Present status of the investigation on the spectra of moderately charged thulium ions

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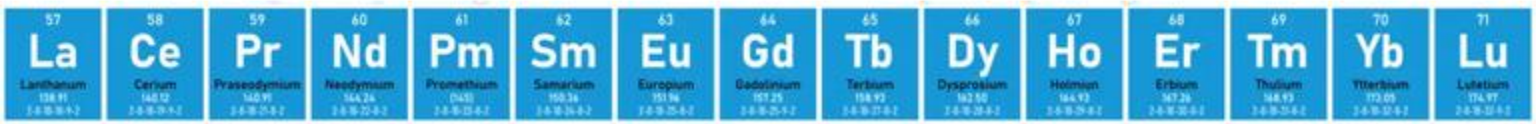
Tribute to Jean-François Wyart

Plan

- Introduction
- Experimental method
- Analysis and Results
- Conclusion

Introduction

Lanthanide properties



- Z = 57 $\longrightarrow$ 71 with open f-shell configurations.
- 4f, 5d, 6s and 6p have similar binding energies:
- Overlapping configurations
- High level densities, even at a few eV

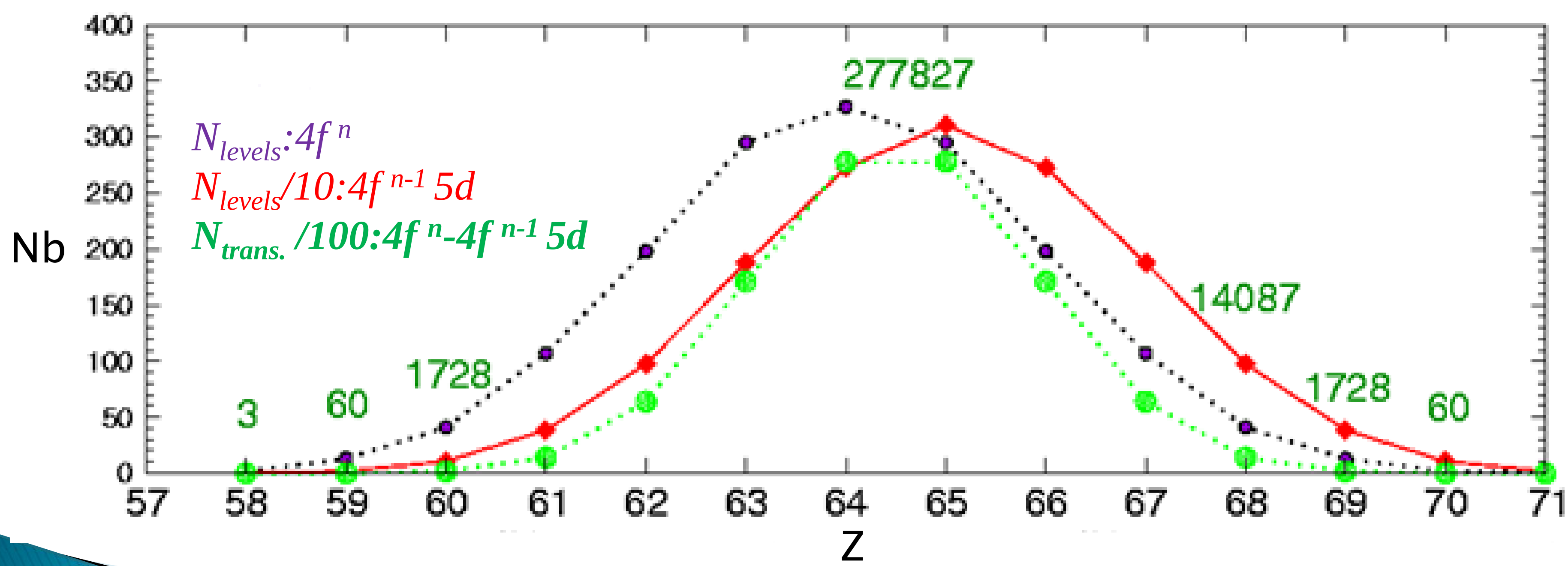
Introduction

- **Lanthanides complexities:**

$4f^{7}$(Gd^{3+}): **327** *levels* ; $4f^{7}5d$ (Tb^{3+}): **3106** *levels*

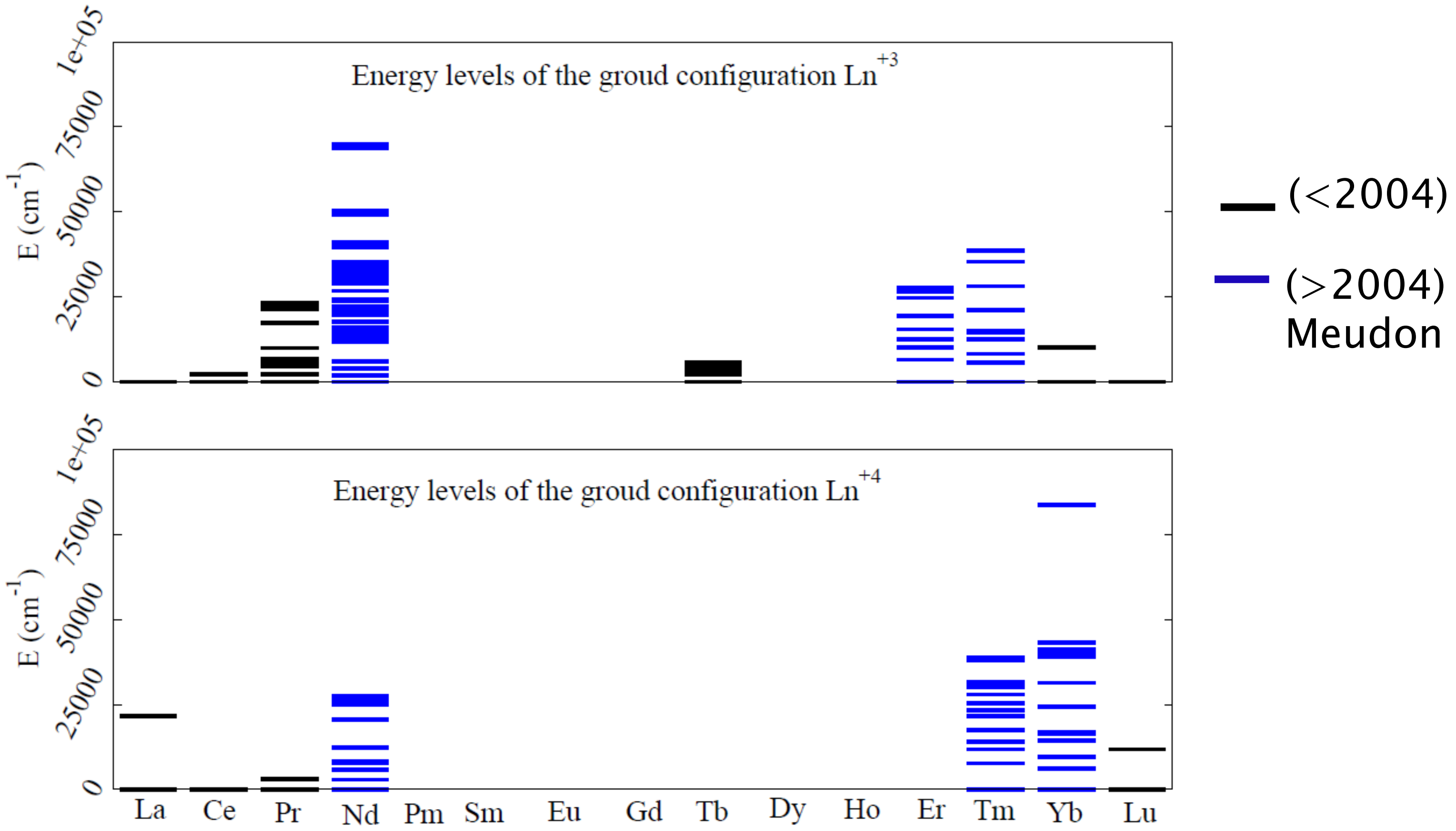
$4f^{7}-4f^{6}5d$ (Gd^{3+}) ; $4f^{8}-4f^{7}5d$ (Tb^{3+})

277827 transitions



Introduction

There are very little experimental data for the lanthanide ions



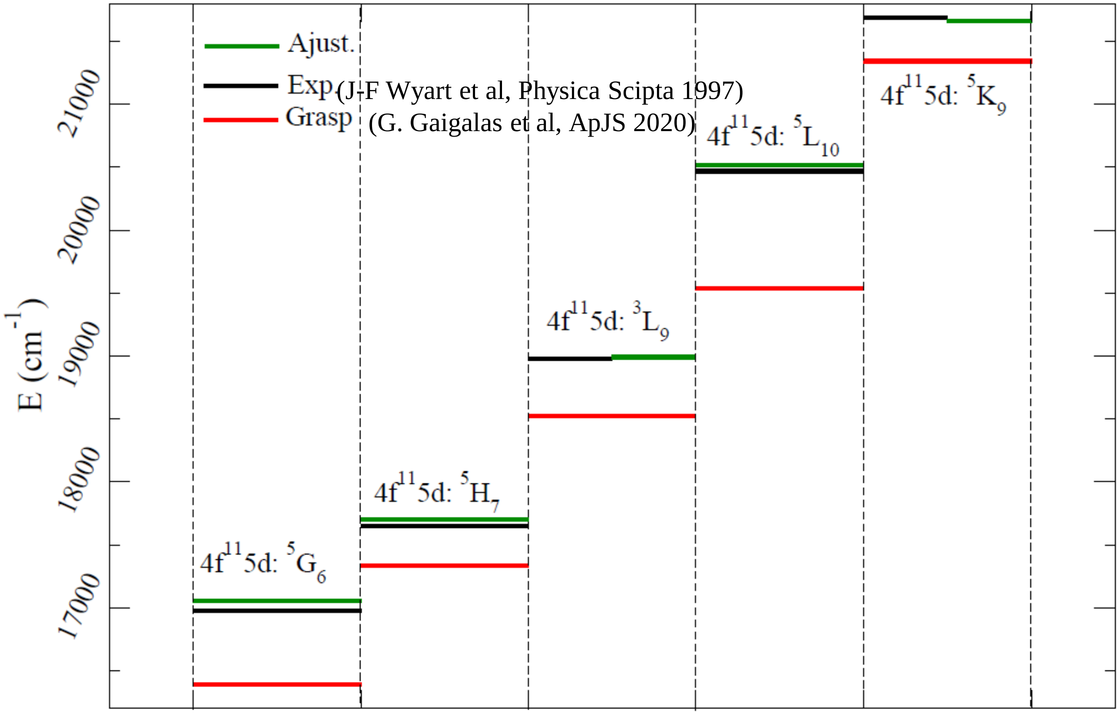
Introduction

- Ab initio atomic structure codes (GRASP, FAC,…)

- ***Experimental levels** are very important to confirm the validity of these codes and accompany their future developments*

- In the semi-empirical approach:

- ***The values of the experimental energies allow to improve very significantly the calculated values by adjusting them with experimental value.***



Ex: Er^{2+}

first levels of $4f^{11}5d$

$E_{exp}-E_{Grasp}$ ~

a few hundred cm^{-1}

- $E_{exp}-E_{Ajust}$ ~

a few tens cm^{-1}

Introduction

- lanthanide ions are of interest for:

- Luminescence of materials doped with lanthanide ions.
- Spectra of chemically peculiar stellar atmospheres
- Study of kilonovae (neutron-star mergers)

Experimental method

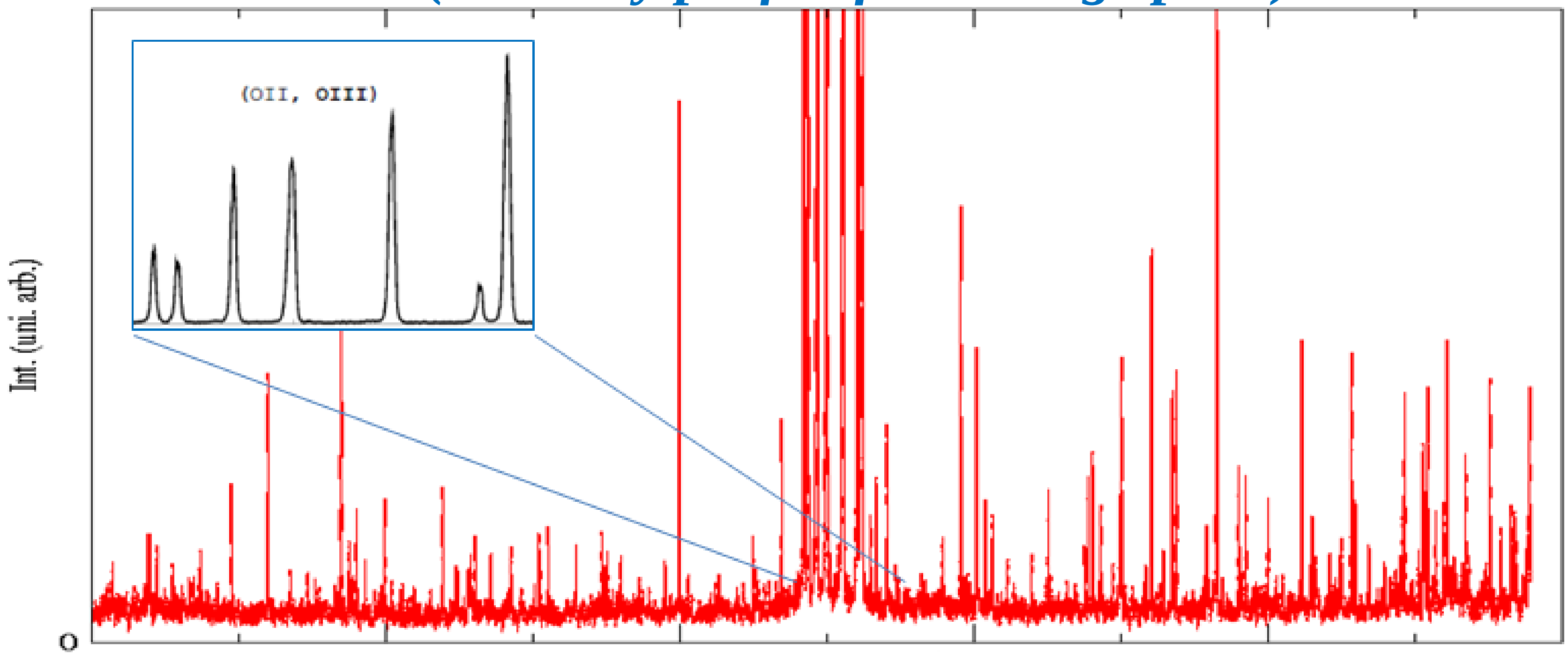
Meudon VUV spectrograph

- **Holographique** Concave grating: **3600 lines/mm**
- Focal length: **10.685 m**
- λ of maximum efficiency: **120 nm**
- Resolving power: **1.5 10^5** (8 mA, slit 30 µm)
- Spectral range: **30-300 nm**

Experimental method

A section of thulium sliding spark spectrum in wavelength range 810-860 Å

(Intensity profile from image plate)



- *The lines of impurities inside the spectrum are used for calibration in wavelength*

Analysis and Results

Principle of Analysis

Exp. λ (σ) list

λ_1 (σ_1)
λ_2 (σ_2)
λ_3 (σ_3)
.
.
.
.
λ_n (σ_n)

+

Atomic structure calc. codes

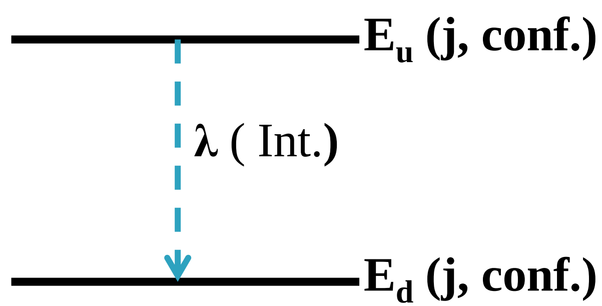
=

Exp. Energy levels

E_1 (j_1, conf.)
E_2 (j_2, conf.)
E_3 (j_3, conf.)
.
.
.
.
E_n (j_n,conf.)

Ritz combination principle

$$\sigma = 1/\lambda = E_u - E_d$$



Consistency between int. and gA

Analysis and Results

Parametric calculations: Cowan code (RCN/RCG/RCE

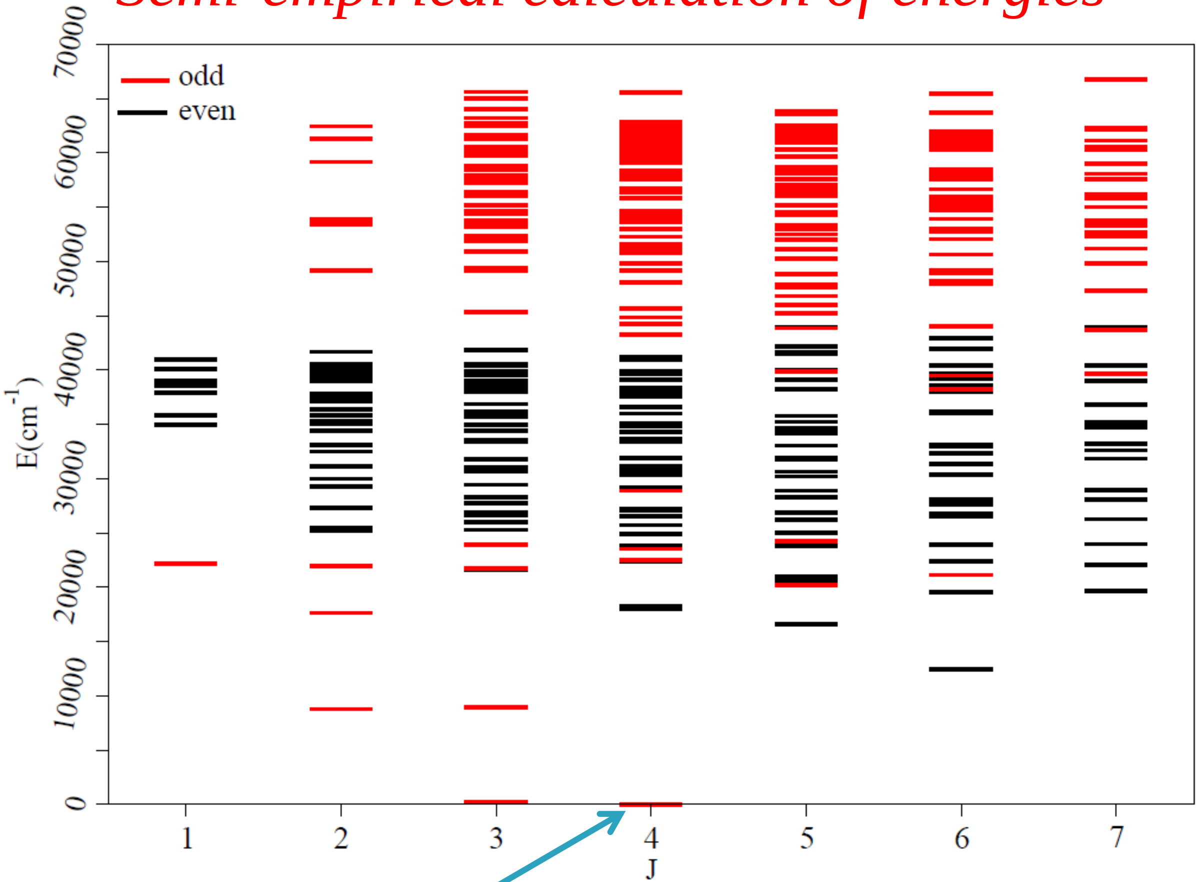
- *Ab initio calculations (Hartree-Fock +relativistic corrections: HFR) of the set of electronic configurations.*

- *Atomic Hamiltonian: H=radial part* x *angular part (Racah algebra).*

- *Least square fitting of the calculated energies by adjusting radial parameters*

Results: Tm^+

Semi-empirical calculation of energies



Experimental levels from NIST/ASD

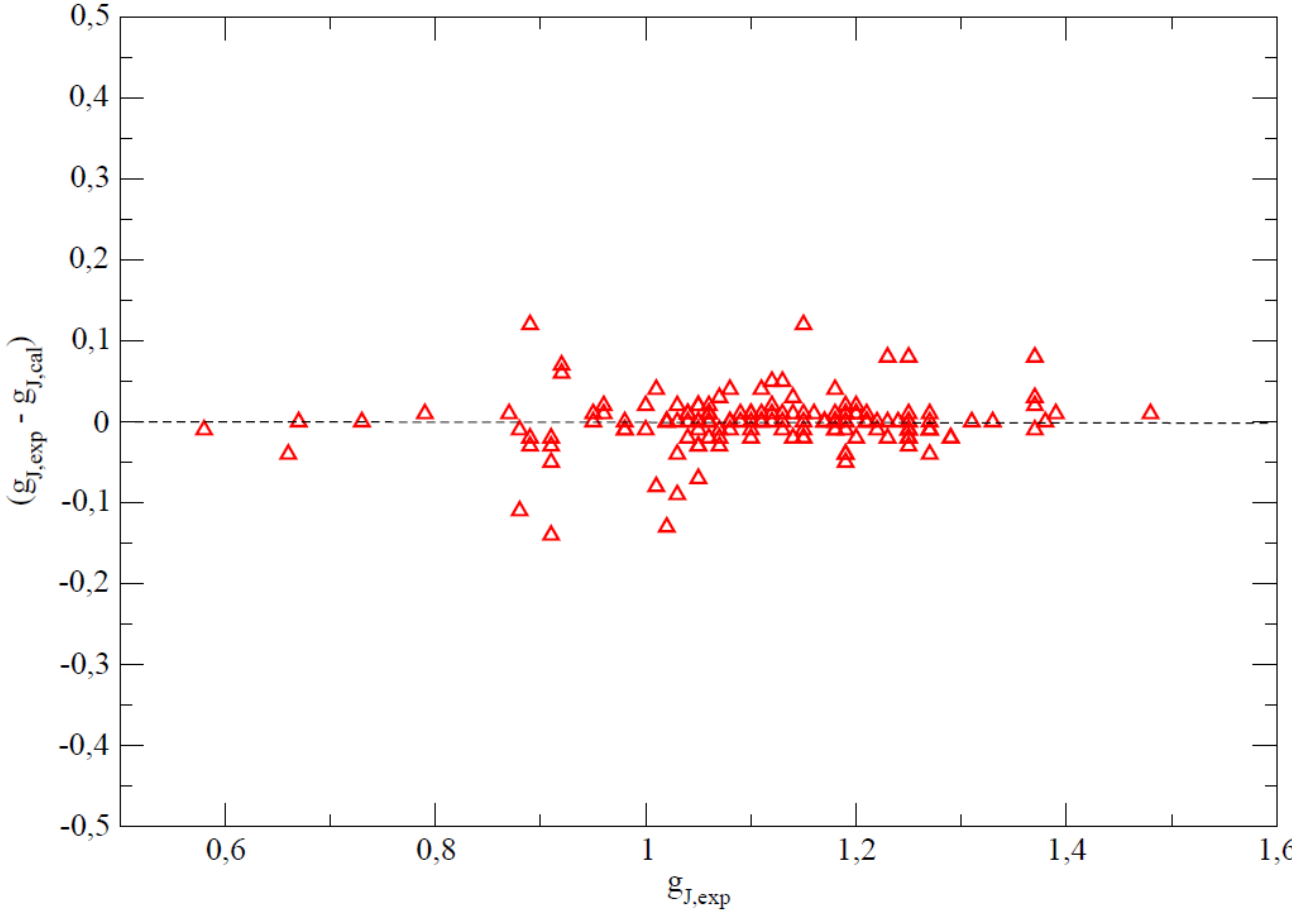
Standard deviation:

$$\sigma_E = \left[\frac{\sum_{i=1}^{N_{lev}} (E_{cal,i} - E_{exp,i})^2}{N_{lev} - N_{par}} \right]^{1/2}$$

Ground level: $4f^{13}6s$: $^5F_4$

Parity	Even	odd
N_{lev}	161	182
N_{par}	23	26
σ_E(cm^{-1})	56	85

Results: Landé g_J factors calculation in Tm^{+1} comparison with measurements



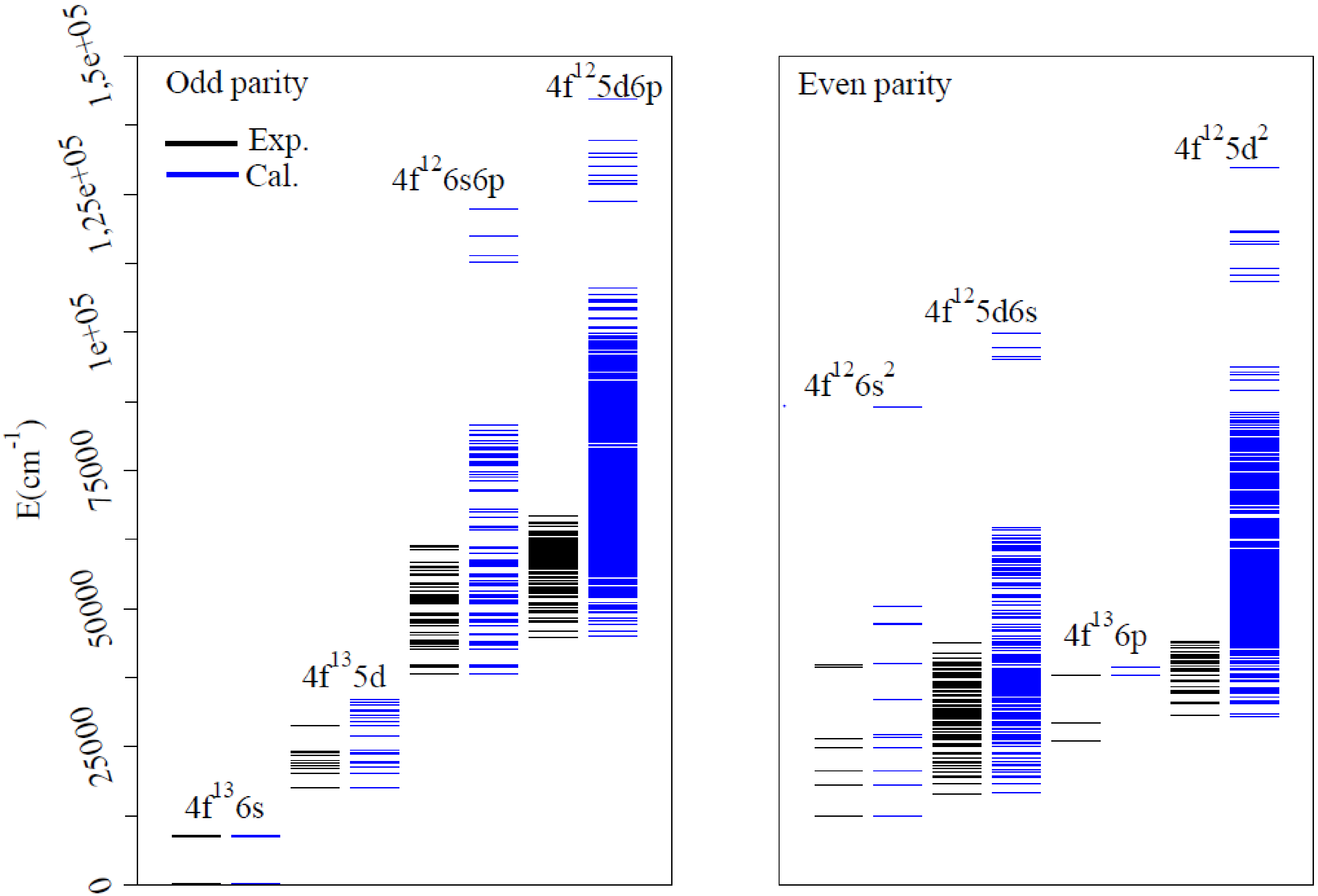
Experimental g_J *from NIST database*

Zeeman shift

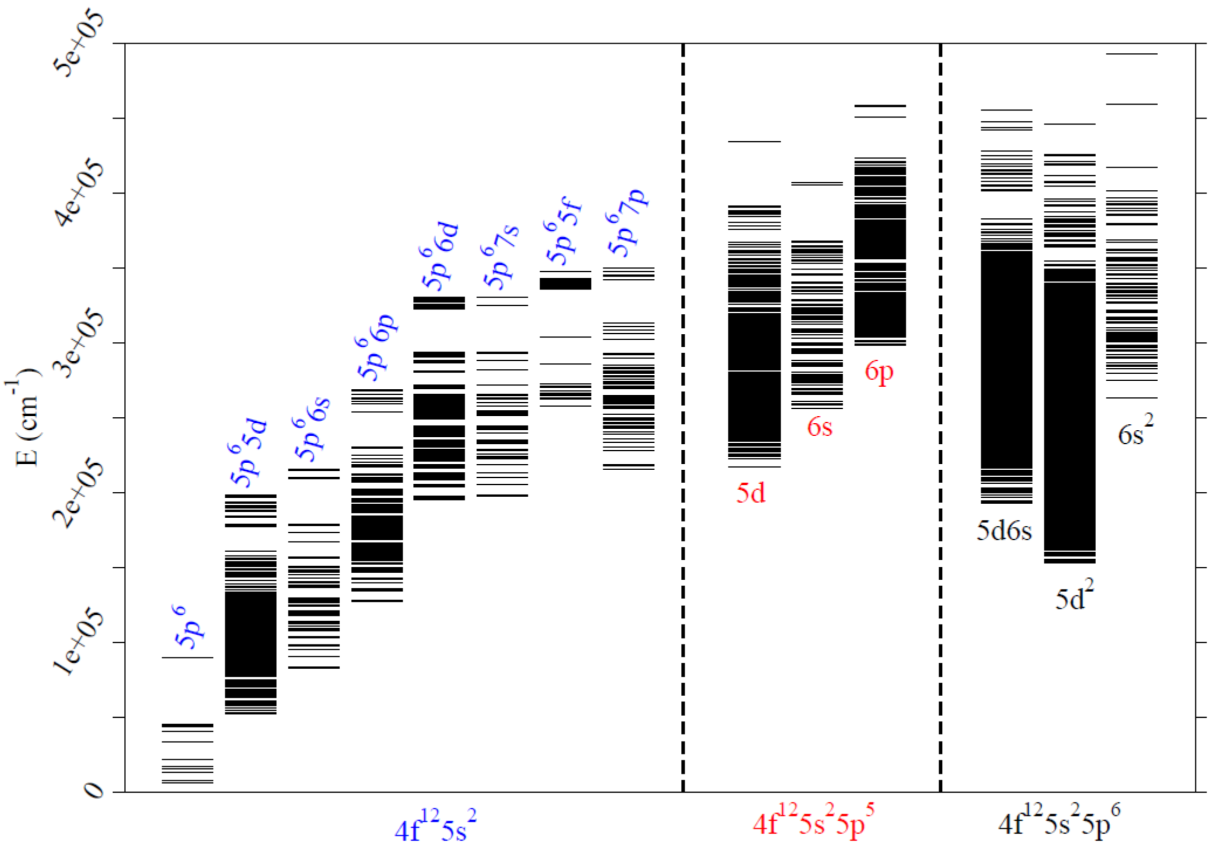
$$\Delta E_{J,M} = \boldsymbol{g_J} M \mu_B B$$

Results: Experimental and predicted levels of Tm^{+1}.

- LSQ fit with known levels improve the prediction of unknown levels



Results: Extended analyse of Tm^{3+}



- First analyse of Tm^{3+}: **209** levels

($4f^{12}$, $4f^{11}5d$, $4f^{11}6s$ and $4f^{11}6p$)

(Meftah et al, EPJD 2007)

- Extended analysis:

More levels for:

$4f^{12}$ → **2** new levels

$4f^{11}5d$ → **69** new levels

$4f^{11}6s$ → **7** new levels

$4f^{11}6p$ → **23** new levels

Results: GRASP calculations in Tm^{3+}

- *Comparison of experimental energies* (cm^{-1}) *and values calculated by GRASP*

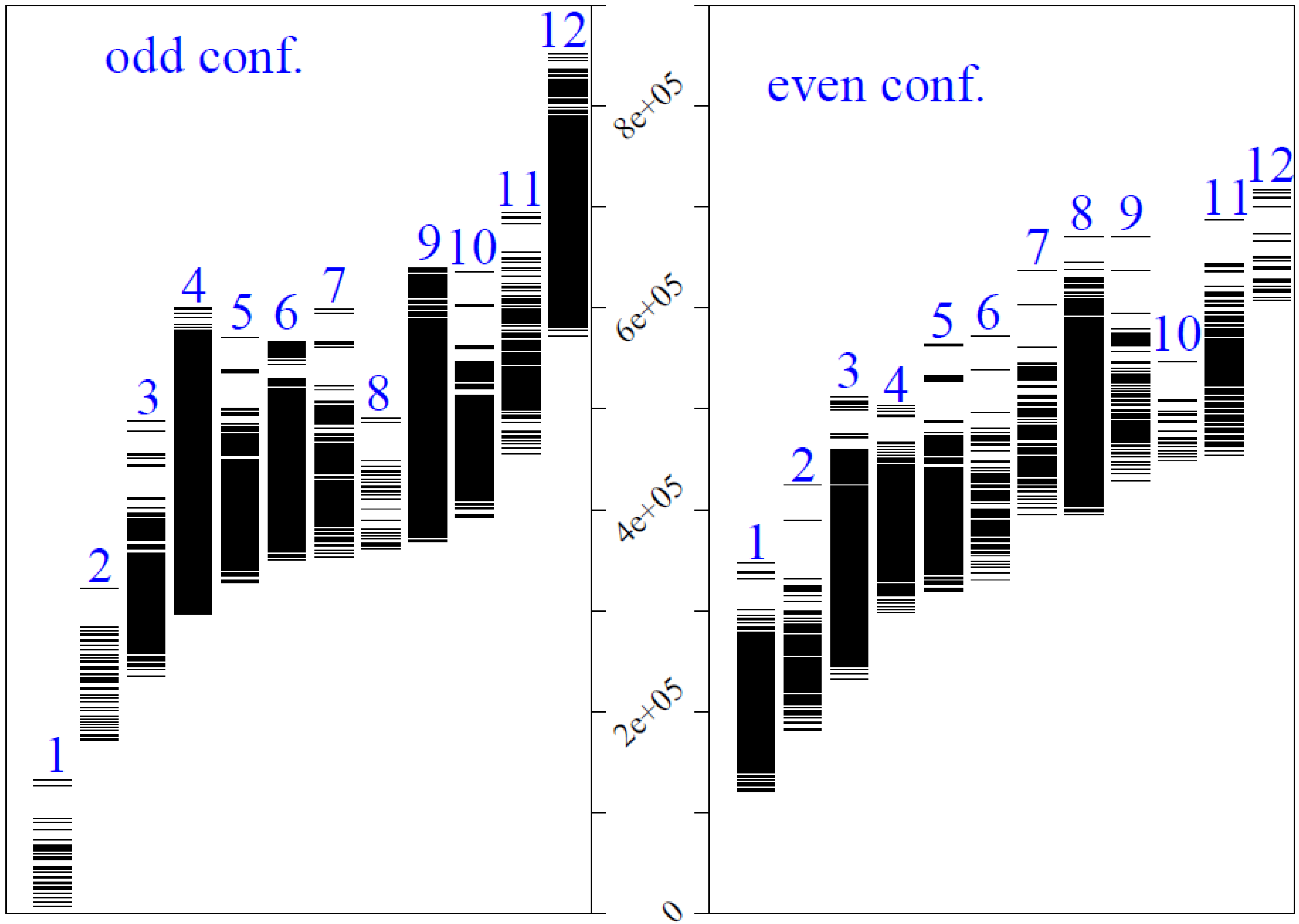
Config.	Term	J	Exp.	Ajust.	Grasp (in%)
$4f^{12}$	^3H	6	0.00	-27	0
	^3F	4	5634.02	5656	6571/-16.17
	^3H	5	8216.73	8192	7315/10.97
	^3H	4	12547.23	12567	11852/5.54
	^3F	3	14410.41	14463	14743/-2.3
$4f^{11}5d$	^5G	6	72011.02	72044	72145/-0.18
	^5H	7	72931.67	72984	73163/-0.30
	^3L	9	74506.41	74526	74735/-0.30
	^5I	8	75585.02	75541	75924/-0.44
	^5G	5	78413.63	78416	78286/0.16
	^5K	9	78677.88	78697	78665/0.01
	^5H	6	79225.87	79212	79203/0.02
	^5I	8	80122.71	80116	80149/-0.03
	^5I	7	80264.65	80226	80459/-0.24
	^5L	8	82258.89	82261	82191/0.08
	^3G	5	83293.13	83289	83613/0.38
	^3I	7	83530.02	83502	83709/-0.21
	^5G	4	83548.79	83549	83524/0.02
	^3H	6	84485.81	84438	84867/-0.45
	^3G	5	85541.93	85500	85641/-0.11
	^5L	9	85504.65	85524	84876/0.73
	^5L	7	86145.56	86115	86157/-0.01
$4f^{11}6s$	^5I	8	98972.81	98968	100975/-2.02
	^3I	7	100145.05	100138	102331/-2.18
	^5I	7	106895.45	106999	108792/-1.77
	^5I	6	107603.36	107541	109124/-1.41
$4f^{11}6p$	^5H	7	144991.40	145008	147541/-1.75
	^3K	8	145564.25	145549	148102/-1.74
	^5H	6	152729.67	152740	155045/-1.51
	^5K	7	153028.54	153032	155283/-1.47
	^5k	9	153217.84	153227	155898/-1.75

- *Good agreement between the calculations with GRASP and the experimental values.*
- *The experimental values are reproduced to few %*
- *But not as clos as the fitted values*

Results: First analyse of Tm^{4+}

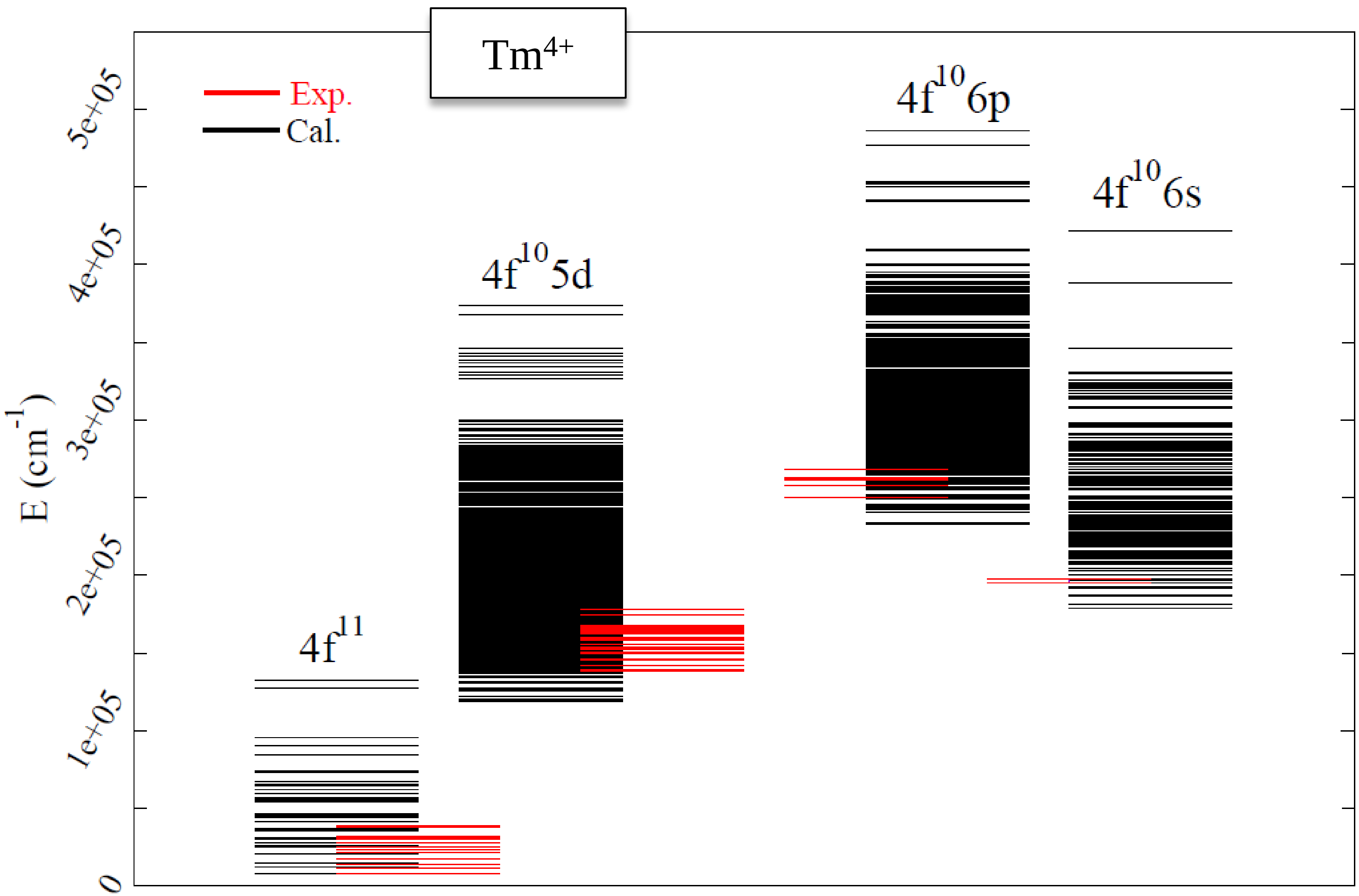
Global view of configurations

1: $4f^{11}$
2: $5p^{5}4f^{12}$
3: $4f^{10}6p$
4: $4f^{9}5d^{2}$
5: $4f^{10}5f$
6: $5p^{5}4f^{11}6p$
7: $4f^{10}7p$
8: $5p^{4}4f^{13}$
9: $4f^{9}5d6s$
10: $4f^{10}6f$
11: $4f^{9}6s^{2}$
12: $4f^{9}6p^{2}$



1: $4f^{10}5d$
2: $4f^{10}6s$
3: $5p^{5}4f^{11}5d$
4: $5p^{5}4f^{11}6s$
5: $4f^{10}6d$
6: $4f^{10}7s$
7: $4f^{10}5g$
8: $5p^{4}4f^{12}5d$
9: $4f^{10}6g$
10: $5s^{1}5p^{6}4f^{12}$
11: $5p^{4}4f^{12}6s$
12: $5s^{1}5p^{5}4f^{13}$

Results: First analysis of Tm^{4+}



4f ^{11}***: 14 levels***

4f ^{10}***5d:37 levels***

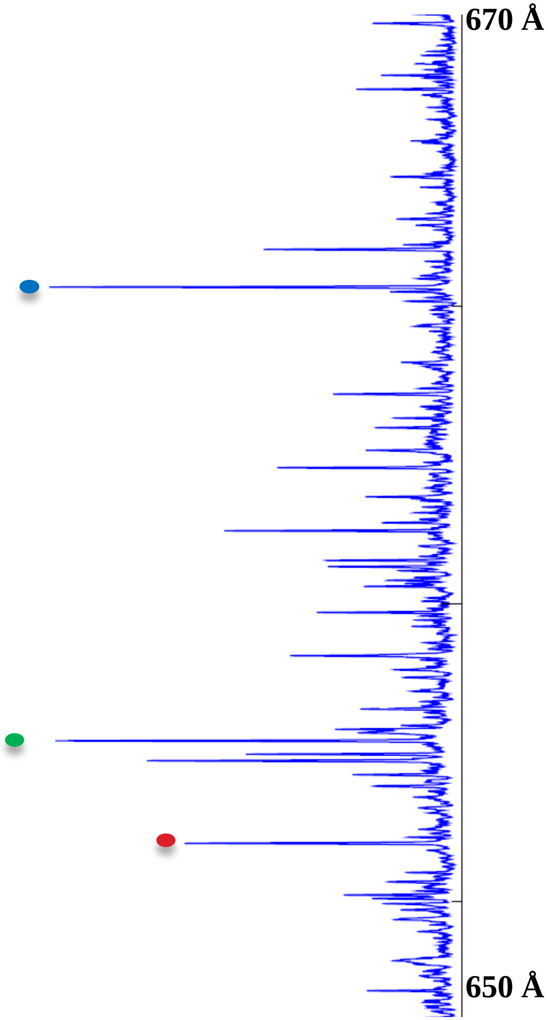
4f ^{10}***6s:2 levels***

4f ^{10}***6p:6 levels***

Results: gA and g*f* calculations in Tm^{4+} (Tm V)

Examples of resonance lines of Tm^{4+}

E_L	Term.	J	E_u	Term.	J	log gf	gA(s^{-1})	λ(Å)	Int.
0.000	^4I	7.5	138325.83	^6H	7.5	-1.910	1.573E+08	722.931	108
			138833.94	^6I	8.5	-2.851	1.815E+07	720.283	6
			139521.49	^6G	6.5	-2.484	4.269E+07	716.731	24
			145671.02	^4K	8.5	-1.125	1.061E+09	686.478	212
			145657.94	^6H	7.5	-1.858	1.966E+08	686.539	83
			149195.71	^6L	8.5	-1.199	9.409E+08	670.259	194
			149687.89	^6K	6.5	-1.251	8.382E+08	668.055	200
			150226.91	^4I	7.5	-0.488	4.895E+09	665.659	292
			152487.62	^4I	7.5	-0.589	3.998E+09	655.790	258
			153156.68	^6K	8.5	-1.624	3.720E+08	652.924	78
			153007.39	^4H	6.5	-0.707	3.069E+09	653.562	238
			153974.90	^6L	7.5	-1.655	3.498E+08	649.454	75
			154312.60	^6H	6.5	-2.078	1.325E+08	648.034	40
7674.36	^4I	6.5	145657.94	^6H	7.5	-2.417	4.866E+07	724.727	25
			149687.89	^6K	6.5	-2.057	1.179E+08	704.158	67
			149824.40	^6I	5.5	-2.335	6.232E+07	703.481	13
			150226.91	^4I	7.5	-2.914	1.653E+07	701.498	7
			152487.62	^4I	7.5	-1.277	7.381E+08	690.544	167
			153007.39	^4H	6.5	-1.595	3.585E+08	688.076	142
			153938.07	^6K	5.5	-2.443	5.141E+07	683.696	7
			153974.90	^6L	7.5	-1.548	4.038E+08	683.526	115
			154312.60	^6H	6.5	-0.920	1.720E+09	681.949	238
			154345.50	^4G	5.5	-1.552	4.030E+08	681.797	143
			155725.21	^6K	5.5	-1.739	2.662E+08	675.440	157
			157952.57	^6F	5.5	-1.908	1.854E+08	665.432	52
			158793.04	^4I	6.5	-0.898	1.924E+09	661.729	224
			159285.39	^6H	6.5	-1.191	9.849E+08	659.582	160
			159515.04	^4H	5.5	-0.993	1.561E+09	658.584	178



Conclusion

- Lower levels of conf.(*f^{11},$4f^{10}5d$, $4f^{10}6s$ and $4f^{10}6p$*) in Tm^{4+} are known, further efforts are needed to determine more excited levels.

- Explore other strategies in GRASP to further improve calculations of Tm^{3+} and Tm^{4+}.

- Predictions on Tm^{1+} will be used to determine other experimental levels.

Contributors to this work

- W.-Ü Lydia Tchang-Brillet, Christian Balança,
- Technical support : Norbert Champion and Christophe Blaess
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