UMONS
Université de Mons
Astrophysics & Spectroscopy

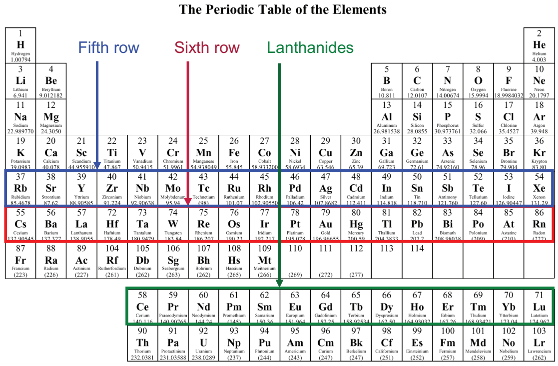
Atomic structure and radiative data calculations for heavy elements of interest in fusion plasma research

Theoretical challenges and recent advances

Pascal Quinet
quinet@umons.ac.be

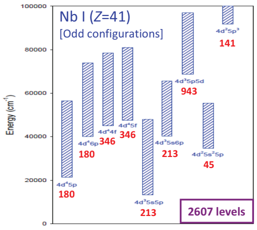
Faculté des Sciences

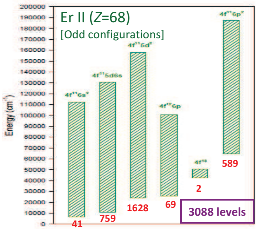
Introduction – Motivations



Introduction – Motivations

Fifth row	Sixth row	Lanthanides
$4d^k nl$	$5d^k nl$	$4f^k nl$
$4d^{k-1} nl n'l'$	$5d^{k-1} nl n'l'$	$4f^{k-1} nl n'l'$
$4d^{k-2} nl n'l' n''l''$	$5d^{k-2} nl n'l' n''l''$	$4f^{k-2} nl n'l' n''l''$
…	…	…





Introduction – Motivations

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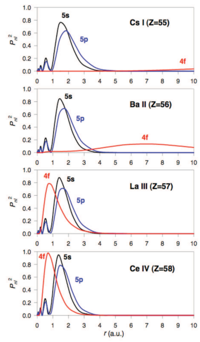
$4d^{k-2} nl n'l' n''l''$	$5d^{k-2} nl n'l' n''l''$	$4f^{k-2} nl n'l' n''l''$
…	…	…

Collapse of the 4f orbital



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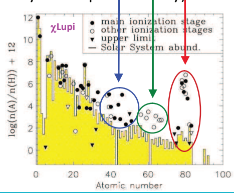
…	…	…

Very complex spectroscopic structures (unfilled 4d, 5d, 4f shells)
→ little investigated up to now (both theoretically and experimentally)

Interest in many other fields :
- Astrophysics (CP stars, nucleosynthesis, …)
- Solid state physics (doped crystals, …)
- New light sources (lasers, lamps, …)
- Plasma physics (fusion, ITER, …)



Progress in computers & laser spectroscopy
→ **New systematic investigations possible**

Determination of atomic data

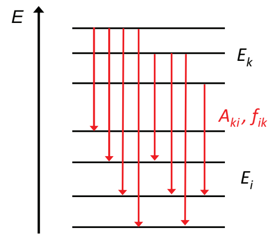
Theoretically and experimentally…

Atomic structure parameters

- Energy levels, E_k, E_i
- Transition energies, ΔE_{ki}
- Wavelengths, λ_{ki}

Radiative parameters

- Transition probabilities, A_{ki}
- Oscillator strengths, f_{ik}
- Radiative lifetimes, $\tau_k = 1/\Sigma_i A_{ki}$



Theoretical approach

Relativistic Hartree-Fock method (HFR)

(R.D. Cowan, *The Theory of Atomic Structure and Spectra*, Univ. California Press, Berkeley, 1981)

Based on the Schrödinger equation (atom with N electrons)

$$H\Psi = E\Psi \quad \text{with} \quad H = \sum_{i=1}^{N}\left[-\frac{\hbar^2}{2m}\nabla_i^2 - \frac{Ze^2}{4\pi\varepsilon_0 r_i} + \sum_{j<i}\frac{e^2}{4\pi\varepsilon_0 r_{ij}}\right]$$

Central field approximation

$$\varphi_{nlm_lm_s}(\boldsymbol{q}) = \frac{1}{r}P_{nl}(r)Y_{lm_l}(\theta,\phi)\chi_{1/2,m_s}(\sigma)$$

Slater determinant

$$\Psi(\mathbf{q}_1,\mathbf{q}_2,\dots,\mathbf{q}_N) = \frac{1}{\sqrt{N!}}\begin{vmatrix}\varphi_1(\mathbf{q}_1) & \varphi_2(\mathbf{q}_1) & \dots & \varphi_N(\mathbf{q}_1)\\ \varphi_1(\mathbf{q}_2) & \varphi_2(\mathbf{q}_2) & \dots & \varphi_N(\mathbf{q}_2)\\ \dots & \dots & & \dots\\ \varphi_1(\mathbf{q}_N) & \varphi_2(\mathbf{q}_N) & \dots & \varphi_N(\mathbf{q}_N)\end{vmatrix}$$

Theoretical approach

Relativistic Hartree-Fock method (HFR)

(R.D. Cowan, *The Theory of Atomic Structure and Spectra*, Univ. California Press, Berkeley, 1981)

Hartree-Fock equations

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr_i^2} + \frac{\hbar^2 l_i(l_i+1)}{2mr_i^2} - \frac{Ze^2}{4\pi\varepsilon_0 r_i}\right]P_i(r_i) + \left[\sum_{j\neq i}\int\left|P_j(r_j)\right|^2\frac{e^2}{4\pi\varepsilon_0 r_{ij}}d\tau_j\right]P_i(r_i)$$

$$-\left[\sum_{j\neq i}\delta_{m_{s_i}}\delta_{m_{s_j}}\int P_j^*(r_j)P_i(r_j)\frac{e^2}{4\pi\varepsilon_0 r_{ij}}d\tau_j\right]P_j(r_i) = E_i\,P_i(r_i)$$

Resolution of Hartree-Fock equations

Iterative method → self-consistent field method

Theoretical approach

Relativistic Hartree-Fock method (HFR)

(R.D. Cowan, *The Theory of Atomic Structure and Spectra*, Univ. California Press, Berkeley, 1981)

Multiconfiguration approach

$$\Psi^k = \sum_b a_b^k \Psi_b$$

Relativistic effects

Included perturbationaly (spin-orbit, mass-velocity, Darwin term)

Good agreement with fully relativistic methods

Ab initio or semi-empirical approach

Experimental energy levels can be used to optimize the radial parameters

Theoretical approach

Relativistic Hartree-Fock method (HFR)

(R.D. Cowan, *The Theory of Atomic Structure and Spectra*, Univ. California Press, Berkeley, 1981)

Multiconfiguration approach

$$\Psi^k = \sum_b a_b^k \Psi_b$$

Example : Lu III (Lu^{2+})
(Ground config. : [Xe]$4f^{14}5s^25p^66s$)

Intravalence correlation (up to n=6, l=3)

Even parity	Odd parity
$5s^25p^66s$	$5s^25p^66p$
$5s^25p^65d$	$5s^25p^65f$
$5s^25p^66d$	$5s^25p^66f$
5 levels	6 levels

+

Core-valence correlation (with 5s, 5p)

Even parity		Odd parity	
$5s^25p^55d5f$	$5s5p^65d^2$	$5s^25p^55d^2$	$5s5p^65d5f$
$5s^25p^55d6p$	$5s5p^65f^2$	$5s^25p^55f^2$	$5s5p^65d6p$
$5s^25p^55d6f$	$5s5p^66s^2$	$5s^25p^56s^2$	$5s5p^65d6f$
$5s^25p^55f6s$	$5s5p^66p^2$	$5s^25p^56p^2$	$5s5p^65f6s$
$5s^25p^55f6d$	$5s5p^66d^2$	$5s^25p^56d^2$	$5s5p^65f6d$
$5s^25p^56s6p$	$5s5p^66f^2$	$5s^25p^56f^2$	$5s5p^66s6p$
$5s^25p^56s6f$	$5s5p^65d6s$	$5s^25p^55d6s$	$5s5p^66s6f$
$5s^25p^56p6d$	$5s5p^65d6d$	$5s^25p^55d6d$	$5s5p^66p6d$
$5s^25p^56d6f$	$5s5p^65f6p$	$5s^25p^55f6p$	$5s5p^66d6f$
	$5s5p^65f6f$	$5s^25p^55f6f$	
	$5s5p^66s6d$	$5s^25p^56s6d$	
	$5s5p^66p6f$	$5s^25p^56p6f$	
885 levels		904 levels	

Core-polarization effects (HFR + CPOL)

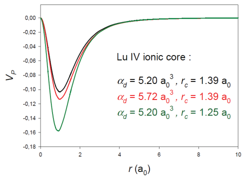
(see e.g. Quinet *et al.*, M.N.R.A.S. **307**, 934, 1999; Quinet *et al.*, J. Alloys Compd **344**, 255, 2002)

Intravalence correlation considered within a configuration interaction scheme

Core-valence correlation represented by a **core-polarization model potential** depending on two parameters (dipole polarizability α_d and cut-off radius r_c)

$$V_{P1} = -\frac{1}{2}\alpha_d \sum_{i=1}^{n} \frac{r_i^2}{(r_i^2 + r_c^2)^3}$$

$$V_{P2} = -\alpha_d \sum_{i>j} \frac{\vec{r}_i \cdot \vec{r}_j}{[(r_i^2 + r_c^2)(r_j^2 + r_c^2)]^{3/2}}$$



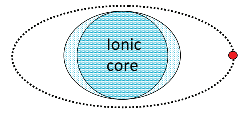
Correction to the dipole radial integral

$$\int_0^\infty P_{nl}(r)\, r\, P_{n'l'}(r)\, dr \quad \text{replaced by} \quad \int_0^\infty P_{nl}(r)\, r \left[1 - \frac{\alpha_d}{(r^2 + r_c^2)^{3/2}}\right] P_{n'l'}(r)\, dr$$

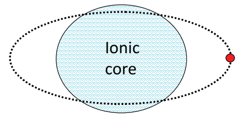
Core-polarization effects (HFR + CPOL)

(see e.g. Quinet *et al.*, M.N.R.A.S. **307**, 934, 1999; Quinet *et al.*, J. Alloys Compd **344**, 255, 2002)

Core-polarization



Core-penetration



Semi-empirical optimization

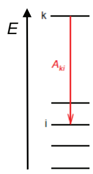
(R.D. Cowan, *The Theory of Atomic Structure and Spectra*, Univ. California Press, Berkeley, 1981)

Radial parameters (average energies, electrostatic integrals, spin-orbit parameters) adjusted in order to minimize the discrepancies between computed Hamiltonian eigenvalues and experimental energy levels

→ Optimization of the transition energies and wavefunctions
→ Optimization of the radiative decay rates

$$A_{ki} = \frac{64\pi^4 e^4 a_0^2}{3h} \frac{(\Delta E_{ki})^3}{2J_k + 1} \left| \langle \gamma_i J_i \| P^{(1)} \| \gamma_k J_k \rangle \right|^2$$

$$= 2.0261 \times 10^{-6} \frac{(\Delta E_{ki})^3}{2J_k + 1} \left| \langle \gamma_i J_i \| P^{(1)} \| \gamma_k J_k \rangle \right|^2$$



→ A good experimental knowledge of the level structure for the atom (or ion) considered is needed

A specific example (Lu III)

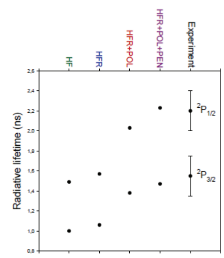
(Biémont *et al.*, J. Phys. B **32**, 3409, 1999)

Radiative lifetimes for 6p $^2P_{1/2}$ (38401 cm^{-1}) and 6p $^2P_{3/2}$ (44705 cm^{-1})

$1s^22s^22p^63s^23p^63d^{10}4s^24p^64d^{10}4f^{14}5s^25p^6$ *nl*

Lu^{3+} ionic core with 68 electrons :
α_d = 5.20 a_0^3 (Fraga *et al.*, 1976)
r_c = $<r>_{5p}$ = 1.39 a_0

Method	$^2P_{1/2}$	$^2P_{3/2}$
HF	1.49	1.00
HFR	1.57	1.06
HFR+POL	2.03	1.38
HFR+POL+PEN	2.23	1.47
Experiment	2.20 ± 0.20	1.55 ± 0.20



Experimental measurements

Time-resolved laser-induced fluorescence (TR-LIF)

(see e.g. Bergström *et al.*, Z. Phys. D **8**, 17, 1988; Xu *et al.*, Phys. Rev. A **70**, 042508, 2004)

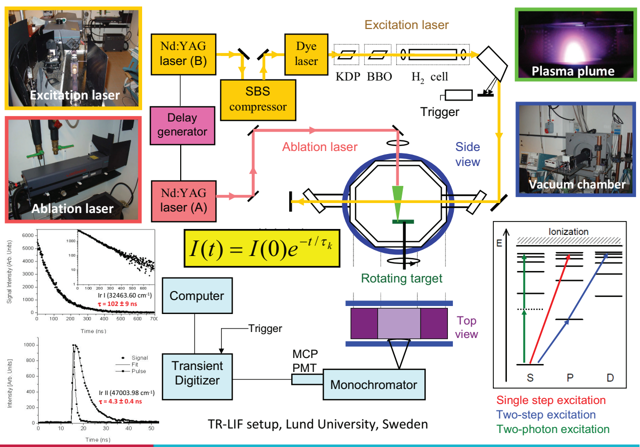
Accurate measurements of radiative lifetimes (within a few %)

Lifetime range from 1 ns to 300 ns

Selective excitation (no cascading problems)

Many levels accessible (using different laser dyes)

Different ionization degrees accessible in the laser-produced plasma (neutral, singly-, doubly- and trebly-ionized atoms)



TR-LIF setup, Lund University, Sweden

Results obtained so far

Calculations and measurements performed during the period 1998 – 2014

Radiative lifetimes, transition rates (lanthanides)

Z	Ion	References
58	Ce II	Palmeri *et al.*, Phys. Scr. **61**, 323 (2000); Zhang *et al.*, Phys. Scr. **63**, 122 (2001)
	Ce III	Biémont *et al.*, MNRAS **336**, 1155 (2002)
	Ce IV	Zhang *et al.*, Phys. Rev. Lett. **87**, 273001 (2001)
59	Pr I	Biémont *et al.*, J. Phys. B **37**, 1381 (2004)
	Pr II	Biémont *et al.*, Eur. Phys. J. D **27**, 33 (2003)
	Pr III	Palmeri *et al.*, ApJS **129**, 367 (2000); Biémont *et al.*, Phys. Rev. A **64**, 022503 (2001)
	Pr IV	Enzonga Yoca & Quinet, J. Phys. B **46**, 145003 (2013)
60	Nd I	Biémont *et al.*, J. Phys. B **37**, 1381 (2004)
	Nd II	Xu *et al.*, MNRAS **346**, 433 (2003)
	Nd III	Zhang *et al.*, A&A **385**, 724 (2002)
	Nd IV	Enzonga Yoca & Quinet, J. Phys. B **47**, 035002 (2014)
61	Pm II	Fivet *et al.*, MNRAS **380**, 771 (2007)
62	Sm II	Xu *et al.*, J. Phys. B **36**, 4773 (2003)
	Sm III	Biémont *et al.*, A&A **399**, 343 (2003)
63	Eu III	Quinet & Biémont, MNRAS **340**, 463 (2003)
64	Gd III	Biémont *et al.*, A&A **393**, 717 (2002)
65	Tb III	Biémont *et al.*, Phys. Rev. A **65**, 052502 (2002)
66	Dy III	Zhang *et al.*, MNRAS **334**, 1 (2002)
67	Ho III	Biémont *et al.*, MNRAS **328**, 1085 (2001); Zhang et al., A&A **384**, 364 (2002)
68	Er II	Xu *et al.*, J. Phys. B **36**, 1771 (2003)
	Er III	Biémont *et al.*, MNRAS **321**, 481 (2001)
69	Tm II	Quinet *et al.*, JQSRT **62**, 625 (1999)
	Tm III	Li *et al.*, J. Phys. B **34**, 1349 (2001)
70	Yb II	Biémont *et al.*, J. Phys. B **31**, 3321 (1998); Li *et al.*, J. Phys. B **32**, 1731 (1999); Biémont *et al.*, J. Phys. B **35**, 4743 (2002)
	Yb III	Biémont *et al.*, J. Phys. B **34**, 1869 (2001); Zhang *et al.*, Eur. Phys. J. D **15**, 301 (2001)
	Yb IV	Wyart *et al.*, Phys. Scr. **63**, 113 (2001)
71	Lu I	Fedchak *et al.*, ApJ **542**, 1109 (2000); Dai *et al.*, J. Phys. B **36**, 479 (2003)
	Lu II	Quinet *et al.*, MNRAS **307**, 934 (1999); Fedchak *et al.*, ApJ **542**, 1109 (2000)
	Lu III	Biémont *et al.*, J. Phys. B **32**, 3409 (1999); Fedchak *et al.*, ApJ **542**, 1109 (2000)

Radiative lifetimes, transition rates (fifth row)

Z	Ion	References
37	Rb III	Zhang *et al.*, Eur. Phys. J. D **68**, 104 (2014)
39	Y II	Biémont *et al.*, MNRAS **414**, 3350 (2011)
	Y III	Biémont *et al.*, MNRAS **414**, 3350 (2011)
40	Zr I	Malcheva *et al.*, MNRAS **395**, 1523 (2009)
	Zr II	Malcheva *et al.*, MNRAS **367**, 754 (2006)
41	Nb I	Malcheva *et al.*, MNRAS **412**, 1823 (2011)
	Nb II	Nilsson *et al.*, A&A **511**, A16 (2010)
	Nb III	Nilsson *et al.*, A&A **511**, A16 (2010)
42	Mo II	Quinet, J. Phys. B **35**, 19 (2002); Lundberg *et al.*, J. Phys. B **43**, 085004 (2010)
	Mo III	Quinet, Phys. Scr., in press (2014)
43	Tc I	Palmeri *et al.*, MNRAS **363**, 452 (2005)
	Tc II	Palmeri *et al.*, MNRAS **374**, 63 (2007)
44	Ru I	Fivet *et al.*, MNRAS **396**, 2124 (2009)
	Ru II	Palmeri *et al.*, J. Phys. B **42**, 165005 (2009)
	Ru III	Palmeri *et al.*, J. Phys. B **42**, 165005 (2009)
45	Rh II	Quinet *et al.*, J. Elec. Spectrosc. Rel. Phen. **184**, 174 (2011); Quinet *et al.*, A&A **537**, A74 (2012)
	Rh III	Zhang *et al.*, Phys. Scr. **88**, 065302 (2013)
46	Pd I	Xu *et al.*, A&A **452**, 357 (2006)
	Pd II	Quinet, Phys. Src. **54**, 483 (1996)
	Pd III	Zhang *et al.*, Phys. Scr. **88**, 065302 (2013)
47	Ag II	Biémont *et al.*, J. Elec. Spectr. Rel. Phen. **144-147**, 27 (2005); Campos *et al.*, MNRAS **363**, 905 (2005)
	Ag III	Zhang *et al.*, Phys. Scr. **88**, 065302 (2013)
48	Cd I	Biémont *et al.*, Phys. Rev. A **62**, 032512 (2000), Xu *et al.* Phys. Rev. **70**, 042508 (2004)
	Cd II	Xu *et al.* Phys. Rev. **70**, 042508 (2004)
49	In II	Biémont *et al.*, Phys. Rev. A **62**, 032512 (2000)
50	Sn I	Zhang *et al.*, Phys. Rev. A **78**, 022505 (2008); Zhang *et al.*, Eur. Phys. J. D **55**, 1 (2009)
	Sn III	Biémont *et al.*, Phys. Rev. A **62**, 032512 (2000)
51	Sb I	Hartman *et al.*, Phys. Rev. A **82**, 052512 (2010)
52	Te II-III	Zhang *et al.*, Astron. Astrophys. **551**, A136 (2013)

Radiative lifetimes, transition rates (sixth row)

Z	Ion	References
56	Ba I	Zhang *et al.*, Phys. Rev. A **82**, 042507 (2010)
57	La I	Biémont *et al.*, Eur. Phys. J. D **30**, 157 (2004)
	La III	Biémont *et al.*, J. Phys. B **32**, 3409 (1999)
72	Hf I	Malcheva *et al.*, MNRAS **396**, 2289 (2009)
	Hf III	Malcheva *et al.*, MNRAS **396**, 2289 (2009)
73	Ta I	Fivet *et al.*, Eur. Phys. J. D **37**, 29 (2006)
	Ta II	Quinet *et al.*, A&A **493**, 711 (2009)
	Ta III	Fivet *et al.*, J. Phys. B **41**, 015702 (2008)
74	W I	Quinet *et al.*, J. Phys. B **44**, 145005 (2011)
	W II	Nilsson *et al.*, Eur. Phys. J. D **49**, 13 (2008)
	W III	Palmeri *et al.*, Phys. Scr. **78**, 015304 (2008)
	W IV	Enzonga Yoca *et al.*, J. Phys. B **45**, 035001 (2012)
	W V	Enzonga Yoca *et al.*, J. Phys. B **45**, 065001 (2012)
	W VI	Enzonga Yoca *et al.*, J. Phys. B **45**, 035002 (2012)
75	Re I	Palmeri *et al.*, Phys. Scr. **74**, 297 (2006)
	Re II	Palmeri *et al.*, MNRAS **362** 1348 (2005)
76	Os I - II	Quinet *et al.*, A&A **448**, 1207 (2006)
77	Ir I - II	Xu *et al.*, JQSRT **104**, 52 (2007)
78	Pt II	Quinet *et al.*, Phys. Rev. A **77**, 022501 (2008)
79	Au I	Fivet *et al.*, J. Phys. B **39**, 3587 (2006)
	Au II	Fivet *et al.*, J. Phys. B **39**, 3587 (2006); Biémont *et al.*, MNRAS **380**, 1581 (2007)
	Au III	Enzonga Yoca *et al.*, Phys. Scr. **78**, 025303 (2008)
80	Hg I	Blagoev *et al.*, Phys. Rev. A **66**, 032509 (2002)
81	Tl I	Biémont *et al.*, J. Phys. B **38**, 3547 (2005)
82	Pb I	Li *et al.*, Phys. Rev. A **57**, 3443 (1998); Biémont *et al.*, MNRAS **312**, 116 (2000)
	Pb II	Quinet *et al.*, J. Phys. B **40**, 1705 (2007)
83	Bi II	Palmeri *et al.*, Phys. Scr. **63**, 468 (2001)
	Bi III	Quinet *et al.*, J. Phys. B **40**, 1705 (2007)

Some recent results : Nb II, Mo II, Rh II

Nb II : lifetimes measured for 17 energy levels belonging to $4d^35p$

Level	E (cm^{-1})	τ (ns) [Theory] This work	τ (ns) [Experiment] This work	Previous
$4d^3(^4F)5p\ ^3D_1$	34886.35	5.9	5.6 ± 0.3	5.5 ± 0.3[a] 5.7 ± 0.3[b]
$4d^3(^4F)5p\ ^3D_2$	35520.82	5.7	5.5 ± 0.3	5.7 ± 0.3[a] 5.7 ± 0.3[b]
$4d^3(^4F)5p\ ^5D_0$	37298.24	2.7	2.6 ± 0.2	3.1 ± 0.3[b]
$4d^3(^4F)5p\ ^5D_2$	37797.32	2.8	2.7 ± 0.2	3.2 ± 0.3[b]
$4d^3(^4F)5p\ ^3G_5$	40103.61	5.0	5.1 ± 0.3	5.2 ± 0.3[b]
$4d^3(^4F)5p\ ^3P_2$	41710.14	8.4	8.5 ± 0.7	
$4d^3(^4F)5p\ ^3P_1$	42132.65	7.2	7.2 ± 0.5	
$4d^3(^4F)5p\ ^5D_0$	42596.55	7.2	7.5 ± 0.7	
$4d^3(^4F)5p\ ^5D_2$	43290.34	7.3	7.5 ± 0.4	
$4d^3(^4F)5p\ ^1D_2$	43618.39	6.7	6.7 ± 0.3	
$4d^3(^2P)5p\ ^3D_1$	43649.19	8.1	7.2 ± 0.4	12.8 ± 0.3[b]
$4d^3(^4P)5p\ ^5D_3$	43887.08	6.3	5.7 ± 0.5	
$4d^3(^4P)5p\ ^5D_1$	44066.67	6.7	6.4 ± 0.5	5.3 ± 0.3[b]
$4d^3(^4P)5p\ ^3P_0$	44285.94	7.5	7.0 ± 0.5	
$4d^3(^2P)5p\ ^3D_2$	44924.60	6.6	6.2 ± 0.3	
$4d^3(^4P)5p\ ^5D_4$	44970.71	5.8	5.2 ± 0.5	
$4d^3(^2P)5p\ ^3D_3$	45802.47	4.6	4.6 ± 0.3	

[a] Salih & Lawer (1983); [b] Hannaford *et al.* (1985)

Mean ratio (Th/Exp) = 1.035 ± 0.048

Some recent results : Nb II, Mo II, Rh II

Mo II : lifetimes measured for 16 energy levels belonging to $4d^45p$

Level	E (cm^{-1})	τ (ns) [Theory] This work	τ (ns) [Experiment] This work	Previous
$4d^4(^5D)5p\ z\ ^4P_{3/2}$	48022.815	4.8	4.9 ± 0.2	4.8 ± 0.4[a] 4.9 ± 0.3[b]
$4d^4(^5D)5p\ z\ ^6D_{7/2}$	50302.913	4.2	4.0 ± 0.3	4.3 ± 0.3[a] 4.0 ± 0.3[b]
$4d^4(^5D)5p\ z\ ^4F_{3/2}$	51373.170	4.7	4.2 ± 0.3	
$4d^4(^5D)5p\ z\ ^4F_{5/2}$	51732.690	4.6	4.2 ± 0.3	
$4d^4(^5D)5p\ z\ ^4F_{7/2}$	52217.587	4.4	4.0 ± 0.3	
$4d^4(^5D)5p\ z\ ^4F_{9/2}$	52843.296	4.3	4.0 ± 0.3	
$4d^4(^5D)5p\ z\ ^4D_{1/2}$	54238.949	5.5	5.1 ± 0.3	
$4d^4(^5D)5p\ z\ ^4D_{3/2}$	54687.002	5.2	5.0 ± 0.3	
$4d^4(^5D)5p\ z\ ^4D_{5/2}$	55216.203	4.9	4.6 ± 0.3	
$4d^4(^5D)5p\ z\ ^4D_{7/2}$	55706.937	4.7	4.5 ± 0.3	
$4d^4(^3H)5p\ z\ ^4H_{7/2}$	57892.289	5.2	4.9 ± 0.3	
$4d^4(^3H)5p\ z\ ^4H_{9/2}$	58196.928	5.2	4.9 ± 0.3	
$4d^4(^3H)5p\ z\ ^4H_{11/2}$	58761.258	5.0	4.8 ± 0.3	
$4d^4(^3H)5p\ z\ ^4H_{13/2}$	59492.157	4.7	4.6 ± 0.3	
$4d^4(^3F)5p\ z\ ^2D_{3/2}$	59841.060	8.5	7.6 ± 1.0	
$4d^4(^3F)5p\ z\ ^2D_{5/2}$	60992.764	7.5	6.6 ± 0.5	

[a] Hannaford & Lowe (1983); [b] Sikström *et al.* (2001)

Mean ratio (Th/Exp) = 1.068 ± 0.039

Some recent results : Nb II, Mo II, Rh II

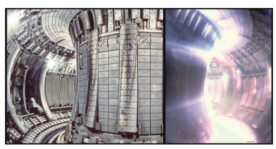
Rh II : lifetimes measured for 17 energy levels belonging to $4d^75p$

Level	E (cm^{-1})	τ (ns) [Theory] This work	τ (ns) [Experiment] This work	Previous
$4d^7(^4F)5p\ ^5F_4$	56547.3	4.4	3.9 ± 0.5	
$4d^7(^4F)5p\ ^5F_5$	57020.8	4.0	3.9 ± 0.3	
$4d^7(^4F)5p\ ^5F_3$	58358.5	4.2	3.8 ± 0.3	
$4d^7(^4F)5p\ ^5D_4$	59161.5	3.9	3.3 ± 0.2	
$4d^7(^4F)5p\ ^5F_2$	59698.6	4.2	3.8 ± 0.3	
$4d^7(^4F)5p\ ^5G_6$	59702.4	3.1	3.0 ± 0.2	
$4d^7(^4F)5p\ ^5G_5$	59729.4	4.0	3.5 ± 0.2	
$4d^7(^4F)5p\ ^5D_3$	60448.4	3.9	3.4 ± 0.4	
$4d^7(^4F)5p\ ^5G_4$	61173.1	3.5	3.3 ± 0.2	
$4d^7(^4F)5p\ ^5D_2$	61355.9	4.0	3.7 ± 0.5	
$4d^7(^4F)5p\ ^5G_3$	61939.8	3.6	3.3 ± 0.3	
$4d^7(^4F)5p\ ^3G_5$	62194.4	3.5	3.2 ± 0.2	
$4d^7(^4F)5p\ ^5G_2$	62288.3	3.6	3.3 ± 0.3	
$4d^7(^4F)5p\ ^3F_4$	62326.1	2.8	2.4 ± 0.2	
$4d^7(^4F)5p\ ^3F_3$	63454.9	2.5	2.3 ± 0.3	
$4d^7(^4F)5p\ ^3G_4$	63959.5	3.7	3.4 ± 0.2	
$4d^7(^4F)5p\ ^3G_3$	65321.2	2.4	2.0 ± 0.2	

Mean ratio (Th/Exp) = 1.107 ± 0.047

The specific case of tungsten

Great interest in plasma physics



Fusion reactors

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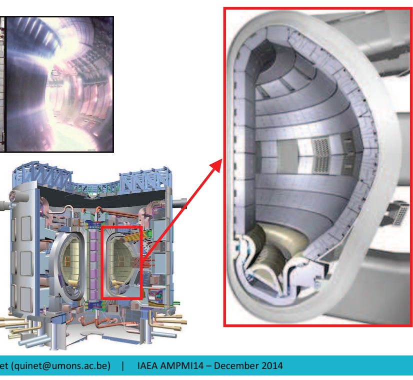


The specific case of tungsten (W I, W II, W III)

Transition rates in W I, W II and W III

W I : 508 experimentally known energy levels within the 5d⁴6s², 5d⁵6s, 5d⁴6s7s, 5d⁵6p, 5d⁴6s6p and 5d³6s²6p configurations
(Kramida & Shirai, J. Phys. Chem. Ref. Data **35**, 423, 2006; Wyart, J. Phys. B 43, 074018, 2010)

W II : 263 experimentally known energy levels within the 5d⁵, 5d⁴6s, 5d³6s², 5d⁴6p, 5d³6s6p and 5d²6s²6p configurations
(Kramida & Shirai, J. Phys. Chem. Ref. Data **35**, 423, 2006)

W III : 235 experimentally known energy levels within the 5d⁴, 5d³6s, 5d²6s², 5d³6p and 5d²6s6p configurations
(Iglesias *et al.*, J. Res. Natl Inst. Stand. Tech. **94**, 221, 1989)

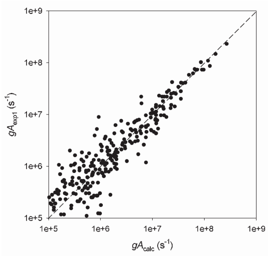
Transition probabilities and oscillator strengths calculated for :

2525 W I lines in the range 223 – 1010 nm (Quinet *et al.*, J. Phys. B. **44**, 145005, 2011)
6086 W II lines in the range 143 – 990 nm (Nilsson *et al.*, Eur. Phys. J. D **49**, 13, 2008)
4822 W III lines in the range 83 – 1494 nm (Palmeri *et al.*, Phys. Scr. **78**, 015304, 2008)

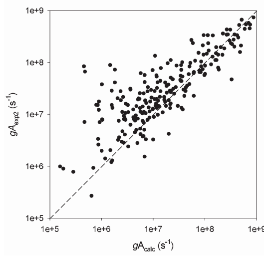
The specific case of tungsten (W I, W II, W III)

Transition rates in W I

Comparison between theoretical transition probabilities and available experimental results



[Den Hartog *et al.*, J.O.S.A. B **4**, 48 (1987)]

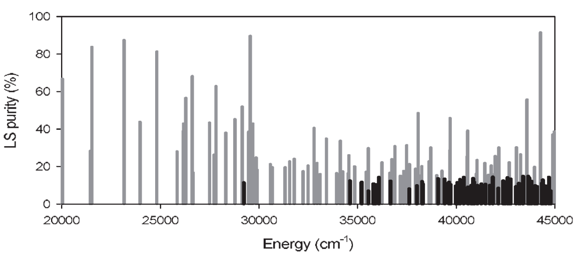


[Kling & Kock, J.Q.S.R.T. **62**, 129 (1999)]

The specific case of tungsten (W I, W II, W III)

Transition rates in W I

Wavefunction purities (in LS coupling) for W I odd-levels below 45000 cm⁻¹
(bold lines represent purities smaller than 15%)



The specific case of tungsten (W I, W II, W III)

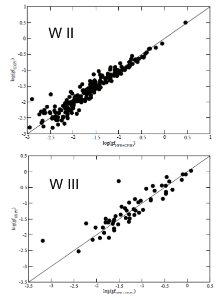
Transition rates in W II and W III

Comparison between theoretical and experimental lifetimes obtained in our work

E (cm⁻¹)	J	Theory	Experiment
W II			
47179.941	3/2	6.8	5.8 ± 0.3
48284.498	5/2	7.6	5.9 ± 0.3
48181.034	9/2	20.4	21.5 ± 1.0
50430.999	3/2	5.3	6.6 ± 0.4
51045.292	7/2	4.3	4.7 ± 0.4
51254.429	3/2	2.2	2.1 ± 0.2
51438.064	5/2	4.7	4.6 ± 0.4
54498.608	7/2	2.9	2.1 ± 0.2
55392.446	9/2	2.4	2.3 ± 0.2
W III			
57231.04	2	2.9	2.9 ± 0.3
61488.36	3	2.3	2.5 ± 0.3

W II: ~ 25%
W III: ~ 10%

Comparison between theoretical oscillator strengths and available experimental results
(W II : Kling *et al.*, JQSRT **67**, 227, 2000)
(W III : Schultz-Johanning *et al.*, Phys. Scr. **63**, 367, 2001)



The specific case of tungsten (W I, W II, W III)

Critical evaluation of available data

IOP Publishing — Journal of Physics B: Atomic, Molecular and Optical Physics
J. Phys. B: At. Mol. Opt. Phys. **43** (2010) 144003 (12pp) doi:10.1088/0953-4075/43/14/144003

Radiative decay rates for W I, W II and W III allowed and forbidden transitions of interest for spectroscopic diagnostics in fusion plasmas

P Quinet[1,2], V Vinogradoff[1], P Palmeri[1] and É Biémont[1,2]
[1] Astrophysique et Spectroscopie, Université de Mons-UMONS, B-7000 Mons, Belgium
[2] IPNAS, Université de Liège, B15 Sart Tilman, B-4000 Liège, Belgium
E-mail: quinet@umons.ac.be

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Abstract
Transition probabilities for allowed and forbidden lines in neutral, singly ionized and doubly ionized tungsten are discussed in the present paper. For the electric dipole transitions, recommended values are proposed from a critical evaluation of the data available in the literature. For the magnetic dipole and electric quadrupole transitions, for which no data have been published so far, a new set of radiative rates has been obtained using a relativistic Hartree–Fock approach including core-polarization effects. The tables summarizing the compiled data are expected to be useful for plasma modelling in fusion reactors.

Recommended *A*-values for the most intense W I, W II and W III E1 lines

+ new decay rates for forbidden lines

The specific case of tungsten (W IV, W V, W VI)

Transition rates in W IV, W V and W VI

W IV : 105 experimentally known energy levels within the 5d³, 5d²6s, 5d6s², 5d²6p and 5d6s6p configurations
(Kramida & Shirai, At. Data Nucl. Data Tables **95**, 305, 2009)

W V : 59 experimentally known energy levels within the 5d², 5d6s, 5d6p, 6s6p, 5d5f and 5d7p configurations
(Kramida & Shirai, At. Data Nucl. Data Tables **95**, 305, 2009)

W VI : 14 experimentally known energy levels within the 5d, 6s, 6p, 6d, 7s, 5f, 5g and 6g configurations
(Kramida & Shirai, At. Data Nucl. Data Tables **95**, 305, 2009)

Transition probabilities and oscillator strengths calculated for :

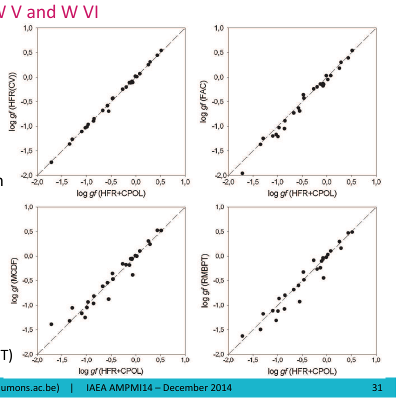
W IV lines in the range 143 – 990 nm (Enzonga Yoca *et al.*, J. Phys. B **45**, 035001, 2012)
W V lines in the range 83 – 1494 nm (Enzonga Yoca *et al.*, J. Phys. B **45**, 065001, 2012)
W VI lines in the range 38 - 1148 nm (Enzonga Yoca *et al.*, J. Phys. B **45**, 035002, 2012)

The specific case of tungsten (W IV, W V, W VI)

Transition rates in W IV, W V and W VI

No experimental radiative data to compare with !

- Use of different and independent theoretical methods
- HFR + CPOL compared with
  - HFR including core-valence (HFR(CV))
  - Flexible Atomic Code (FAC)
  - Multiconfiguration Dirac-Fock (MCDF)
  - Relativistic Many-Body Perturbation Theory (RMBPT)



Conclusions

New radiative data (lifetimes, transition probabilities, oscillator strengths) obtained for a large number of lines belonging to heavy neutral and lowly ionized atoms (fifth row, sixth row, lanthanides)
[~ 90 ions considered, ~ 700 lifetimes measured, ~ 100000 *A*-values calculated]

Semi-empirical model based on the relativisitic Hartree-Fock method including core-polarization effects

Good agreement between theoretical approach and experimental results

New data very useful in astrophysics, plasma physics, …

Level structure still too poorly known for many ions to perform semi-empirical calculations (→ new term analyses needed)

Collaborations

Atomic structure calculations

Astrophysics & Spectroscopy, UMONS, Belgium (* also ULg, Liège, Belgium)

(E. Biémont*, V. Fivet, P. Palmeri, P. Quinet*)

Department of Physics, University of Brazzaville, Congo

(S. Enzonga Yoca)

Experimental measurements

Department of Physics, Lund University, Lund, Sweden

(L. Engström, H. Hartman, Z. Li, H. Lundberg, H. Nilsson, S. Svanberg, H. Xu, Z. Zhang)

Department of Physics, Jilin University, Changchun, China

(Z. Dai, L. Han, Z. Jiang, P. Li, Z. Ma, G. Sun, S. You, J. Xu, W. Zhang, Y. Zhang)

Also collaboration with

Institute of Solid State Physics, Bulgarian Academy of Sciences, Sofia, Bulgaria

(K. Blagoev, G. Malcheva)

Faculty of Physics, Universidad Complutense de Madrid, Spain

(R. Mayo, M. Ortiz)

UMONS Université de Mons

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Thank you for your attention !

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