Spectra of moderately charged ions of heavy elements around tungsten. Some recent results in W IX sequence: The Yb V spectrum

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The determination of radiative data needed for plasma models depends on the classification of spectra

The energy levels are calculated by means of the Cowan codes, the radial integrals (Hartree-Fock) being treated as adjustable parameters (Racah-Slater parametric method).

The steps are:

I- choice of a set of configurations that can describe the levels in a long sequence of ions and determination of the HFR radial integrals.

II- Application of scaling factors (P_{fit} / P_{HFR}) derived from known cases and shifts of average energies to get E^{th}, Landé factors $g_L{}^{th}$, transition probabilities gA^{th} in good agreement with E^{exp}, gL^{exp}, intensities or lifetimes … from the first diagonalisation.

III- The least squares minimisation of E^{exp}- E^{th}, from a large number of firmly identified levels leads to refined parameter values, better energy E^{th} predictions and reliable eigenfunctions.

The configuration interaction (CI) requires an extended basis set and the use of second order effective parameters for cumulated effects due to far lying configurations.

Scaling factors SF are consistent data in long periods and isoelectronic sequences.
Weird values of SF or fitted parameters generally indicate that some Eexp value(s) is wrong. Correct predictions for the levels of unknown ions have to be supported by a preliminary knowledge of near-by ions.

About consistency of scaling factor (SF) values $SF=P_{fit}/P_{HFR}$ **and effective CI parameters**

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

SF=0.85 Recommanded by R.D. Cowan for Slater integrals in TASS (1981) p.465

Advances in the isoelectronic sequence of **W IX**

Ho II, Er III, Tm IV, **Yb V**, Lu VI, Hf VII, Ta VIII, **W IX**, Re X

Ho II: FS and HFS calculations in Physica Scripta 79 (2009) 035306 (14pp), Gurell, Wahlgren, Nave, Wyart

Er III: Old line lists, new calculations >> gA^{th} values, new levels; application to identifications in CP star HR465 Wyart, Blaise, Bidelman, Cowley Physica Scripta 56 (1997) 446-458

Tm IV: First analysis (Meftah, Wyart, Champion,Tchang-Brillet Eur. Phys. J. D 44,35-45 (2007) is being extended by Meftah (2014)

Yb V: Measurements of NBS spectrograms (Sugar, Kaufman, ~1979) led to lower levels of first 4 configurations $4f^{12}$, $4f^{11}5d$, $4f^{11}6s$ and $4f^{11}6p$

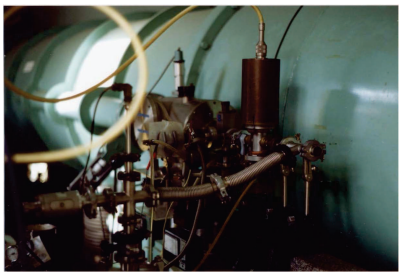
Lu VI and beyond: unknown

Spectrum and energy levels of the Yb^{4+} free ion (Yb V)

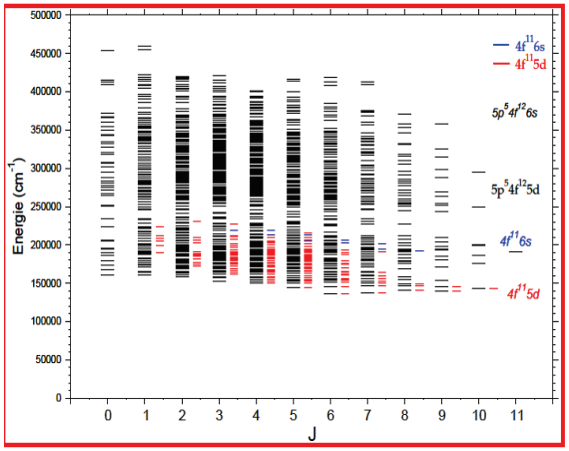
A. Meftah, J.-F. Wyart, W.-Ü L. Tchang-Brillet, C. Blaess, N. Champion
Physica Scripta **88**, 045305 (2013)

New experiments in Meudon: Low inductance vacuum spark source, Al cathode, pure ytterbium (99%) as a cathode. Normal incidence vacuum spectrograph with concave grating (3600 l.mm^{-1}) and resolution ~ 150000. Kodak SWR and Ilford Q plates.
Digitization by high resolution optical scanner iQsmart1.
Polynomial interpolation with wavelengths (Ritz) of Yb III, Yb IV and usual impurities (C,N,O, Al,Si). Overall uncertainty is about 0.005 Å for isolated lines.
Search for levels with IDEN package (Azarov, 1991,1993).
Stepwise interpretation of energy levels with the Cowan codes,
with mean errors in final steps:
55 cm^{-1} for the 56 even parity levels $4f^{12}$, $4f^{11}6p$ + ($5p^54f^{13}$ + $5p^54f^{12}6p$)
51 cm^{-1} for the 186 odd parity levels $4f^{11}5d$, $4f^{11}6s$ + ($5p^54f^{12}5d$ + $5p^54f^{12}6s$).
The ground configuration $4f^{12}$ is completely known.

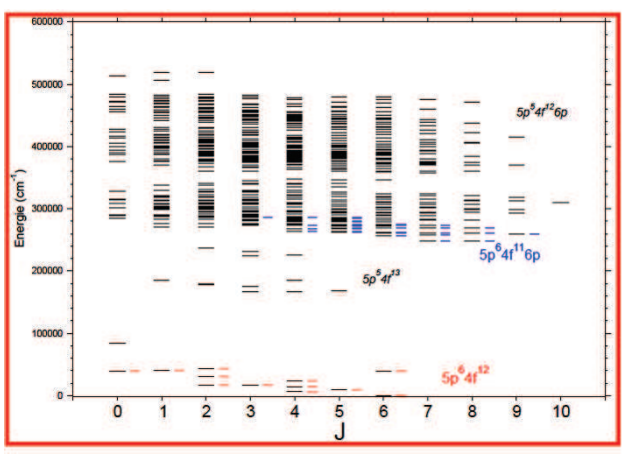
The Meudon 10m VUV spectrograph



Yb V Odd parity levels E_{th} in black



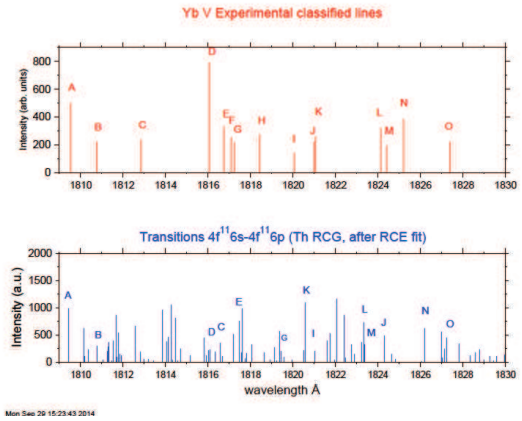
Yb V Even parity levels E_{th} in black, E_{exp} coloured



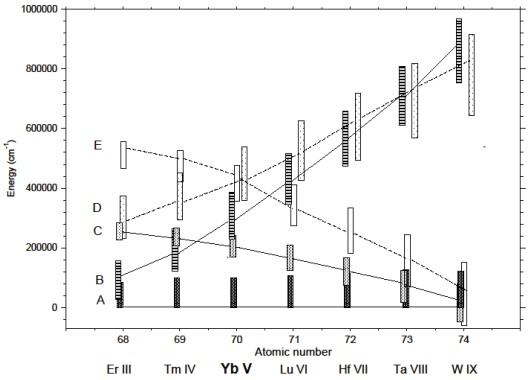
Transitions for the level E=14405.00cm^{-1} ($4f^{12}\ ^3H_4$) in 505-561Å region

Ritz wl Å	exp	Int	gA 10^6 s^{-1}	Ritz wavn cm^{-1}	Even lev	J	Odd lev	J	Note
505.7215	.721	42	2300	197737.300	14405.000	4	212142.300	3	
508.0457	.047	20	761	196832.700	14405.000	4	211237.700	3	
510.0602	.061	11	480	196055.300	14405.000	4	210460.300	3	
513.3921	.393	11	552	194782.900	14405.000	4	209187.900	4	
518.8444	.841	10	265	192736.000	14405.000	4	207141.000	3	
523.7327	.732	10	329	190937.100	14405.000	4	205342.100	4	
524.8502	.851	7	140	190530.550	14405.000	4	204935.550	5	
529.2876	.285	6	301	188933.200	14405.000	4	203338.200	4	
530.7966	.797	5	231	188396.100	14405.000	4	202801.100	4	
533.2531	.251	23	1570	187528.200	14405.000	4	201933.200	5	
535.6579	.658	10	230	186686.300	14405.000	4	201091.300	3	
536.0769	.077	10	604	186540.400	14405.000	4	200945.400	4	
540.9874	.990	45	1322	184847.200	14405.000	4	199252.200	3	
546.3770	.377	44	1392	183023.800	14405.000	4	197428.800	3	
548.6384	.638	59	1273	182269.400	14405.000	4	196674.400	4	
550.6647	.664	20	415	181598.700	14405.000	4	196003.700	3	
551.0525	.052	9	87	181470.900	14405.000	4	195875.900	5	
553.9865	.988	8	158	180509.800	14405.000	4	194914.800	4	
554.9322	.934	93	7415	180202.200	14405.000	4	194607.200	5	
557.4593	.458	39	647	179385.300	14405.000	4	193790.300	5	
558.4517	.450	8	145	179066.500	14405.000	4	193471.500	3	
560.0879	.089	42	1260	178543.400	14405.000	4	192948.400	4	DCL
561.4183	.418	60	613	178120.300	14405.000	4	192525.300	4	

Comparison of experimental and calculated transitions in Yb V



Isoelectronic trends for $5p^64f^{11}6p$ (B), $5p^54f^{13}$(C), $5p^54f^{12}6p$(D), $5p^44f^{14}$(E) *vs.* $5p^64f^{12}$) (A)



Extended analysis of W III – W VII and isoelectronic ions

Sequence of (Yb I) Lu II:
Lowest configurations known in Lu II-Hg XI spectra.
High odd configurations 5d5f and 5d7p known from transitions to the ground $5d^2$ till Pt IX in the UV.
Lower charge ions are more complex with unsolved interpretation of overlapping configurations $(6s+5d)_{el}$ and $6p^2$

In Hf III, upper even levels (with ambiguous J values and lacking an interpretation) are listed by Noorman (Physica, 1961). Additional levels are derived from the Corliss&Meggers linelist (1958) E=105120.5 cm^{-1}, 5d6d ($^3D_3$?)

In Ta IV, we have identified the 5d6p-(5d6d+5d7s) transitions in the same spectra as used for Ta III (Azarov, Wyart, Tchang-Brillet,Meijer, Physica Scripta, 2003).

Fitted energy parameters in Ta IV even parity

Parameter		fitted	st dev	Scaling
EAV 5d^2		11384	66	
F2(11)		46482	324	0.888
F4(11)		29228	397	0.778
ALPHA	fix	10		
ZETA 5d	R1	2295	21	0.923
EAV 5d6s		33947	71	
ZETA 5d	R1	2462	22	0.923
G2(5d,6s)	R2	19501	463	0.891
EAV 6s^2		70229	148	
EAV 5d7s		162490	100	
ZETA 5d	R1	2578	23	0.923
G2(5d,7s)	R2	3515	84	0.891
EAV 5d6d		163246	40	
ZETA 5d	R1	2578	23	0.923
ZETA 6d	R1	460	4	0.923
F2(5d,6d)	R3	12992	404	0.880
F4(5d,6d)	R3	6210	193	0.880
G0(5d,6d)	R4	2966	55	0.630
G2(5d,6d)	R4	3273	60	0.630
G4(5d,6d)	R4	2654	49	0.630
EAV 6s6d	fix	191972		
EAV 6p^2	fix	180372		
EAV 6s7s	fix	191706		

All Slater C.I. Parameters fixed at S.F.= 0.700

Fit with
34 levels and
11 free parameters.
Parameters marked Rn vary in the ratio of HFR values.

Mean error 139 cm^{-1}

Extended analysis of W $^{4+}$ (W V) : 5d6p - 5d(6d,7s) transitions

Classified lines in the
1125 – 1300 Å region:
In black, 5d6p-5d6s (NIST database)
In green, 5d6p -5d7s New
In red, 5d6p – 5d6d New

Ritz wl	exp	Int	Ritz wn	Odd level	J	Even level	J
1125.3075	.315	408	88864.600	149160.100	1	60295.500	2
1143.2726	.266	501	87468.200	149160.100	1	236628.300	2
1157.8630	.874	655	86366.000	133430.000	2	219796.000	2
1164.4738	.469	388	85875.700	144389.900	2	58514.200	1
1169.9683	.964	242	85472.400	145767.900	3	60295.500	2
1170.0683	.073	226	85465.100	137709.300	1	223174.400	0
1189.1398	.136	707	84094.400	144389.900	2	60295.500	2
1191.5784	.520	41	83922.300	139252.100	0	223174.400	0
1192.3826	.395	226p	83865.700	136887.800	3	220753.500	4
1206.1533	.120	373	82908.200	136887.800	3	219796.000	2
1210.0985	.139	526	82637.900	144389.900	2	227027.800	2
1211.6307	.635	268p	82533.400	142907.900	4	225441.300	3
1216.5213	.489	210	82201.600	144389.900	2	226591.500	3
1218.2241	.235	752	82086.700	137709.300	1	219796.000	2
1230.6193	.618	362	81259.900	145767.900	3	227027.800	2
1233.7850	.819	205	81051.400	144389.900	2	225441.300	3
1237.2624	.289	46	80823.600	145767.900	3	226591.500	3
1238.5757	.562	793	80737.900	139252.100	0	58514.200	1
1255.1240	.141	477	79673.400	145767.900	3	225441.300	3
1262.7044	.709	960	79195.100	137709.300	1	58514.200	1
1264.0595	.064	933	79110.200	145767.900	3	66657.700	3
1284.2295	.259	20	77867.700	149160.100	1	227027.800	2
1284.5941	.538	1	77845.600	142907.900	4	220753.500	4
1286.4682	.466	300	77732.200	144389.900	2	66657.700	3
1291.7594	.746	200	77413.800	137709.300	1	60295.500	2

Parametric interpretation in progress Example of W IV

Transitions of the level $5d^26p$ o402 115422.93 cm^{-1}

(second lowest odd parity level with J=9/2)

λ(Å) [1]	Int [1]	Even parity E^e cm^{-1}	J^e		gA (10^6s^{-1})	log(gf)
920.147	350	6744.63	7/2		291	-1.434
941.916	10	9256.39	9/2		1513	-0.697
998.382	-	15260.92	7/2		64	-2.02
1007.889	2	16204.85	9/2		158	-1.619
1072.963	800	22223.06	11/2		21650	0.571
1094.970	200	24096.03	9/2		2332	-0.379
1149.287	3 H	28412.13	7/2		162	-1.496
1309.020	10	39029.73	7/2		40	-1.988
1385.070	400	43224.40	9/2		3824	0.040
1597.573	300	52828.24	7/2		5284	0.303
1713.124	50	57050.05	9/2		907	-0.398
1752.833	100	58372.54	7/2		2752	0.101

The use of orthogonal parameters for mixed configurations of d,s,p electrons was successful in iron group elements (Raassen, Uylings, Physica Scripta T65,1995)
It should be tried in W ions (see Azarov, Tchang-Brillet, Physica Scripta T, 2002).