UMONS
Université de Mons

Atomic Data for Lowly-Charged Tungsten Ions

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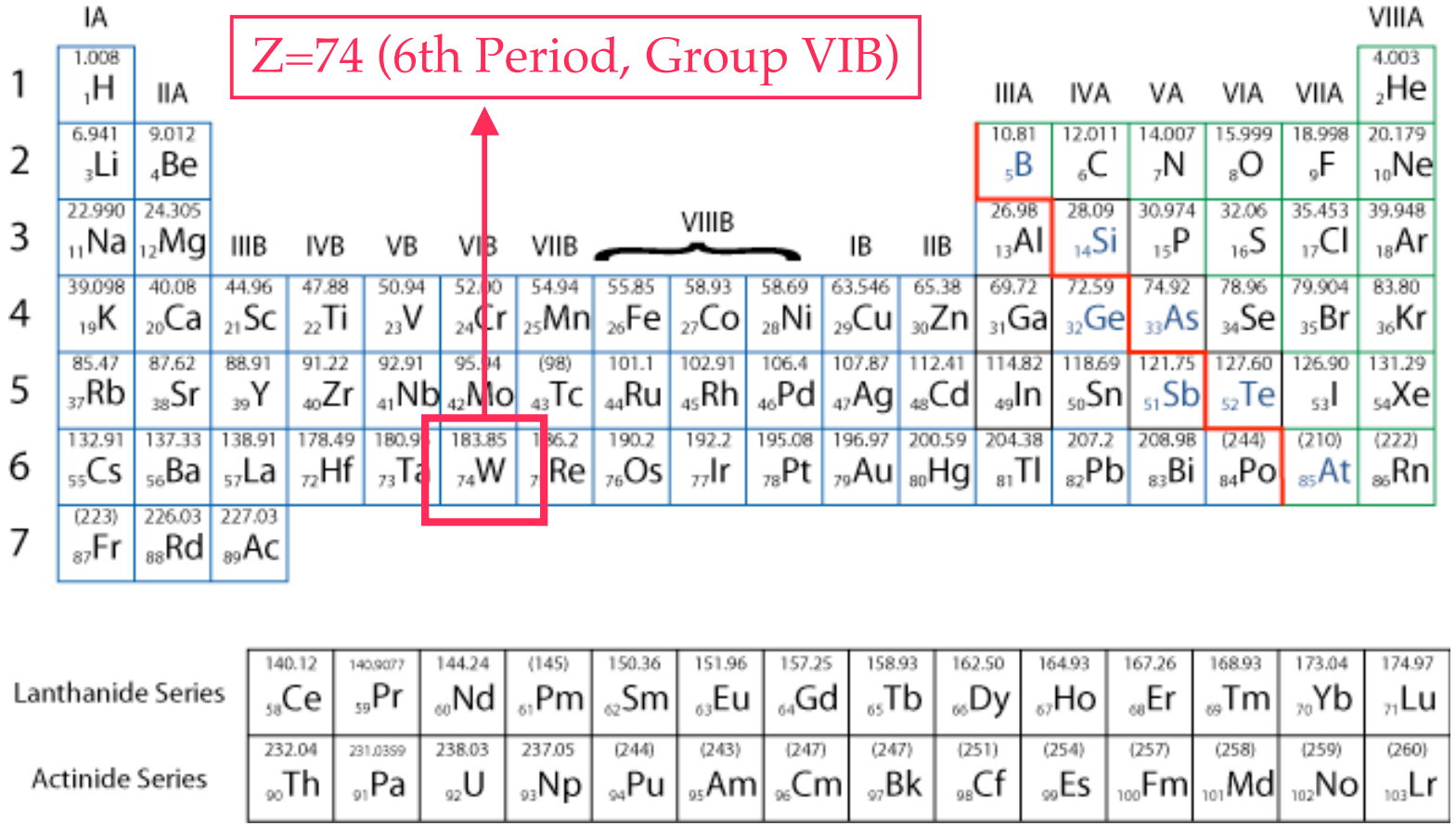
Outline

- Introduction
- HFR+CPOL Method
- Results: W^{0}, $W^{3\text{-}5+}$
- Conclusions & Perspectives

Introduction



Lanthanide Series	140.12 Ce	140.9077 Pr	144.24 Nd	(145) Pm	150.36 Sm	151.96 Eu	157.25 Gd	158.93 Tb	162.50 Dy	164.93 Ho	167.26 Er	168.93 Tm	173.04 Yb	174.97 Lu
Actinide Series	232.04 Th	231.0359 Pa	238.03 U	237.05 Np	(244) Pu	(243) Am	(247) Cm	(247) Bk	(251) Cf	(254) Es	(257) Fm	(258) Md	(259) No	(260) Lr

Introduction

Ground Configurations of Lowly-Charged W Ions:

W^{0} $[Xe]4f^{14}5d^{4}4s^{2}$ (W-like: 74 electrons)
W^{+} $[Xe]4f^{14}5d^{4}4s$ (Ta-like: 73 electrons)
W^{2+} $[Xe]4f^{14}5d^{4}$ (Hf-like: 72 electrons)
W^{3+} $[Xe]4f^{14}5d^{3}$ (Lu-like: 71 electrons)
W^{4+} $[Xe]4f^{14}5d^{2}$ (Yb-like: 70 electrons)
W^{5+} $[Xe]4f^{14}5d$ (Tm-like: 69 electrons)

→ Complex open 5d shell configurations !

Introduction

Status of the UMONS Tungsten Project:

Ion	Transition Rates
W^{0+}	M1+E2 lines (Quinet et al 2010, J Phys B 43, 144003)
W^{+}	Nilsson et al 2008, Eur Phys J D 49, 13
W^{2+}	Palmeri et al 2008, Phys Scr 78, 015304
W^{3+}	to be done
W^{4+}	to be done
W^{5+}	to be done

Introduction

Transition Rates in W^{+} and W^{2+}:

6086 W^{+} lines in the range 143 - 990 nm

4822 W^{2+} lines in the range 83 - 1494 nm

→ Along with Landé g-factors are available in the DESIRE database
(URL: w3.umons.ac.be/astro/desire.shml)

Introduction

W^{+} and W^{2+} data transfered to ADAS:

Not only the published data have been transfered to ADAS but also the HFR+CPOL models in order to compute plane wave Born collision strengths.

The HFR+CPOL Method

The Relativistic Hartree-Fock (HFR) method of R.D. Cowan:
(The Theory of Atomic Structure and Spectra, Univ. of California Press, Berkeley, 1981)

Multiconfiguration approach through superpositions of configurations

Most important relativistic effects included (spin-orbit, mass-velocity correction, Darwin term, kappa-averaged orbitals)

Good agreement with fully relativistic methods

Convergence problems do occur very rarely

Can be used both in *ab initio* or semi-empirically

The HFR+CPOL Method

The Semi-Empirical Optimization:
(R.D. Cowan, The Theory of Atomic Structure and Spectra, Univ. of California Press, Berkeley, 1981)

Radial parameters (average energies, electrostatic integrals, spin-orbit parameters) adjusted to minimize the discrepancies between the Hamiltonian eigenvalues and the experimental level energies

→ Optimization of the wavefunctions

→ Optimization of the wavelengths

→ Optimization of the transition rates

→ Depends on the availability of experimental level energies!

The HFR+CPOL Method

The Core-Polarization Effects (HFR+CPOL):
(see e.g. Quinet et al 1999, MNRAS 307,934 & 2002, J. Alloys Comp. 344, 255)

Intravalence correlation: explicit multiconfiguration expansions

Core-valence correlation: core-polarization model potential depending upon two parameters:
(Migdalek & Baylis 1978, J Phys B 11, L497)

1-electric dipole polarizability of the ionic core, α_d
2-cut-off radius (size of the ionic core), r_c

Penetration of the core by valence electrons: core penetration correction
(Hameed et al 1968, J Phys B 1, 822; Hameed 1972, J Phys B 5, 746)

Neutral Tungsten

HFR+CPOL model:

Intravalence Correlation:

$5d^46s^2+5d^56s+5d^57s+5d^6+5d^46s7s+5d^46s6d+5d^56d+5d^46p^2+5d^46d^2+5d^36s6p^2+5d^26s^26p^2$ (even parity)

$5d^46s6p+5d^46s7p+5d^56p+5d^57p+5d^46s5f+5d^55f+5d^36s^26p+5d^36p^3+5d^26s6p^3$ (odd parity)

Core-Polarization Potential:

Yb-like W^{4+} $[Xe]4f^{14}5d^2$ ionic core with $\alpha_d = 4.59\ a_0^3$ (Fraga et al 1976, Handbook of Atomic Data, Amsterdam: Elsevier) and $r_c = \langle r \rangle_{5d} = 1.99\ a_0$

Neutral Tungsten

HFR+CPOL model:

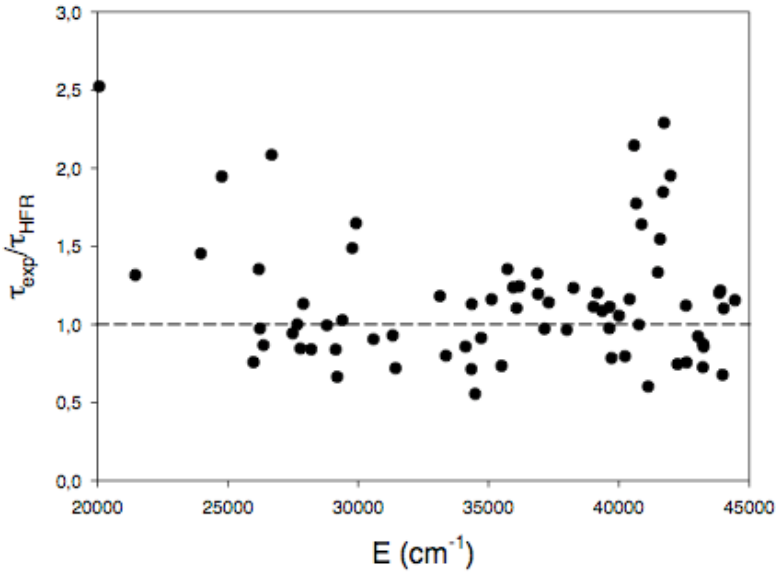
Semi-Empirical Optimization:

All the 70 even-parity levels belonging to $5d^46s^2$ and $5d^56s$ published in Kramida & Shirai (2006, J Chem Ref Data 35, 423) have been considered. The average deviation between the experimental and calculated level energies was 57 cm^{-1}.

141 odd-parity levels with E < 45000 cm^{-1} belonging to $5d^46s6p$, $5d^56p$ and $5d^36s^26p$ published in Wyart (2010, J Phys B 43, 074018) have been considered. The average deviation was 64 cm^{-1}.

Neutral Tungsten

Comparison of radiative lifetimes, and LS purities

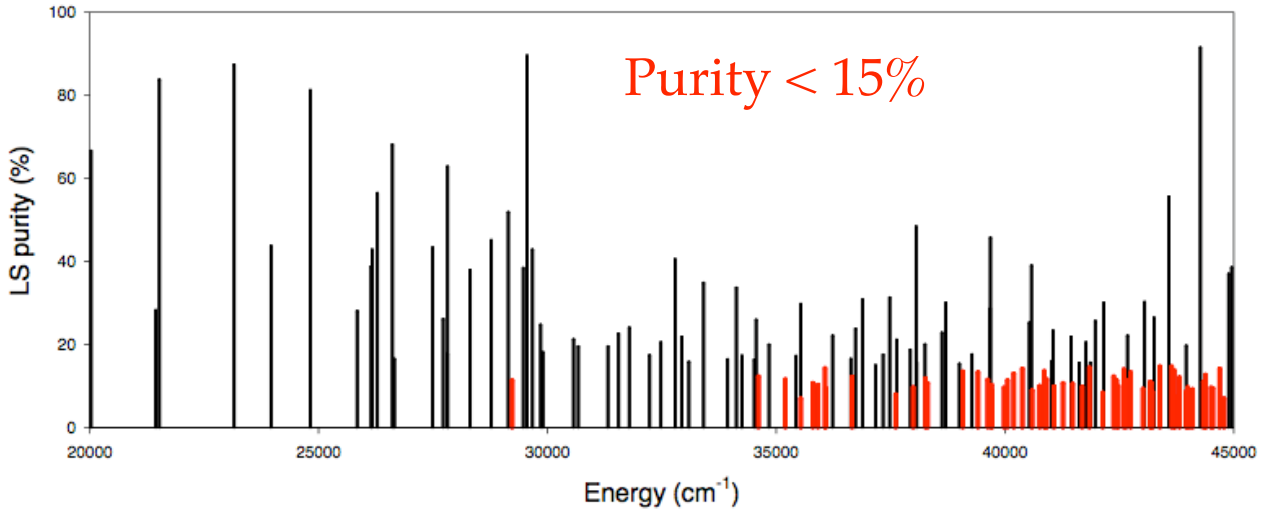


TR-LIF measurements
(Den Hartog et al 1987, JOSA B 4, 48; Kling & Kock 1999, JQSRT 62, 129)

Average exp / calc ratio = 1.12±0.40

E < 30 000 cm^{-1}: a lot of τ > 500 ns

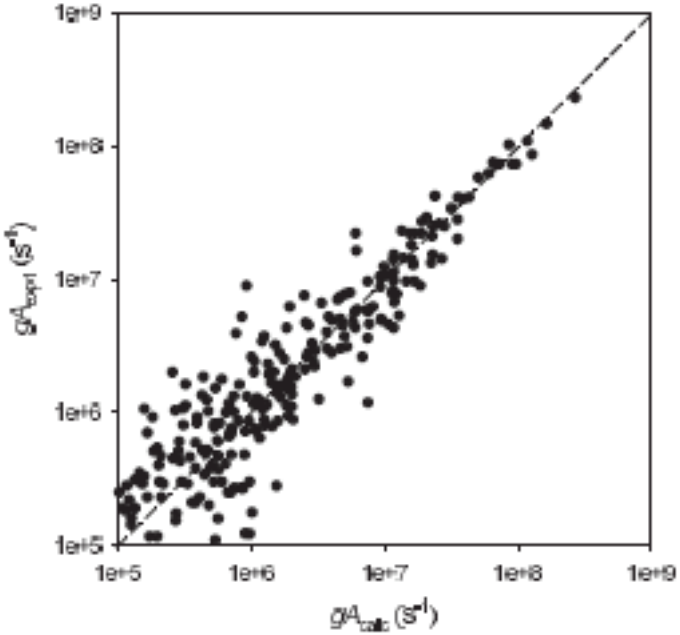
E > 40 000 cm^{-1}: strong mixings



Neutral Tungsten

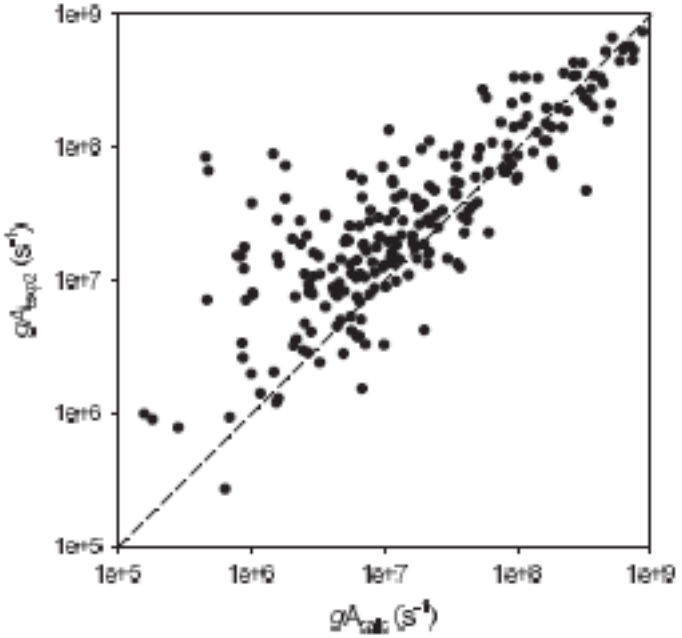
Comparison of transition probabilities (gA)
(Average exp/calc ratio = 1.10±0.74)

TR-LIF+FTS of Den Hartog et al (1987, JOSA B 4, 48)



Good agreement here!
Average exp/calc = 0.95±0.17
for gA > 5E+7 s^{-1}

TR-LIF+FTS of Kling & Kock (1999, JQSRT 62, 129)



Measurements here focused on high lying levels most of which are affected by strong mixings!

W^{3+}

HFR+CPOL model:

Similar model as in Ta^{2+} (Fivet et al 2008, J Phys B 41, 015702) which gave a good agreement with the TR-LIF lifetimes of the $5d^26p$ levels.

Intravalence Correlation:

$5d^3+5d^26s+5d6s^2+5d^26d+5d6p^2+5d6d^2+5d5f^2+5d6f^2+$
$5d6s6d+5d6p5f+5d6p6f+5d5f6f+6s^26d+6s6p^2+6s6d^2+6d^3+$
$6s5f^2+6d5f^2+6s6f^2+6d6f^2$ (even parity)

$5d^26p+5d^25f+5d^26f+5d6s6p+5d6s5f+5d6s6f+5d6p6d+$
$5d6d5f+5d6d6f+6s^26p+6s^25f+6s^26f+6p^25f+6p^26f+6p^3+6p6d^2+$
$6d^25f+6d^26f+6p5f^2+6p6f^2+5f^26f+5f6f^2$ (odd parity)

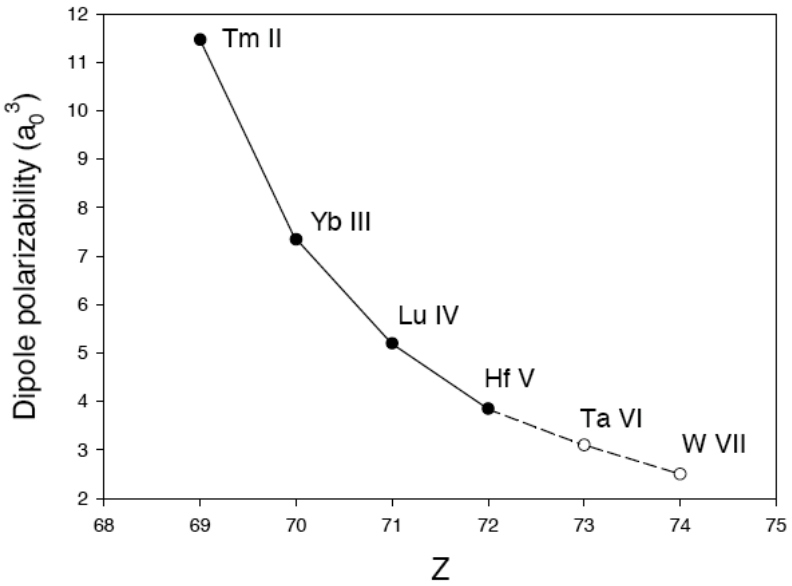
W^{3+}

Core-Polarization Potential:

Er-like W^{6+} $[Xe]4f^{14}$ ionic core: $\alpha_d = 2.50\ a_0^3$

(extrapolated value from Fraga et al 1976)

$r_c = \langle r \rangle_{5p} = 1.18\ a_0$



W^{3+}

Semi-Empirical Optimization:

Even parity: 36 $5d^3+5d^26s+5d6s^2$ experimental levels in Kramida & Shirai (2009, ADNDT 95, 305). Average deviation = 40 cm^{-1}.

Odd parity: 68 $5d^26p+5d6s6p$ experimental levels in Kramida & Shirai (2009, ADNDT 95, 305). Average deviation = 159 cm^{-1}.

W^{3+}

The transition probabilities and oscillator strengths have been calculated for:

- 278 strong (log gf > -1) E1 transitions in the range 93 - 237 nm

- 103 forbidden (M1+E2) transitions in the range 130 - 1517 nm

No measurements are available for comparison!

→Comparison with an independent model (MCDF) to assess the reliability

W^{3+}

Multiconfiguration Dirac-Fock (MCDF) model:

Fully relativistic method that takes into account QED effects

The GRASP code has been used (Grant et al 1980, CPC 21, 207; McKenzie et al 1980, CPC 21, 233; Norrington 2009, http://www.am.qub.ac.uk/DARC/) with the EAL option where the spin-orbitals are optimized self-consistently minimizing an energy functional built from the trace of the Hamiltonian matrix.

The configurations considered in the CI expansions: $5d^3+5d^26s+5d6s^2+5d^26d+5d6p^2+5d6d^2+ 6s^26d+6s6p^2+6s6d^2+6d^3$ (even parity); $5d^26p+5d6s6p+5d6p6d+6s^26p+6p^3+6p6d^2$ (odd parity) → only intravalence correlations!

W^{3+}

Comparison with the MCDF lifetimes of the 6p levels:

10-20% agreement

Level[a]	Energy[a] (cm^{-1})	Lifetime (ns)			
		$MCDF_{16}$	HFR_{16}	HFR_{43}	HFR_{43}+CPOL
$5d(^2D)6s6p(^3P^o)\ ^2F^o_{5/2}$	155752.99	0.29	0.35	0.35	0.40
$5d(^2D)6s6p(^3P^o)\ ^2P^o_{3/2}$	157 726.0	0.32	0.23	0.24	0.29
$5d(^2D)6s6p(^3P^o)\ ^2F^o_{7/2}$	157 984.23	0.24	0.26	0.27	0.30
$5d(^2D)6s6p(^3P^o)\ ^2P^o_{1/2}$	162 651.8	0.35	0.34	0.39	0.44
$5d(^2D)6s6p(^1P^o)\ ^2F^o_{5/2}$	163375.42	0.15	0.14	0.15	0.18
$5d(^2D)6s6p(^1P^o)\ ^2D^o_{3/2}$	163536.02	0.12	0.18	0.17	0.20
$5d(^2D)6s6p(^1P^o)\ ^2P^o_{1/2}$	168767.50	0.17	0.17	0.16	0.20
$5d(^2D)6s6p(^1P^o)\ ^2D^o_{5/2}$	169912.91	0.12	0.13	0.12	0.15
$5d(^2D)6s6p(^1P^o)\ ^2F^o_{7/2}$	171306.23	0.16	0.17	0.18	0.22
$5d(^2D)6s6p(^1P^o)\ ^2P^o_{3/2}$	174786.10	0.15	0.15	0.14	0.17

[a] Level designations and energies from Kramida and Shirai (2009).

30-40% lengthening

HFR_{16}: HFR with same CI as MCDF; HFR_{43}: HFR+CPOL without polarization

W^{4+}

HFR+CPOL model:

Similar model as in Hf^{2+} (Malcheva et al 2009, MNRAS 396, 2289) which gave a good agreement with the TR-LIF lifetimes of the 5d6p and 6s6p levels.

Intravalence Correlation:

$5d^2$+5d6s+5d7s+5d6d+5d7d+$6s^2$+6s6d+6s7d+6s7s+$6p^2$+6p7p+ 6p5f+6p6f+6p7f+$6d^2$+6d7s+6d7d+$7s^2$+$7p^2$+7s7d+7p5f+7p6f+ 7p7f (even parity)

5d6p+5d7p+5d5f+5d6f+5d7f+6s6p+6s7p+6s5f+6s6f+6s7f+6p6d+ 6p7d+6p7s+6d7p+6d5f+6d6f+6d7f+7s5f+7s6f+7s7f+7s7p+7p7d (odd parity)

W^{4+}

Core-Polarization Potential:

Er-like W^{6+} $[Xe]4f^{14}$ ionic core: $\alpha_d = 2.50\ a_0$(extrapolated)

$r_c = \langle r \rangle_{5p} = 1.20\ a_0$

Semi-Empirical Optimization:

Even parity: 14 $5d^2$+5d6s experimental levels in Kramida & Shirai (2009, ADNDT 95, 305). Average deviation = 20 cm^{-1}.

Odd parity: 30 5d6p+6s6p+5d5f+5d7p experimental levels in Kramida & Shirai (2009, ADNDT 95, 305). Average deviation = 132 cm^{-1}.

W^{4+}

The transition probabilities and oscillator strengths have been calculated for:

- 110 strong (log gf > -1) E1 transitions in the range 39 - 119 nm

- 40 forbidden (M1+E2) transitions in the range 137 - 1896 nm

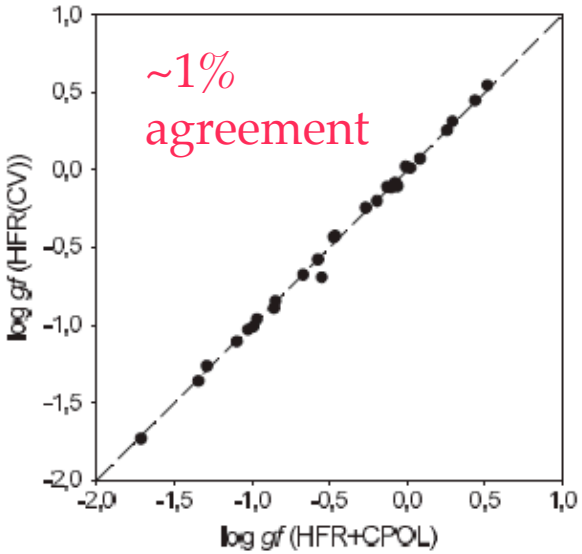
Here again no measurements are available for comparison!

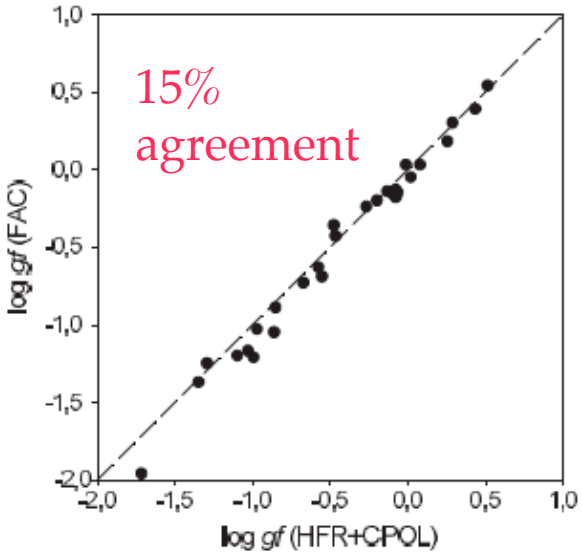
→Comparison with independent models (MCDF, FAC, RMBPT) to assess the reliability

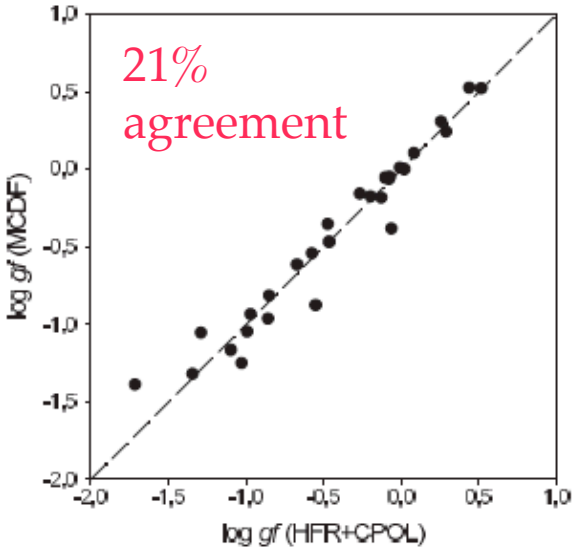
W^{4+}

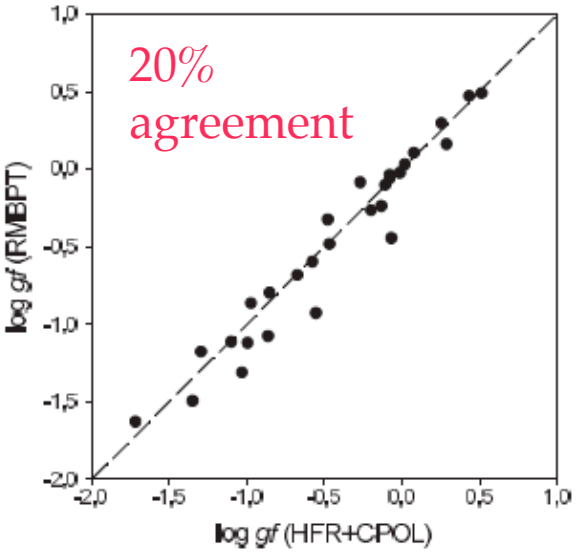
HFR(CV)	MCDF	FAC (Gu 2003, ApJ 582, 1241)	RMBPT
$5d^2$+5d6s+5d6d+ $6s^2$+6s6d+$6p^2$+6p5f +6p6f+$6d^2$+5d6p+ 5d5f+5d6f+6s6p+ 6s5f+6s6f+6p6d+ 6d5f+6d6f+ $5p^5 5d^2 6p$+ $5p^5 5d6s6p$+ $5s5p^6 5d^3$+ $5s5p^6 5d^2 6s$+ $5s5p^6 5d6s^2$+$5p^5 5d^3$+ $5p^5 5d^2 6s$+$5p^5 5d6s^2$+ $5s5p^6 5d^2 6p$+ $5s5p^6 5d6s6p$ S-E optimization: Av. dev.= 20 cm^{-1}(even) 135 cm^{-1}(odd)	$5d^2$+5d6s+5d6d+$6s^2$ +$6p^2$+$6d^2$+5d6p+ 6s6p+$5p^5 5d^2 6p$+ $5p^5 5d6s6p$+ $5s5p^6 5d^3$+ $5s5p^6 5d^2 6s$+ $5s5p^6 5d6s^2$+$5p^5 5d^3$+ $5p^5 5d^2 6s$+$5p^5 5d6s^2$+ $5s5p^6 5d^2 6p$+ $5s5p^6 5d6s6p$ EAL optimization	$5d^2$+5d6s+5d6d+ $6s^2$+6s6d+$6p^2$+6p5f +6p6f+$6d^2$+5d6p+ 5d5f+5d6f+6s6p+ 6s5f+6s6f+6p6d+ 6d5f+6d6f+ $5p^5 5d^2 6p$+ $5p^5 5d6s6p$+ $5s5p^6 5d^3$+ $5s5p^6 5d^2 6s$+ $5s5p^6 5d6s^2$+$5p^5 5d^3$+ $5p^5 5d^2 6s$+$5p^5 5d6s^2$+ $5s5p^6 5d^2 6p$+ $5s5p^6 5d6s6p$ DFS potential minimizing the average energy of $5d^2$+5d6s+5d6p	Calculations by Safronova & Safronova (2010, J Phys B 43, 074026) DF core potential: Er-like [Xe]$4f^{14}$ Zero order model space: $5d^2$+5d6s+$6s^2$+5d6p+ 5d5f+6s6p PT corrections up to second order

W^{4+}


~1%
agreement
log gf (HFR(CV))
log gf (HFR+CPOL)


15%
agreement
log gf (FAC)
log gf (HFR+CPOL)


21%
agreement
log gf (MCDF)
log gf (HFR+CPOL)


20%
agreement
log gf (RMBPT)
log gf (HFR+CPOL)

W^{4+}

Influence of the level mixing on the log gf of the $5d^2\ {}^1G_4$ - $5d6p\ {}^3F^o_4$ intercombination line

Method	Mixing of $5d^2\ {}^1G_4$	log gf
HFR+CPOL	91% ^{1}G + 9% ^{3}F	-1.03
	92% ^{1}G + 8% ^{3}F	-1.09
	93% ^{1}G + 7% ^{3}F	-1.14
	94% ^{1}G + 6% ^{3}F	-1.24
MCDF	94% ^{1}G + 6% ^{3}F	-1.25

W^{5+}

HFR+CPOL model:

Intravalence Correlation:

ns (n=6-7) + nd (n=5-6) + ng (n=5-7) (even parity)

np (n=6-7) + nf (n=5-7) (odd parity)

Core-Polarization Potential:

Er-like W^{6+} $[Xe]4f^{14}$ ionic core: $\alpha_d = 2.50\ a_0$(extrapolated)
$r_c = \langle r \rangle_{5p} = 1.20\ a_0$

W^{5+}

Semi-Empirical Optimization:

Even parity: 10 5d+6s+6d+7s+5g+6g experimental levels in Kramida & Shirai (2009, ADNDT 95, 305). Average deviation = 0 cm^{-1}.

Odd parity: 4 6p+5f experimental levels in Kramida & Shirai (2009, ADNDT 95, 305). Average deviation = 0 cm^{-1}.

W^{5+}

	Lower level[a]		Upper level[a]				
λ^a(nm)	E (cm^{-1})	Designation	E (cm^{-1})	Designation	Type	Log gf_{ik}^c	gA_{ki}^c(s^{-1})
38.2145	0.0	$5d\ ^2D_{3/2}$	261 681	$5f\ ^2F^o_{5/2}$	E1	0.28	8.68(10)
39.4133	8709.3	$5d\ ^2D_{5/2}$	262 430	$5f\ ^2F^o_{7/2}$	E1	0.42	1.13(11)
39.5301	8709.3	$5d\ ^2D_{5/2}$	261 681	$5f\ ^2F^o_{5/2}$	E1	−0.88	5.60(9)
60.5929	0.0	$5d\ ^2D_{3/2}$	165 036.7	$6p\ ^2P^o_{3/2}$	E1	−0.86	2.49(9)
63.9687	8709.3	$5d\ ^2D_{5/2}$	165 036.7	$6p\ ^2P^o_{3/2}$	E1	0.07	1.91(10)
66.9315	261 681	$5f\ ^2F^o_{5/2}$	411 087	$6g\ ^2G_{7/2}$	E1	−0.07	1.28(10)
67.2726	262 430	$5f\ ^2F^o_{7/2}$	411 079	$6g\ ^2G_{9/2}$	E1	0.05	1.64(10)
67.7718	0.0	$5d\ ^2D_{3/2}$	147 553.1	$6p\ ^2P^o_{1/2}$	E1	−0.21	8.91(9)
76.1252	147 553.1	$6p\ ^2P^o_{1/2}$	278 915.5	$7s\ ^2S_{1/2}$	E1	−0.27	6.21(9)
87.6106	147 553.1	$6p\ ^2P^o_{1/2}$	261 694.6	$6d\ ^2D_{3/2}$	E1	0.41	2.25(10)
87.8128	165 036.7	$6p\ ^2P^o_{3/2}$	278 915.5	$7s\ ^2S_{1/2}$	E1	−0.03	8.09(9)
99.4502	261 681	$5f\ ^2F^o_{5/2}$	362 234	$5g\ ^2G_{7/2}$	E1	0.85	4.78(10)
100.1964[b]	262 430	$5f\ ^2F^o_{7/2}$	362 234	$5g\ ^2G_{7/2}$	E1	−0.58	1.75(9)
100.2085	262 430	$5f\ ^2F^o_{7/2}$	362 222	$5g\ ^2G_{9/2}$	E1	0.96	6.11(10)
100.6289	165 036.7	$6p\ ^2P^o_{3/2}$	264 411.7	$6d\ ^2D_{5/2}$	E1	0.61	2.68(10)
103.4575	165 036.7	$6p\ ^2P^o_{3/2}$	261 694.6	$6d\ ^2D_{3/2}$	E1	−0.36	2.74(9)
116.8151	79 431.3	$6s\ ^2S_{1/2}$	165 036.7	$6p\ ^2P^o_{3/2}$	E1	0.18	7.32(9)
125.8950[b]	0.0	$5d\ ^2D_{3/2}$	79 431.3	$6s\ ^2S_{1/2}$	E2	−6.16	2.88(3)
141.3987[b]	8709.3	$5d\ ^2D_{5/2}$	79 431.3	$6s\ ^2S_{1/2}$	E2	−6.14	2.42(3)
146.7958	79 431.3	$6s\ ^2S_{1/2}$	147 553.1	$6p\ ^2P^o_{1/2}$	E1	−0.23	1.85(9)
1147.8836[b]	0.0	$5d\ ^2D_{3/2}$	8709.3	$5d\ ^2D_{5/2}$	M1	−6.07	4.30(1)
1147.8836[b]	0.0	$5d\ ^2D_{3/2}$	8709.3	$5d\ ^2D_{5/2}$	E2	−9.51	1.55(−2)

Here again no measurements are available for comparison!

→Comparison with an independent model to assess the reliability

W^{5+}

Relativistic Configuration Interaction (RCI) model:

The GRASP2K code has been used (Jonsson et al 2007, CPC 117, 597)

The CI expansions have been generated through single and double electron promotions from the multireference configurations 5d+5f+6p to the active set of orbitals {5s,5p,5d,5f,6s,6p,6d,6f}
→intravalence, core-valence and core-core correlations!

1s to 5d orbitals : MCDF-EAL optimization of ground config.
5f orbitals : MCDF-EAL opt. of 5d+5f conf.
n=6 orbitals : MCDF-EOL opt. of the 9 lowest levels of 5d+5f+6s+6p+6d+6f conf.

W^{5+}

Comparison of radiative lifetimes (in s)

Level	HFR+CPOL	RCI
$5d\ ^2D_{5/2}$	1.40E-1	1.40E-1
$6s\ ^2S_{1/2}$	3.77E-4	3.60E-4
$6p\ ^2P^o_{1/2}$	1.86E-10	1.71E-10
$6p\ ^2P^o_{3/2}$	1.39E-10	1.34E-10
$5f\ ^2F^o_{5/2}$	6.50E-11	5.47E-11
$5f\ ^2F^o_{7/2}$	7.10E-11	5.21E-11
$6d\ ^2D_{3/2}$	1.58E-10	1.65E-10
$6d\ ^2D_{5/2}$	2.24E-10	2.02E-10

Agreement is 10% on average

Conclusions & Perspectives

- New radiative data have been calculated in $W^{0,3-5+}$ using the HFR+CPOL method
- Accuracies of ~10-20% have been estimated through comparisons with available measurements in W^{0} and independent calculations in W^{3-5+}
- Measurements are needed in W^{3-5+}!
- Publications: Quinet et al (2011, J Phys B 44, 145005); Enzonga Yoca et al (2012, J Phys B 45, 035001; 035002; 065001)
- Data transfer to DESIRE and ADAS is in progress (W^{0} already transfered to ADAS!)

Collaborations

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  V. Vinogradoff (*also ULg, Belgium)
- Université Marien Ngouabi (Congo-Brazzaville):
  S. Enzonga Yoca
- ULB (Belgium): G. Jumet
- Lund University (Sweden): H. Nilsson
- Lund Institute of Technology (Sweden):
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- ADAS-EU Team

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Thank you for your attention!

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