the parameters :
HFR values or multiplied by a scaling factor $SF=P_{fit}/P_{HFR}$

Consistency of scaling factor (SF) values and effective CI parameters

Parameters	**Nd IV**	Nd V	**Tm IV**	Er II	**Yb V**	**Er IV**
	$4f^3$+… $4f^25d$+…	$4f^2$+4f6p 4f5d+….	$4f^{12}+4f^{11}6p$ $4f^{11}5d$+…	$4f^{12}6p$ $4f^{12}5d$….	$4f^{12}+4f^{11}6p$ $4f^{11}5d$+…	$4f^{11}+4f^{10}6p$ $4f^{10}5d$+…
F^2(4f,4f)	0.768	0.761	0.785	0.763	0.800	0.779
F^4(4f,4f)	0.839	0.852	0.868	0.844	0.898	0.880
F^6(4f,4f)	0.797	0.766	0.855	0.930	0.864	0.877
ζ_{4f}	0.932	0.927	0.982	0.981	0.982	0.991
F^2(4f,5d)	0.758	0.763	0.806	0.816	0.807	0.804
F^4(4f,5d)	1.082	1.100	1.132	1.174	1.129	1.152
G^1(4f,5d)	0.846	0.860	0.751	0.683	0.774	0.693
G^3(4f,5d)	0.954	0.983	0.974	1.013	0.960	0.966
G^5(4f,5d)	0.839	0.868	0.830	0.753	0.843	0.822
F^2(4f,6p)	0.797	0.815	0.867	0.820	0.844	0.803
ζ_{6p}	1.207	1.168	1.17	1.320	1.143	1.173
Effective CI parameter F^1(4f,5d)	**758±57**	**839±147**	**866±106**	**902±62**	**819±81**	**1066±109**

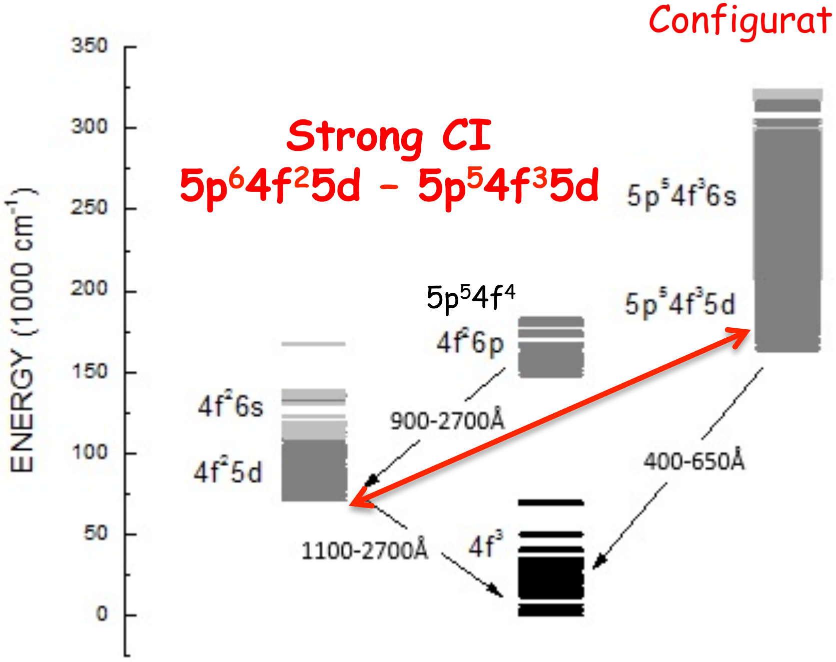
Tm V
Lines & levels

E_{upper} (cm^{-1})	J_{upper}	4f^{10}6p	λ(Å)	σ(cm^{-1})	Int_{exp}	gA(s^{-1})	E_{lower} (cm^{-1})	J_{lower}	4f^{10}5d +6s
249871.29	7.5	^{6}H	896.49	111546.14	150	1.585E+10	138325.83	7.5	^{6}H
			900.59	111038.31	157 P	8.208E+09	138833.94	8.5	^{6}I
			906.20	110350.91	141	1.989E+10	139521.49	6.5	^{6}G
			1837.74	54414.58	181	9.472E+09	195456.43	8.5	^{6}I
			1903.77	52527.23	22	2.197E+09	197343.07	7.5	^{4}I
250401.53	8.5	4K	892.25	112076.21	45	7.533E+09	138325.83	7.5	^{6}H
			896.32	111567.29	169	1.536E+10	138833.94	8.5	^{6}I
			918.04	108927.71	180	2.331E+10	141474.16	9.5	^{6}K
			959.40	104231.81	38	2.887E+09	146171.21	9.5	^{6}K
			1820.03	54943.94	156	6.833E+09	195456.43	8.5	^{6}I
			1884.74	53057.54	121	5.137E+09	197343.07	7.5	^{4}I
257574.44	7.5	^{6}K	893.63	111903.42	51	3.305E+09	145671.02	8.5	^{4}K
260932.23	8.5								
261034.65	9.5								

Configurations	J	E_{exp} (cm^{-1})	E_{calc} (cm^{-1})	ΔE (cm^{-1})	$g_{Landé}$	LS level composition Comp.1	Perc.	Comp.2	Perc.
Odd 4f^{11}	7.5	0.00	0.2	-0.2	1.196	^{4}I	97%	^{2}K	3%
	6.5	7674.92	7708.8	-33.9	1.106	^{4}I	99%	^{2}K	1%
4f^{10}6p	7.5	249871.29	249704.1	167.2	1.276	(^{5}I) ^{6}H	56%	(^{5}I) ^{4}I	19%
	8.5	250401.53	250211.8	189.7	1.215	(^{5}I) ^{4}K	41%	(^{5}I) ^{6}I	33%
	7.5	257574.44	257362.2	212.2	1.148	(^{5}I) ^{6}K	34%	(^{5}I) ^{4}K	30%
	8.5	260932.23	261033.9	-101.7	1.240	(^{5}I) ^{6}I	57%	(^{5}I) ^{4}K	32%
	9.5	261034.65	261133.6	-99.0	1.254	(^{5}I) ^{6}K	91%	(^{3}K) ^{4}L2	7%
	7.5	261938.10	261980.8	-42.7	1.235	(^{5}I) ^{4}I	57%	(^{5}I) ^{6}H	31%
	7.5	268153.00	268229.6	-76.6	1.184	(^{5}I) ^{6}I	54%	(^{5}I) ^{4}K	27%
Even 4f^{10}5d	7.5	138325.83	138487.4	-161.6	1.272	(^{5}I) ^{6}H	48%	(^{5}I) ^{6}I	28%
	8.5	138833.94	138935.7	-101.8	1.254	(^{5}I) ^{6}I	63%	(^{5}I) ^{6}K	18%
	6.5	139521.49	139674.7	-153.2	1.324	(^{5}I) ^{6}G	58%	(^{5}I) ^{6}H	22%
	9.5	141474.16	141568.5	-94.3	1.210	(^{5}I) ^{6}K	48%	(^{5}I) ^{4}I	23%

Nd IV

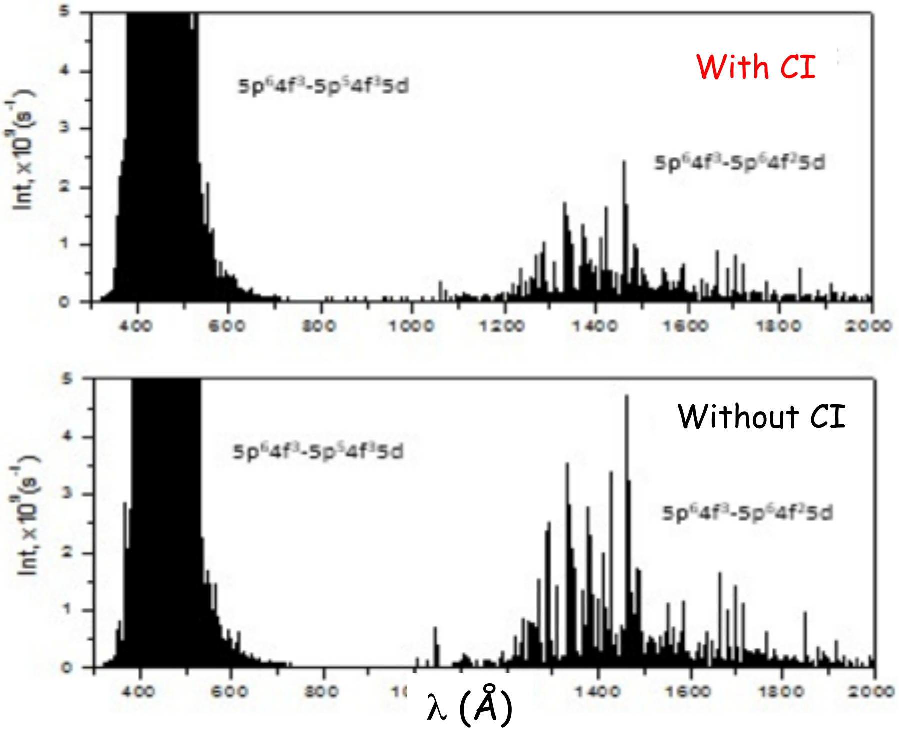
Core-excited Configurations



Strong CI

$5p^64f^25d$ – $5p^54f^35d$

Resonance transition intensities reduced by 1/2
due to CI $5p^64f^25d$ - $5p^54f^35d$



Low configurations (Wyart et al 2007)

1426 lines (900 -2700Å)

Odd $4f^3 + 4f^26p + 5p^54f^4$:

111 levels, 27 param., rms 91 cm^{-1}

Even $4f^25d + 4f^26s + 5p^54f^35d$:

121 levels, 38 param., rms 37 cm^{-1}

Predicted $E_{av}(5p^54f^35d) = 221000$ cm^{-1}

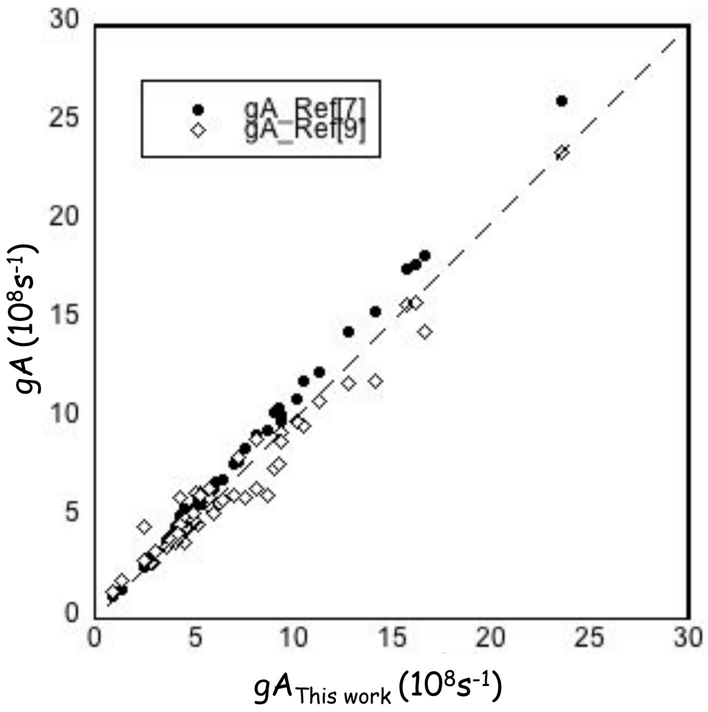
Core-excited configurations (Arab et al 2019)

313 lines (400-650Å), 125 new levels

19 param. rms 182 cm^{-1}

$E_{av}(5p^54f^35d) = 221076$ cm^{-1}

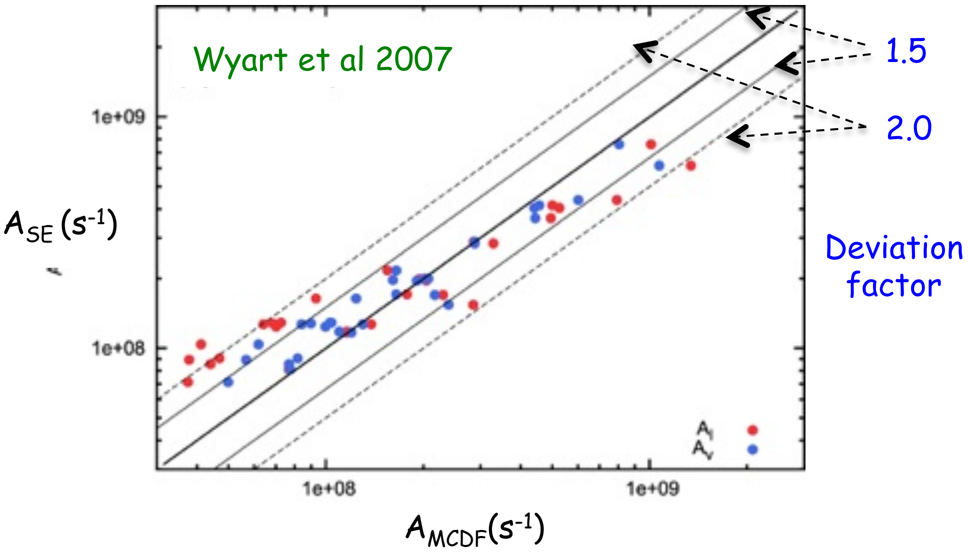
Nd IV

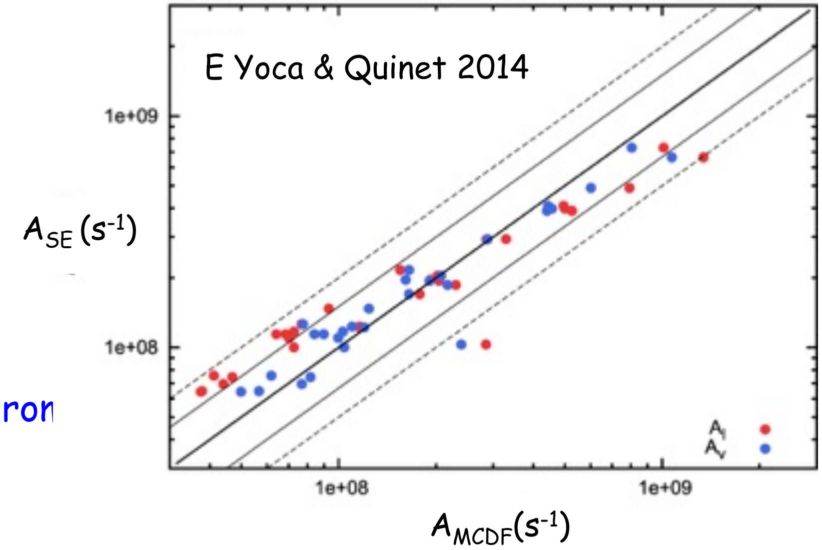


Comparison of semi-empirical gA values fron
parametric calculations
Diagonal : Arab et al 2019

- ● : Wyart et al 2007
- ◇ : same experimental levels

Core-polarization, larger basis,
Enzonga Yoca & Quinet 2014





Comparison of MCDF
and semi-empirical values of
Einstein coeff. A in s^{-1}
G. Gaigalas et al. ApJS 2019

Conclusions

- Knowledge of experimental energy levels

\+ parametric interpretation of atomic configurations

⇒ E_{exp} for validation of ab initio E_{th} (E_{th} could deviate up to 30%)

⇒ Reliable semi-empirical values of gA or log(gf), lifetimes, branching ratios, Landé factors, partition fonctions

⇒ improved predictions for unknown levels and transition probabilities

- Systematic trends by isoelectronic or isoionic sequences

⇒ better estimation of scaling factors for the initial parameter values

⇒ disentangling complex spectra

Identified lines and experimental level energies on molat.obspm.fr

Tm IV (EPJD 2007)

- 760 lines, 209 energy levels

Nd IV (J. Phys. B 2007)

- 1426 lines, 232 levels

Eu III (A&A 2008)

- 90 new lines, 30 new levels
- (1150 Ritz wavelengths)

Nd V (Physica Scripta 2008)

- 160 lines 48 levels

More recent

Yb V (Physica Scripta 2013)

- 1080 lines, 242 energy levels

Nd V (Physica Scripta 2015) for core-excited configurations

- 304 lines, 104 energy levels

Er IV (J. Phys. B 2016)

- 591 lines, 120 energy levels

Nd IV (2019) for $5p^5 4f^3 5d$ core-excited configuration

- 313 lines, 125 energy levels

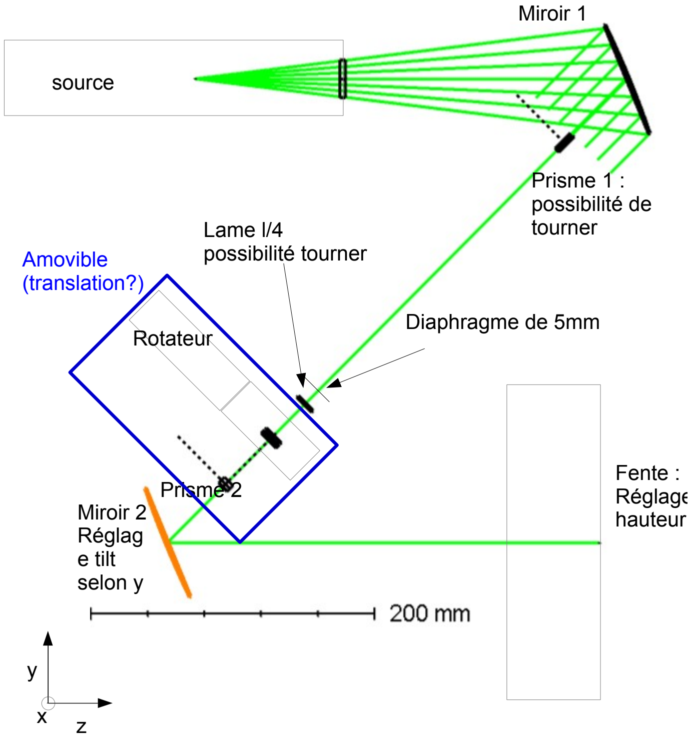
Coming soon

U II (Atoms 2017)

541 UV lines, interpretation of 253 odd levels and 125 even levels

Calibration of a prototype UV polarimeter
Schematics
(C. Neiner LUVOIR/POLLUX)

Schéma design banc de test prototype polarimètre UV



→ VUV 10m spectrograph

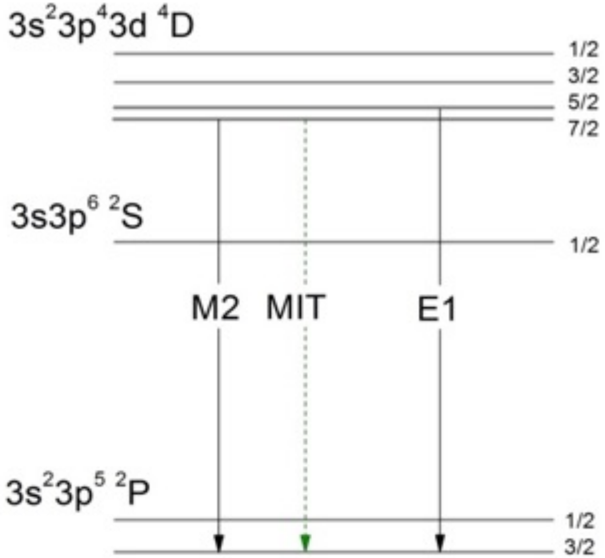
Measurement of magnetic field without polarization ?

Fe X : magnetic field induced transition (MIT)

Coll. R. Hutton, Y. Yang (Shanghai), T. Brage (Lund)

$I_{MIT}/I_{E1} \propto B^2$

Observation and modeling of an assymetric profile from two unresolved lines ?



⇕ $\Delta E(5/2-7/2)$ = ?
(~ 5 cm^{-1})

EBIT ion source
+
Meudon 10m Spectrograph

Schematic energy-level diagram for Cl-like ions with $Z < 26$ and zero nuclear spin, where $E(^4D_{7/2}) < E(^4D_{5/2})$ in $3s^23p^43d$. For $Z > 26$, $E(^4D_{5/2}) < E(^4D_{7/2})$.

B=0, E1 transition allowed from $^4D_{5/2}$ to the ground state, forbidden from $^4D_{7/2}$.
When B ≠ 0, $^4D_{7/2}$ is mixed with $^4D_{5/2}$, an E1 transition opens up from the $^4D_{7/2}$ to the ground state (MIT)

Thank you for your attention !