UMONS
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Atomic Data for Lowly-Charged Heavy Ions

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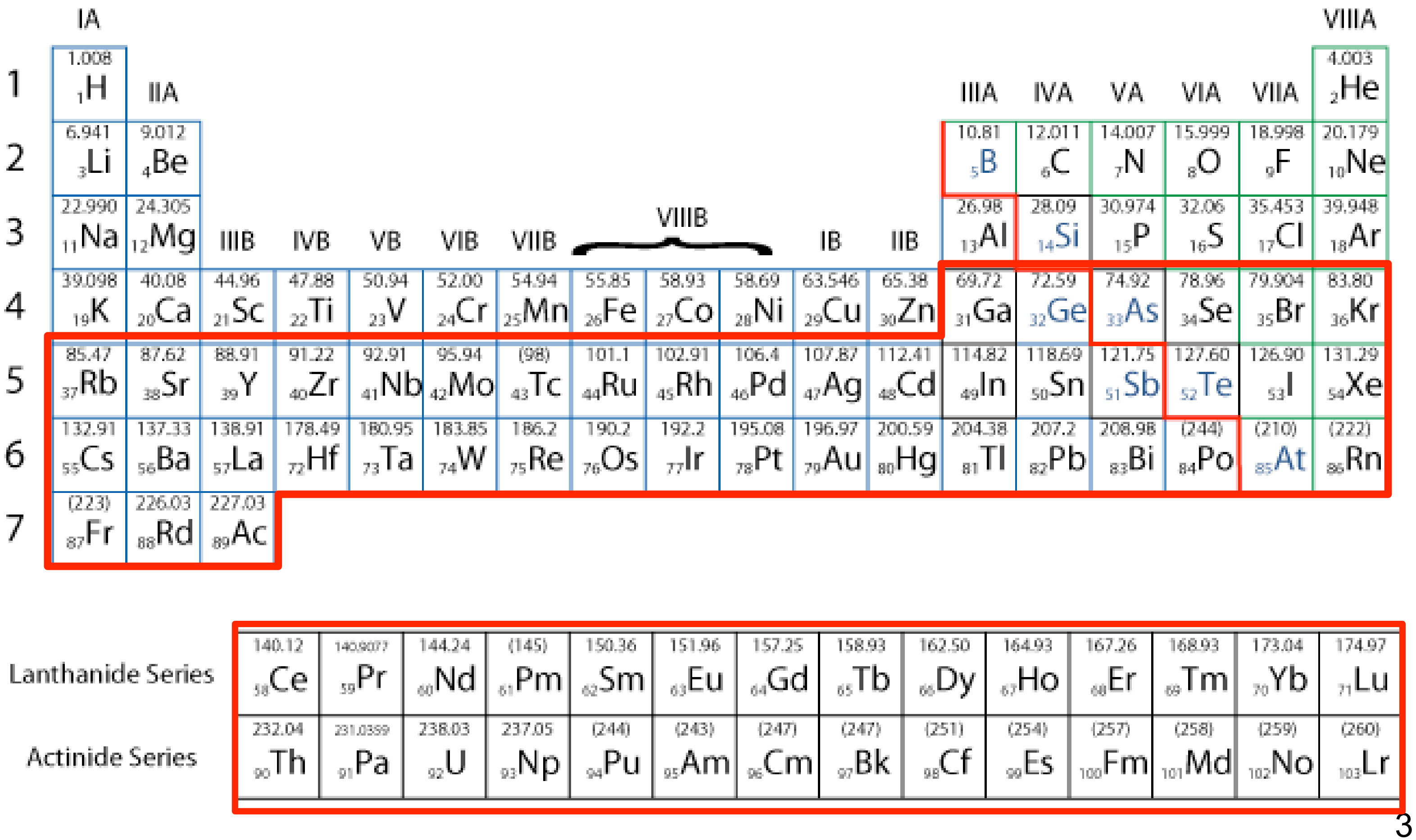
Outline

- Introduction
- HFR+CPOL Method
- Results: Te II-III, Rh III, Pd III, Ag III, Pr IV
- Conclusions & Perspectives

Introduction



	IA	IIA	IIIB	IVB	VB	VIB	VIIB	VIIIB			IB	IIB	IIIA	IVA	VA	VIA	VIIA	VIIIA
1	1.008 $_{1}$H																	4.003 $_{2}$He
2	6.941 $_{3}$Li	9.012 $_{4}$Be											10.81 $_{5}$B	12.011 $_{6}$C	14.007 $_{7}$N	15.999 $_{8}$O	18.998 $_{9}$F	20.179 $_{10}$Ne
3	22.990 $_{11}$Na	24.305 $_{12}$Mg											26.98 $_{13}$Al	28.09 $_{14}$Si	30.974 $_{15}$P	32.06 $_{16}$S	35.453 $_{17}$Cl	39.948 $_{18}$Ar
4	39.098 $_{19}$K	40.08 $_{20}$Ca	44.96 $_{21}$Sc	47.88 $_{22}$Ti	50.94 $_{23}$V	52.00 $_{24}$Cr	54.94 $_{25}$Mn	55.85 $_{26}$Fe	58.93 $_{27}$Co	58.69 $_{28}$Ni	63.546 $_{29}$Cu	65.38 $_{30}$Zn	69.72 $_{31}$Ga	72.59 $_{32}$Ge	74.92 $_{33}$As	78.96 $_{34}$Se	79.904 $_{35}$Br	83.80 $_{36}$Kr
5	85.47 $_{37}$Rb	87.62 $_{38}$Sr	88.91 $_{39}$Y	91.22 $_{40}$Zr	92.91 $_{41}$Nb	95.94 $_{42}$Mo	(98) $_{43}$Tc	101.1 $_{44}$Ru	102.91 $_{45}$Rh	106.4 $_{46}$Pd	107.87 $_{47}$Ag	112.41 $_{48}$Cd	114.82 $_{49}$In	118.69 $_{50}$Sn	121.75 $_{51}$Sb	127.60 $_{52}$Te	126.90 $_{53}$I	131.29 $_{54}$Xe
6	132.91 $_{55}$Cs	137.33 $_{56}$Ba	138.91 $_{57}$La	178.49 $_{72}$Hf	180.95 $_{73}$Ta	183.85 $_{74}$W	186.2 $_{75}$Re	190.2 $_{76}$Os	192.2 $_{77}$Ir	195.08 $_{78}$Pt	196.97 $_{79}$Au	200.59 $_{80}$Hg	204.38 $_{81}$Tl	207.2 $_{82}$Pb	208.98 $_{83}$Bi	(244) $_{84}$Po	(210) $_{85}$At	(222) $_{86}$Rn
7	(223) $_{87}$Fr	226.03 $_{88}$Rd	227.03 $_{89}$Ac															

Lanthanide Series	140.12 $_{58}$Ce	140.9077 $_{59}$Pr	144.24 $_{60}$Nd	(145) $_{61}$Pm	150.36 $_{62}$Sm	151.96 $_{63}$Eu	157.25 $_{64}$Gd	158.93 $_{65}$Tb	162.50 $_{66}$Dy	164.93 $_{67}$Ho	167.26 $_{68}$Er	168.93 $_{69}$Tm	173.04 $_{70}$Yb	174.97 $_{71}$Lu
Actinide Series	232.04 $_{90}$Th	231.0359 $_{91}$Pa	238.03 $_{92}$U	237.05 $_{93}$Np	(244) $_{94}$Pu	(243) $_{95}$Am	(247) $_{96}$Cm	(247) $_{97}$Bk	(251) $_{98}$Cf	(254) $_{99}$Es	(257) $_{100}$Fm	(258) $_{101}$Md	(259) $_{102}$No	(260) $_{103}$Lr

Introduction

- Astrophysics: nucleosynthesis, neutron capture elements (s- and r-processes)
- Fusion: plasma facing materials, contamination, radiative loss, influx …
- Lightening technology: richness of lanthanide spectra
- Photonics, lasers: triply-ionized lanthanides

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)

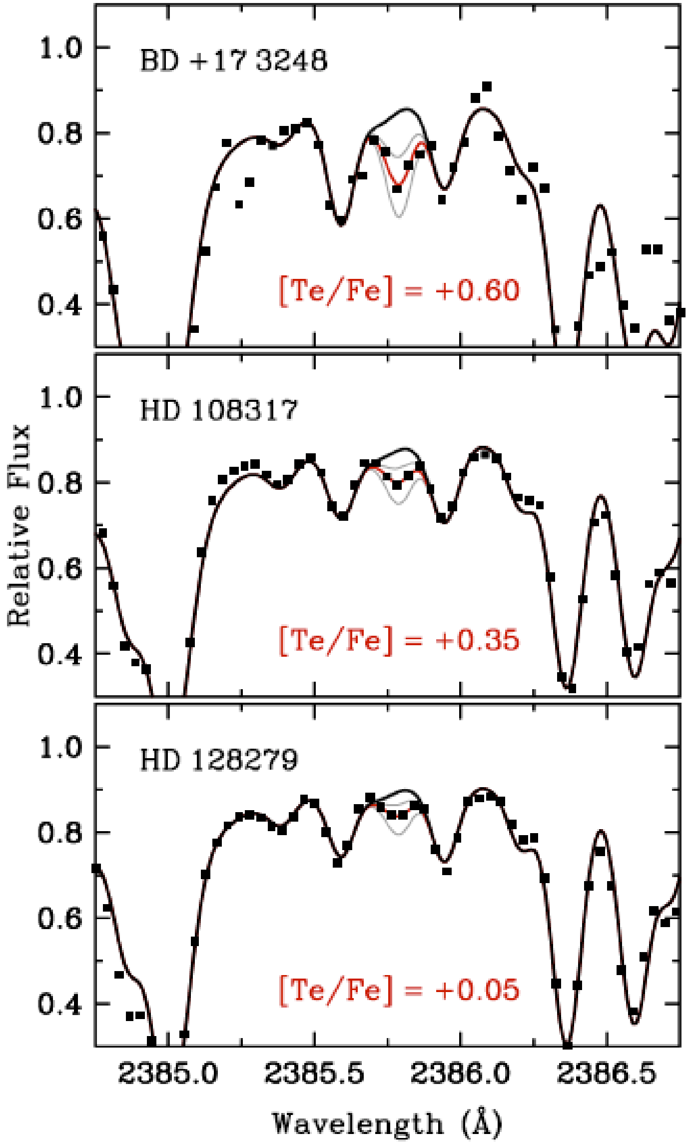
Intravalence correlation: explicit multiconfiguration expansions

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)

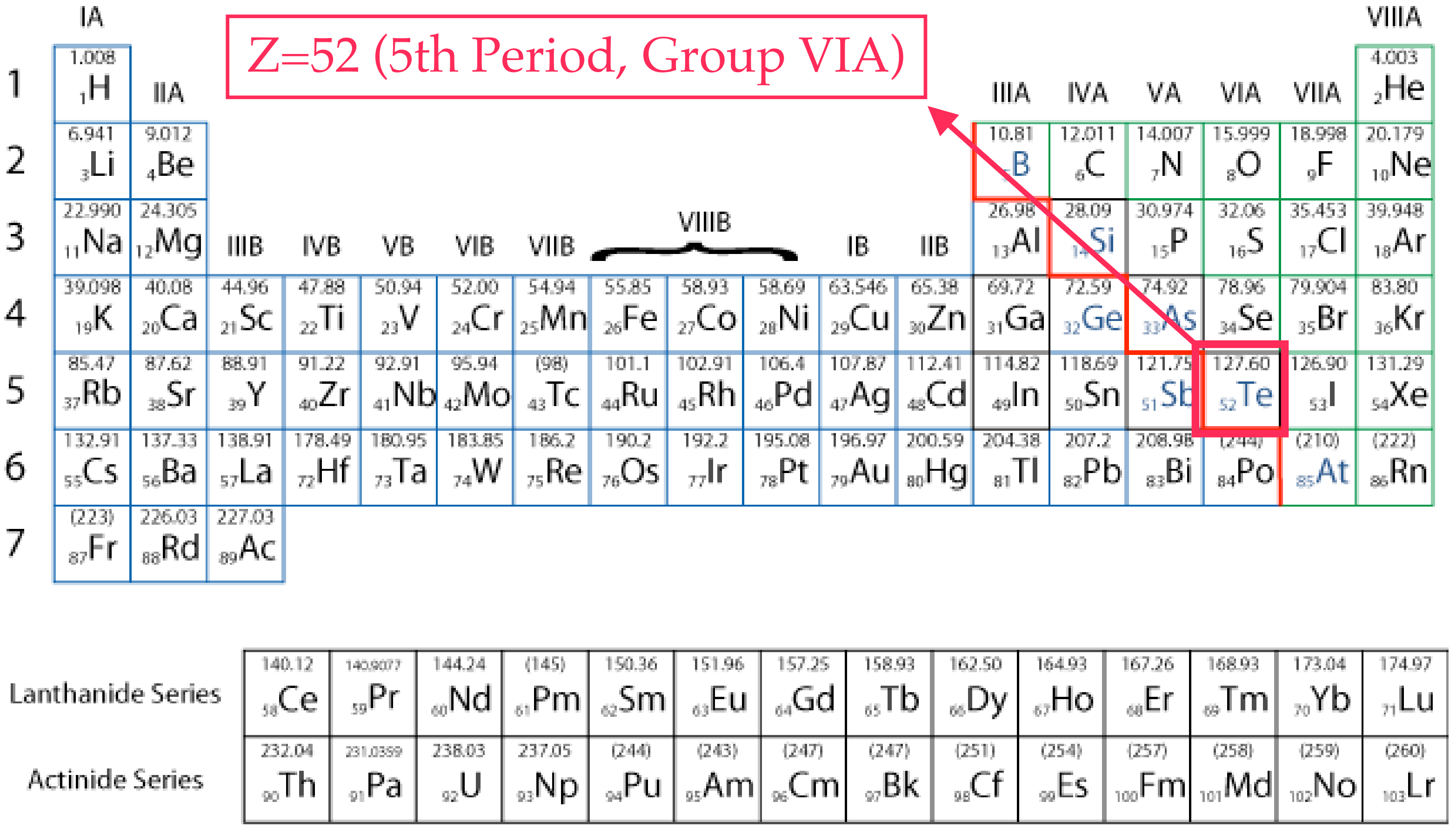
Tellurium is seen in stars (Te I)



Roederer et al 2012 ApJ 747, L8:

Te I λ2385 in HST spectra of metal-poor stars

Tellurium: no radiative data available for Te II-III



Z=52 (5th Period, Group VIA)

	IA	IIA	IIIB	IVB	VB	VIB	VIIB	VIIIB			IB	IIB	IIIA	IVA	VA	VIA	VIIA	VIIIA
1	1.008 ${}_{1}$H																	4.003 ${}_{2}$He
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Te II

HFR+CPOL model:

Intravalence Correlation (43 configurations):

$5p^3+5p^2 6p+5p^2 7p+5p^2 4f+5p^2 5f+5p^2 6f+5d^2 6p+5d^2 6f+6s^2 7p+$
$5d^2 7p+4f^2 5p+4f^2 6p+5s5p^3 6s+5s5p^3 5d+5s5p^3 6d+5s5p^2 6p5d+$
$5s5p^2 6p6d+$ $5s5p^2 4f5d+$ $5s5p^2 4f6d+5p^5$ (odd parity)

$5s5p^4+5p^2 5d+$ $5p^2 6d+$ $5p^2 7d+$ $5p^2 6s+5p^2 7s+$ $5p^2 8s+$ $5p^2 5g+$
$5p^2 6g+5d^2 5g+$ $5d^2 6g+$ $5f^2 5g+$ $5f^2 6g+5s5p^3 6p+5s5p^3 4f+$
$5s5p^3 5f+$ $5s5p^3 6f+5s5p^2 6s5d+$ $5s5p^2 6s6d+$ $5s5p^2 5d6d+$
$5s5p^2 6s^2+$ $5s5p^2 5d^2$ (even parity)

Te II

HFR+CPOL model:

Core-Polarization Potential:

Pd-like Te^{6+} [Kr]$4d^{10}$ ionic core with $\alpha_d = 1.295\ a_0^3$ (Fraga et al 1976, Handbook of Atomic Data, Amsterdam: Elsevier) and $r_c = \langle r \rangle_{4d} = 0.964\ a_0$.

Semi-Empirical Optimization:

Odd parity: 45 experimental levels belonging to the configurations $5p^3+5p^2nl$ (nl=6p,7p,4f) (NIST database).
Average deviation = 87 cm^{-1}.

Even parity: 81 experimental levels belonging to the configurations $5s5p^4+5p^2nl$ (nl=6s,7s,8s,5d,6d,7d)(NIST database).
Average deviation = 217 cm^{-1}.

Te II

The transition probabilities and oscillator strengths for 439 strong (log gf > -1) E1 transitions in the spectral range 77-997 nm.

No lifetime measurements are available for comparison!

→ f-values have been compared with an independent model to assess the reliability: the MCDHF method has been used.

Te II

Multiconfiguration Dirac-Hartree-Fock (MCDHF) model:

Fully relativistic method that takes into account the QED effects

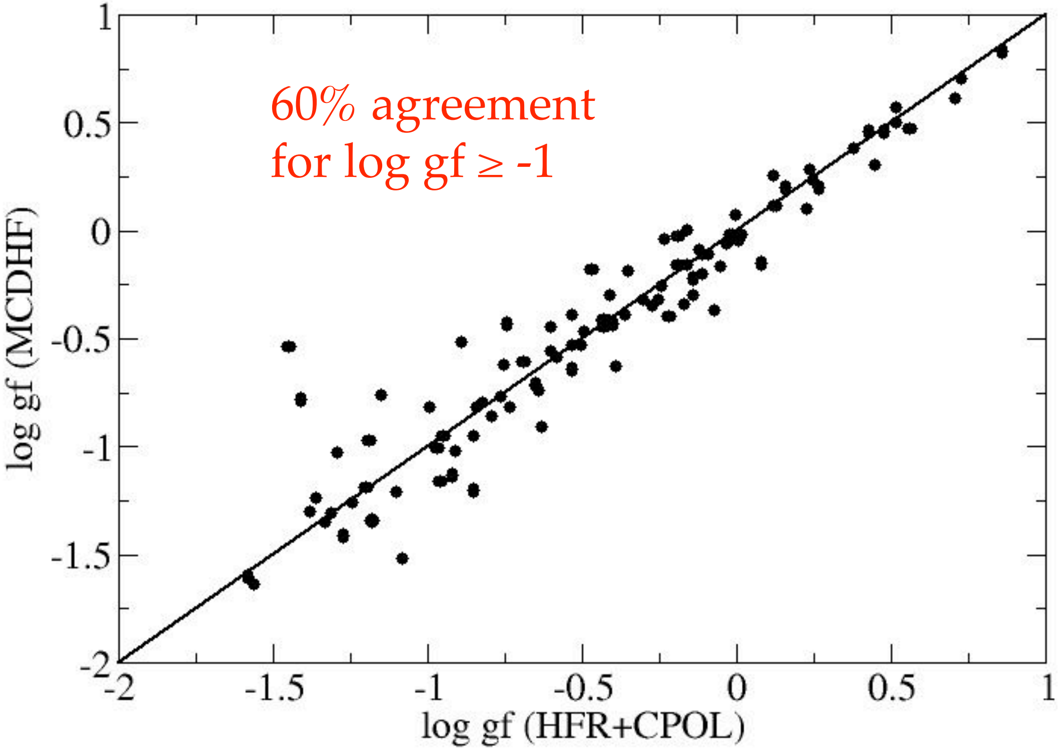
The GRASP2K package has been used (Jonsson et al 2007, CPC 177, 597)

Configuration space: generated from the multireference $5s^25p^3$+$5s5p^4$+$5s^25p^2nl$ (nl=5d,6s,6p) by single & double electron excitations involving the orbitals 4f,ns,np,nd (n=5,6,7,8) (102,359 CSFs).

Orbital optimization: EOL on the 70 levels of the multireference.

→ No core-valence effets due to the opening of the $n \leq 4$ shells !

Te II


60% agreement
for log gf ≥ -1
log gf (MCDHF)
log gf (HFR+CPOL)
1
0.5
0
-0.5
-1
-1.5
-2
-2
-1.5
-1
-0.5
0
0.5
1

Te III

HFR+CPOL model:

Intravalence Correlation (48 configurations):

$5p^2$+5p6p+5p7p+5p4f+5p5f+5p6f+5d6p+5d6d+$6s^2$+
$5d^2$+$4f^2$+$5f^2$+$5s5p^26s$+$5s5p^25d$+$5s5p^26d$+5s5p6p5d+
5s5p6p6d+ 5s5p4f5d+ 5s5p4f6d+$5p^4$+$5p^34f$+$5p^35f$+
$5p^36f$ (odd parity)

$5s5p^3$+5p5d+5p6d+5p7d+5p6s+5p7s+5p8s+5p5g+
5p6g+$5d^25g$+5d6p+5d4f+5d5f+5d6f+$5s5p^26p$+$5s5p^24f$+
$5s5p^25f$+$5s5p^26f$+5s5p6s5d+5s5p6s6d+5s5p5d6d+
$5s5p6s^2$+$5s5p5d^2$+$5p^36s$+$5p^35d$+$5p^36d$ (even parity)

Te III

HFR+CPOL model:

Core-Polarization Potential:

Pd-like Te^{6+} [Kr]$4d^{10}$ ionic core with $\alpha_d = 1.295\ a_0^3$ (Fraga et al 1976, Handbook of Atomic Data, Amsterdam: Elsevier) and $r_c = \langle r \rangle_{4d} = 0.964\ a_0$.

Semi-Empirical Optimization:

Even parity: 14 experimental levels belonging to the configurations $5p^2$+5p6p (NIST database; Tauheed & Naz 2011, J. Korean Phys. Soc. 59, 2910).
Average deviation = 100 cm^{-1}.

Odd parity: 55 experimental levels belonging to the configurations $5s5p^3$+5pnl (nl=6s,7s,8s,5d,6d,7d) (Tauheed & Naz 2011, J. Korean Phys. Soc. 59, 2910). Average deviation = 126 cm^{-1}.

Te III

The transition probabilities and oscillator strengths for 284 E1 transitions in the spectral range 52-901 nm.

Here again no lifetime measurements are available for comparison!

→ f-values have been also compared with a similar MCDHF model using GRASP2K.

Te III

Multiconfiguration Dirac-Hartree-Fock (MCDHF) model:

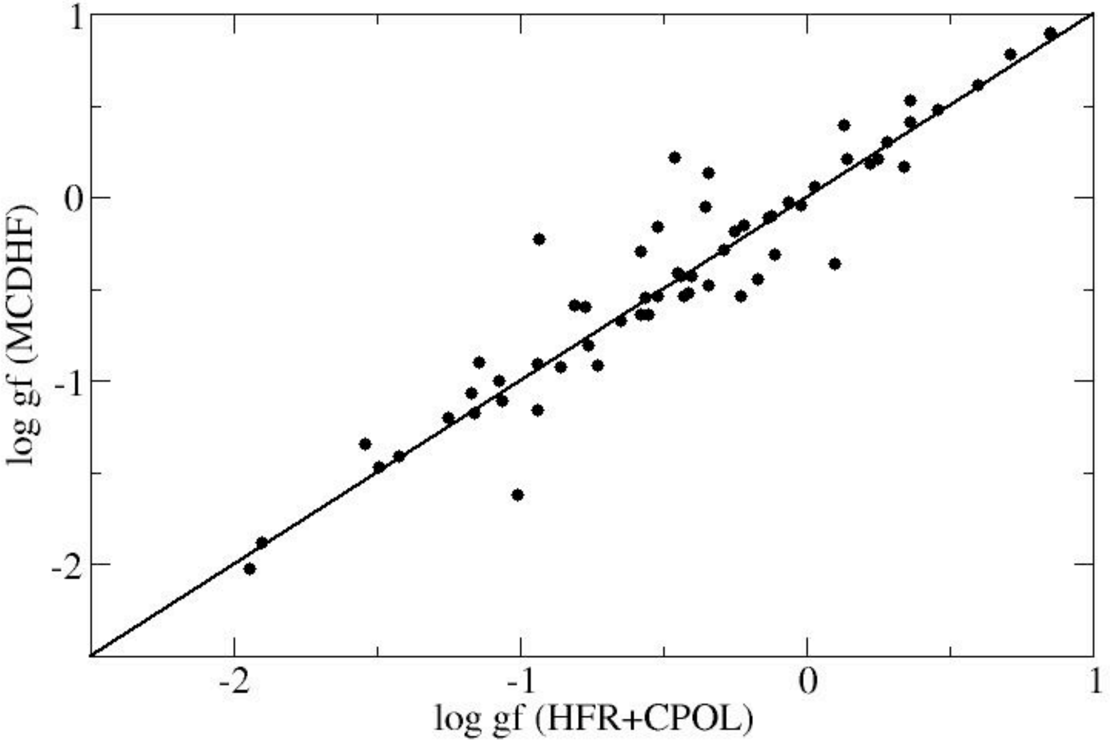
Configuration space: generated from the multireference $5s^2 5p^2 + 5s5p^3 + 5s^2 5pnl$ (nl=5d,6s,6p) by single & double electron excitations involving the orbitals 4f,ns,np,nd (n=5,6,7,8) (32,724 CSFs).

Orbital optimization: EOL on the 41 levels of the multireference.

→ Here also no core-valence effets due to the opening of the $n \leq 4$ shells.

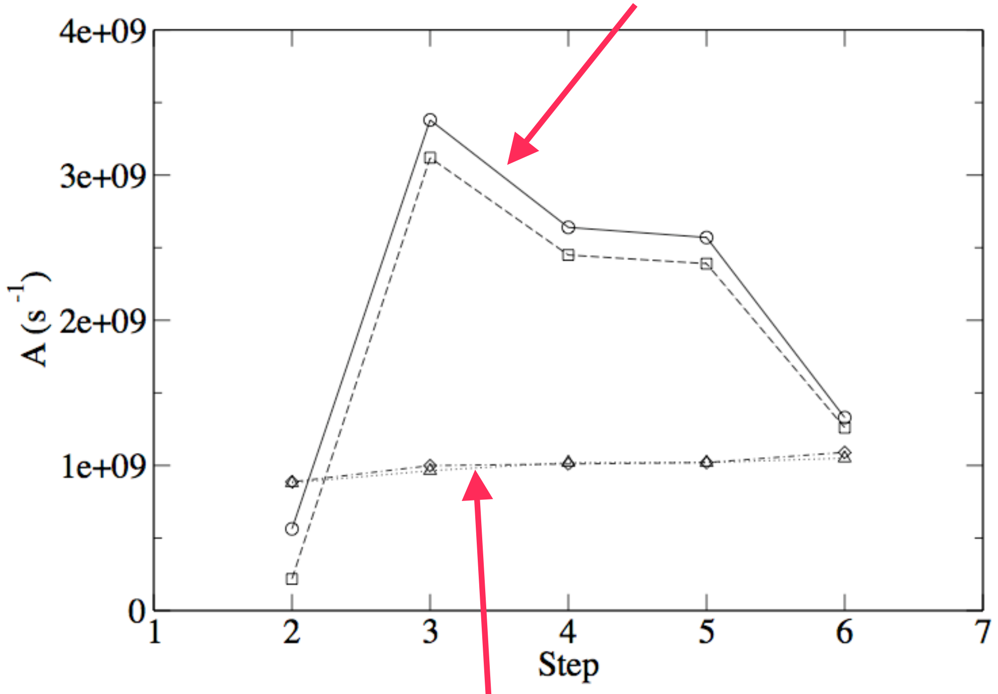
Te III

60% agreement excluding 9 transitions with convergence problem in MCDHF.



Te III: MCDHF convergence

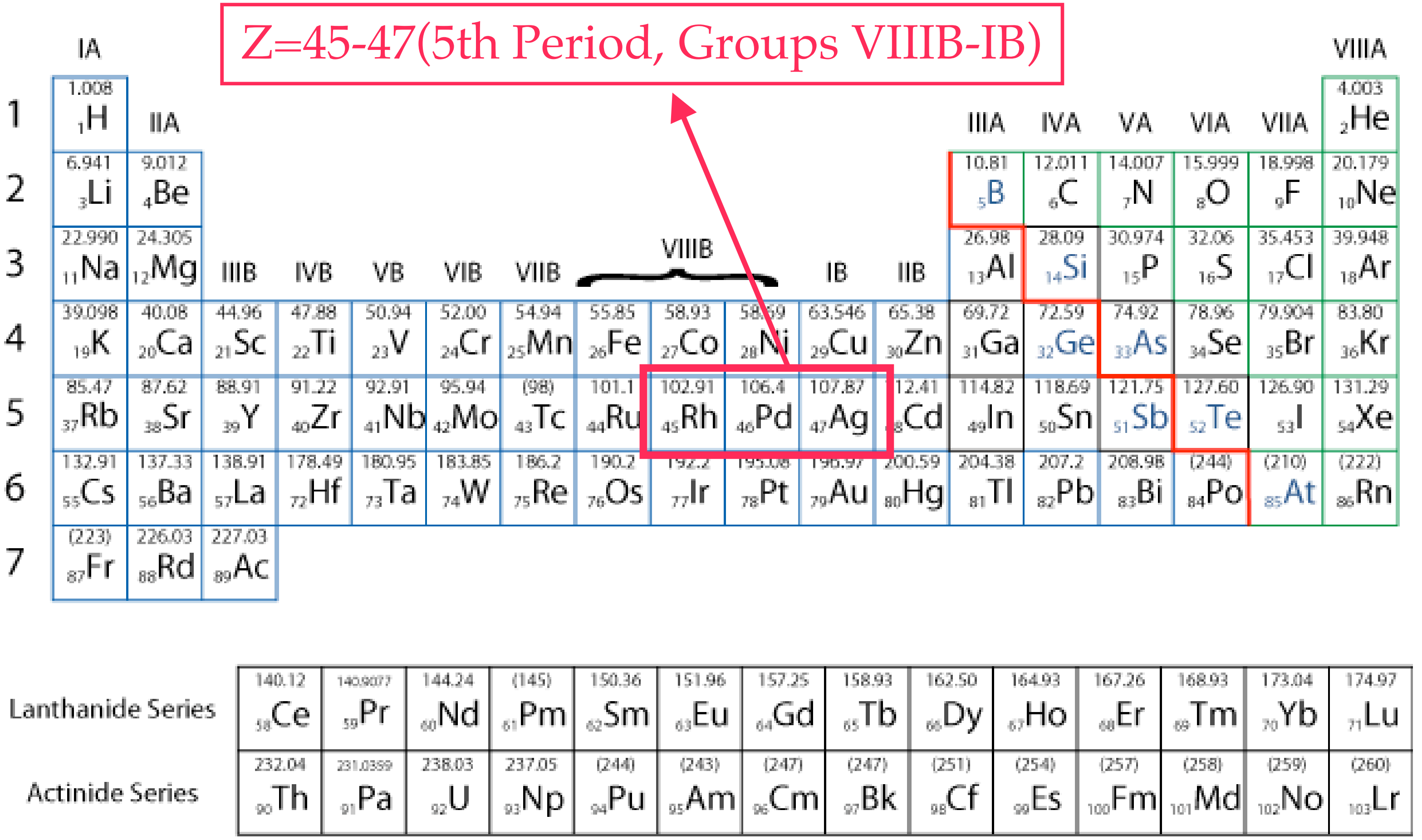
$5p^2\ ^3P_1$ - $5p6s\ ^1P^\circ_1$: convergence problem!
(circles: Babushkin ; squares: Coulomb)



$5p^2\ ^3P_2$ - $5p6s\ ^3P^\circ_1$: converged!
(diamonds: Babushkin ; triangles: Coulomb)

- Step 1: ground configuration orbitals (no transition calculated)
- Step 2: multiref {5s,5p,5d,6s,6p}
- Step 3: SD {5s,5p,5d,6s,6p,6d}
- Step 4: SD {5s,5p,5d,6s,6p,6d, 7s,7p,7d}
- Step 5: SD {5s,5p,5d,6s,6p,6d, 7s,7p,7d,8s,8p,8d}
- Step 6: SD {5s,5p,5d,6s,6p,6d, 7s,7p,7d,8s,8p,8d,4f}

Rh III, Pd III & Ag III: no radiative rates available!



Z=45-47(5th Period, Groups VIIIB-IB)

	IA	IIA	IIIB	IVB	VB	VIB	VIIB	VIIIB			IB	IIB	IIIA	IVA	VA	VIA	VIIA	VIIIA
1	1.008 $_{1}$H																	4.003 $_{2}$He
2	6.941 $_{3}$Li	9.012 $_{4}$Be											10.81 $_{5}$B	12.011 $_{6}$C	14.007 $_{7}$N	15.999 $_{8}$O	18.998 $_{9}$F	20.179 $_{10}$Ne
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4	39.098 $_{19}$K	40.08 $_{20}$Ca	44.96 $_{21}$Sc	47.88 $_{22}$Ti	50.94 $_{23}$V	52.00 $_{24}$Cr	54.94 $_{25}$Mn	55.85 $_{26}$Fe	58.93 $_{27}$Co	58.69 $_{28}$Ni	63.546 $_{29}$Cu	65.38 $_{30}$Zn	69.72 $_{31}$Ga	72.59 $_{32}$Ge	74.92 $_{33}$As	78.96 $_{34}$Se	79.904 $_{35}$Br	83.80 $_{36}$Kr
5	85.47 $_{37}$Rb	87.62 $_{38}$Sr	88.91 $_{39}$Y	91.22 $_{40}$Zr	92.91 $_{41}$Nb	95.94 $_{42}$Mo	(98) $_{43}$Tc	101.1 $_{44}$Ru	102.91 $_{45}$Rh	106.4 $_{46}$Pd	107.87 $_{47}$Ag	112.41 $_{48}$Cd	114.82 $_{49}$In	118.69 $_{50}$Sn	121.75 $_{51}$Sb	127.60 $_{52}$Te	126.90 $_{53}$I	131.29 $_{54}$Xe
6	132.91 $_{55}$Cs	137.33 $_{56}$Ba	138.91 $_{57}$La	178.49 $_{72}$Hf	180.95 $_{73}$Ta	183.85 $_{74}$W	186.2 $_{75}$Re	190.2 $_{76}$Os	192.2 $_{77}$Ir	195.08 $_{78}$Pt	196.97 $_{79}$Au	200.59 $_{80}$Hg	204.38 $_{81}$Tl	207.2 $_{82}$Pb	208.98 $_{83}$Bi	(244) $_{84}$Po	(210) $_{85}$At	(222) $_{86}$Rn
7	(223) $_{87}$Fr	226.03 $_{88}$Rd	227.03 $_{89}$Ac															

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Actinide Series	232.04 $_{90}$Th	231.0359 $_{91}$Pa	238.03 $_{92}$U	237.05 $_{93}$Np	(244) $_{94}$Pu	(243) $_{95}$Am	(247) $_{96}$Cm	(247) $_{97}$Bk	(251) $_{98}$Cf	(254) $_{99}$Es	(257) $_{100}$Fm	(258) $_{101}$Md	(259) $_{102}$No	(260) $_{103}$Lr

Rh III, Pd III & Ag III: Computational Strategy

- Rh III: similar model as in the isoelectronic ion Ru II (Palmeri et al 2009, J Phys B 42, 165005) → good agreement with the TR-LIF lifetime measurements (within a few percents).

- Pd III: similar model as in Rh II (Quinet et al 2012, A&A 537, A74) → also good agreement with the TR-LIF lifetime measurements (within a few percents).

- Ag III: similar model as in Pd III adding one electron to the 4d subshell

→ An accuracy of a few percents for the radiative rates is expected at least for the strongest lines

Rh III, Pd III & Ag III: HFR+CPOL Models (CI)

- Rh III: $4d^7 + 4d^65s + 4d^66s + 4d^65d + 4d^66d + 4d^55s^2 + 4d^55p^2 + 4d^55d^2 + 4d^55s6s$ (even parity) & $4d^65p + 4d^66p + 4d^64f + 4d^65f + 4d^55s5p + 4d^55s6p + 4d^55p6s$ (odd parity); CPOL: Rh V $4d^5$ core with $\alpha_d=3.31\ a_0^3$ (Fraga et al, 1976) & $r_c=\langle r\rangle_{4d}=1.43\ a_0$; Fit:

- Pd III: $4d^8 + 4d^75s + 4d^76s + 4d^75d + 4d^76d + 4d^65s^2 + 4d^65p^2 + 4d^65d^2 + 4d^65s6s + 4d^65s5d + 4d^65s6d$ (even parity) & $4d^75p + 4d^76p + 4d^74f + 4d^75f + 4d^65s5p + 4d^65s6p + 4d^65p5d + 4d^65p6s$ (odd parity)

- Ag III: $4d^9 + 4d^85s + 4d^86s + 4d^85d + 4d^86d + 4d^75s^2 + 4d^75p^2 + 4d^75d^2 + 4d^75s6s + 4d^75s5d + 4d^75s6d$ (even parity) & $4d^85p + 4d^86p + 4d^84f + 4d^85f + 4d^75s5p + 4d^75s6p + 4d^75p5d + 4d^75p6s$ (odd parity)

Rh III, Pd III & Ag III: HFR+CPOL Models (CPOL)

- Rh III: Rh V $4d^5$ core with α_d=3.31 a_0^3 (Fraga et al, 1976) & r_c=$<r>_{4d}$=1.43 a_0

- Pd III: Pd V $4d^6$ core with α_d=3.17 a_0^3 (Fraga et al, 1976) & r_c=$<r>_{4d}$=1.36 a_0

- Ag III: Ag V $4d^7$ core with α_d=3.04 a_0^3 (Fraga et al, 1976) & r_c=$<r>_{4d}$=1.04 a_0

Rh III, Pd III & Ag III: HFR+CPOL Models (Fits)

- Rh III: 196 experimental levels belonging to $4d^7$, $4d^65s$ & $4d^65p$ (NIST database). Average deviations: 28 cm^{-1} (even parity) & 84 cm^{-1} (odd parity).

- Pd III: 177 experimental levels belonging to $4d^8$, $4d^75s$, $4d^76s$, $4d^75p$ & $4d^65s5p$ (NIST database). Average deviations: 80 cm^{-1} (even parity) & 68 cm^{-1} (odd parity).

- Ag III: 64 experimental levels belonging to $4d^9$, $4d^85s$ & $4d^85p$ (NIST database). Average deviations: 117 cm^{-1} (even parity) & 66 cm^{-1} (odd parity).

Experimental and Calculated Even-Parity Energy Levels in Ag III

E_{exp}[a] (cm^{-1})	E_{calc}[b] (cm^{-1})	ΔE (cm^{-1})	J	LS composition[c] (%)
				Even parity
0.0	0059	-59	5/2	99 $4d^9\ ^2D$
4609.2	4550	59	3/2	99 $4d^9\ ^2D$
63246.3	63269	-23	9/2	99 $4d^8(^3F)5s\ ^4F$
65759.2	65714	46	7/2	90 $4d^8(^3F)5s\ ^4F$ + 9 $4d^8(^3F)5s\ ^2F$
68139.1	68050	89	5/2	95 $4d^8(^3F)5s\ ^4F$
69345.7	69268	77	3/2	91 $4d^8(^3F)5s\ ^4F$ + 8 $4d^8(^1D)5s\ ^2D$
71686.4	71715	-29	7/2	89 $4d^8(^3F)5s\ ^2F$ + 9 $4d^8(^3F)5s\ ^4F$
73928.9	74127	-198	5/2	46 $4d^8(^3F)5s\ ^2F$ + 27 $4d^8(^3P)5s\ ^4P$ + 26 $4d^8(^1D)5s\ ^2D$
76402.3	76480	-78	5/2	54 $4d^8(^3P)5s\ ^4P$ + 42 $4d^8(^3F)5s\ ^2F$
77408.7	77555	-147	3/2	65 $4d^8(^3P)5s\ ^4P$ + 22 $4d^8(^1D)5s\ ^2D$ + 8 $4d^8(^3P)5s\ ^2P$
78893.2	78959	-66	1/2	98 $4d^8(^3P)5s\ ^4P$
80127.4	80279	-151	3/2	47 $4d^8(^1D)5s\ ^2D$ + 34 $4d^8(^3P)5s\ ^4P$ + 14 $4d^8(^3P)5s\ ^2P$
82228.4	82421	-193	5/2	70 $4d^8(^1D)5s\ ^2D$ + 17 $4d^8(^3P)5s\ ^4P$ + 10 $4d^8(^3F)5s\ ^2F$
85179.8	85157	23	3/2	76 $4d^8(^3P)5s\ ^2P$ + 22 $4d^8(^1D)5s\ ^2D$
85505.5	85421	84	1/2	97 $4d^8(^3P)5s\ ^2P$
85596.1	85293	303	9/2	98 $4d^8(^1G)5s\ ^2G$
85724.1	85351	373	7/2	98 $4d^8(^1G)5s\ ^2G$
111436.4	111551	-115	1/2	96 $4d^8(^1S)5s\ ^2S$

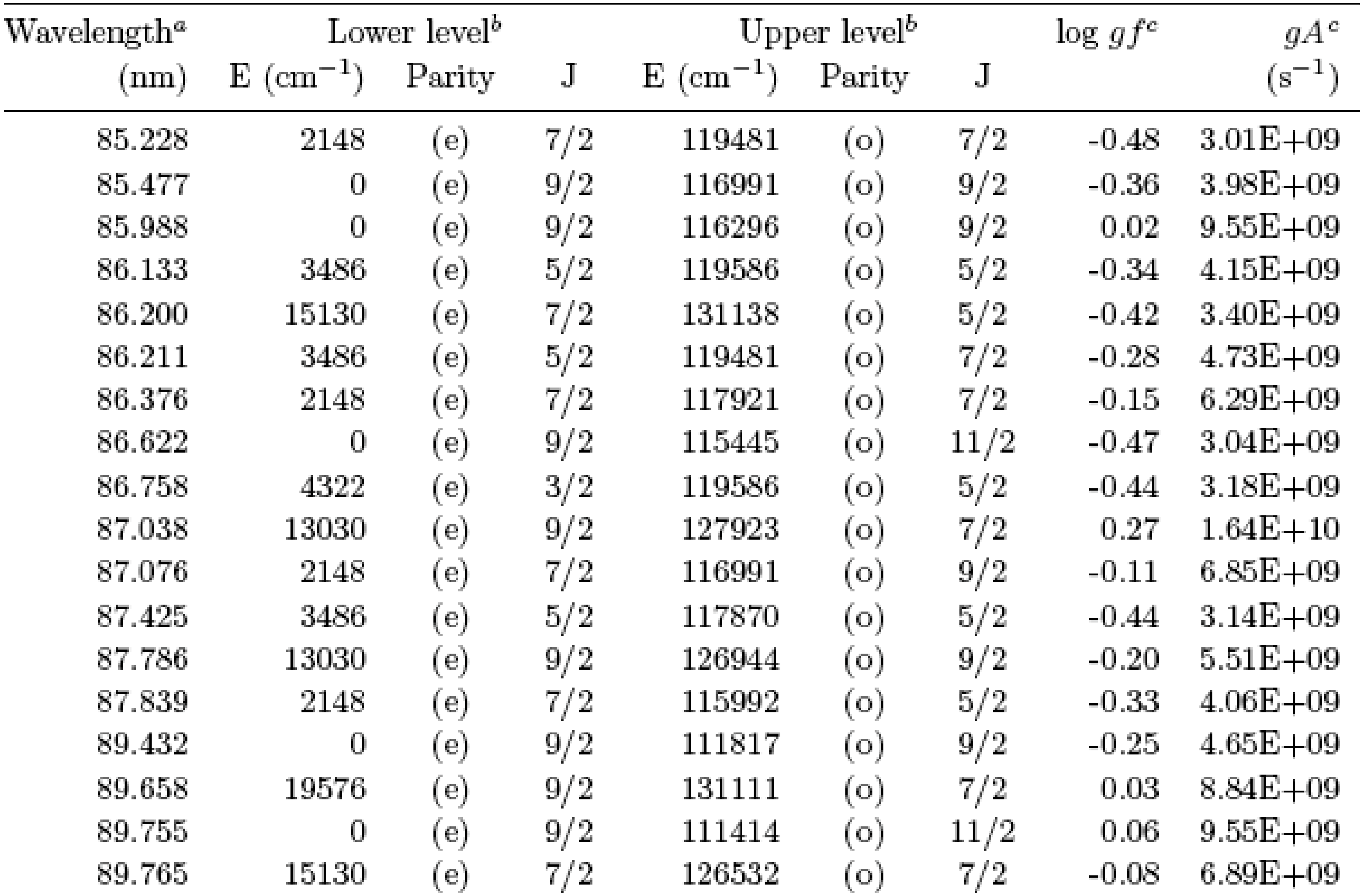
Rh III, Pd III & Ag III: Radiative Rates

- Rh III: 2150 E1 transitions in the spectral region 76-519 nm

- Pd III: 2120 E1 transitions in the spectral region 61-975 nm

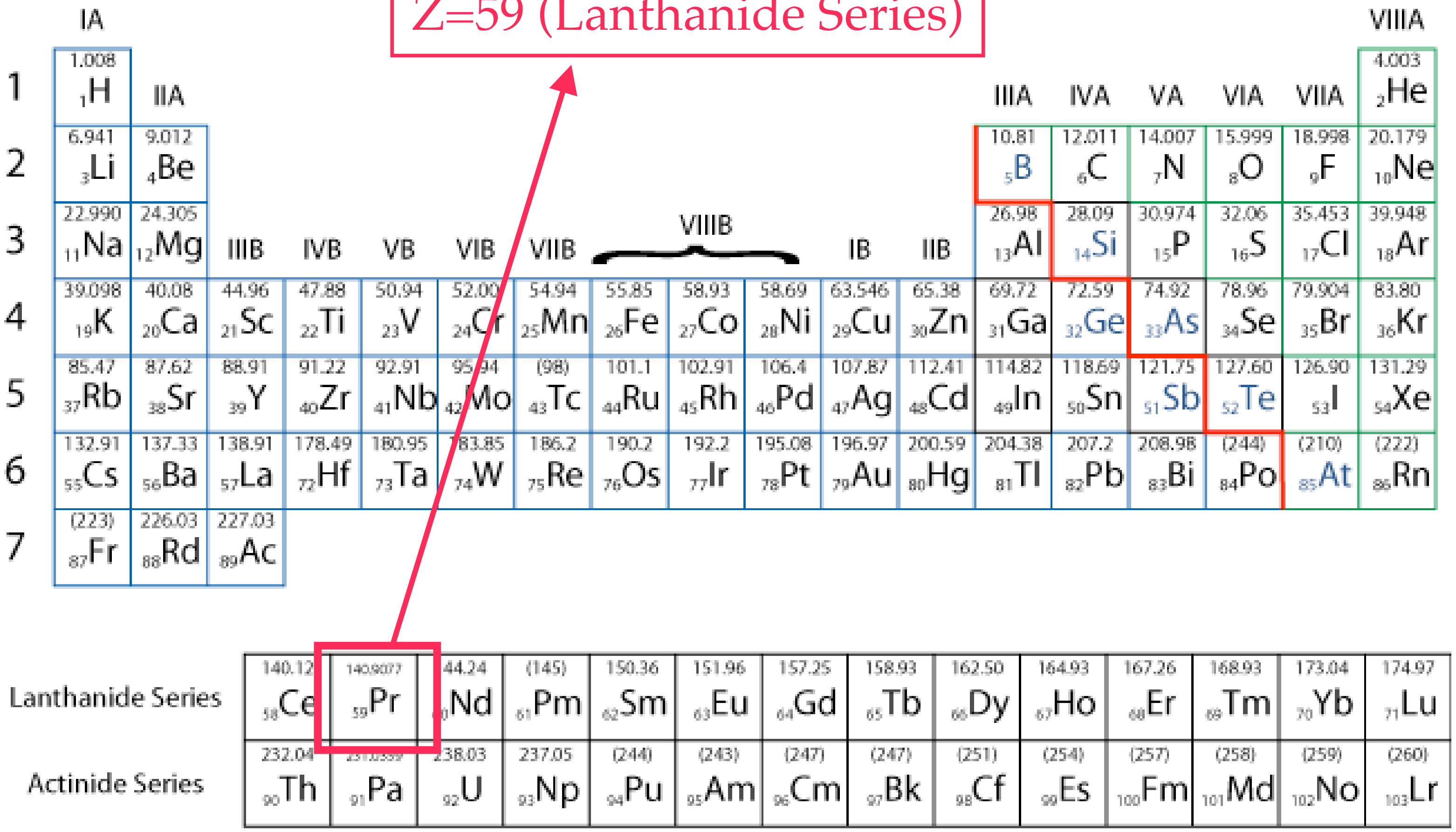
- Ag III: 440 E1 transitions in the spectral region 59-801 nm

Sample of E1 Radiative Rates (log gf > -0.5) in Rh III



Wavelength[a]	Lower level[b]			Upper level[b]			log gf[c]	gA[c]
(nm)	E (cm^{-1})	Parity	J	E (cm^{-1})	Parity	J		(s^{-1})
85.228	2148	(e)	7/2	119481	(o)	7/2	-0.48	3.01E+09
85.477	0	(e)	9/2	116991	(o)	9/2	-0.36	3.98E+09
85.988	0	(e)	9/2	116296	(o)	9/2	0.02	9.55E+09
86.133	3486	(e)	5/2	119586	(o)	5/2	-0.34	4.15E+09
86.200	15130	(e)	7/2	131138	(o)	5/2	-0.42	3.40E+09
86.211	3486	(e)	5/2	119481	(o)	7/2	-0.28	4.73E+09
86.376	2148	(e)	7/2	117921	(o)	7/2	-0.15	6.29E+09
86.622	0	(e)	9/2	115445	(o)	11/2	-0.47	3.04E+09
86.758	4322	(e)	3/2	119586	(o)	5/2	-0.44	3.18E+09
87.038	13030	(e)	9/2	127923	(o)	7/2	0.27	1.64E+10
87.076	2148	(e)	7/2	116991	(o)	9/2	-0.11	6.85E+09
87.425	3486	(e)	5/2	117870	(o)	5/2	-0.44	3.14E+09
87.786	13030	(e)	9/2	126944	(o)	9/2	-0.20	5.51E+09
87.839	2148	(e)	7/2	115992	(o)	5/2	-0.33	4.06E+09
89.432	0	(e)	9/2	111817	(o)	9/2	-0.25	4.65E+09
89.658	19576	(e)	9/2	131111	(o)	7/2	0.03	8.84E+09
89.755	0	(e)	9/2	111414	(o)	11/2	0.06	9.55E+09
89.765	15130	(e)	7/2	126532	(o)	7/2	-0.08	6.89E+09

Praseodymium: radiative parameters are sparse in Pr IV



Z=59 (Lanthanide Series)

	IA	IIA	IIIB	IVB	VB	VIB	VIIB	VIIIB			IB	IIB	IIIA	IVA	VA	VIA	VIIA	VIIIA
1	1.008 $_{1}$H																	4.003 $_{2}$He
2	6.941 $_{3}$Li	9.012 $_{4}$Be											10.81 $_{5}$B	12.011 $_{6}$C	14.007 $_{7}$N	15.999 $_{8}$O	18.998 $_{9}$F	20.179 $_{10}$Ne
3	22.990 $_{11}$Na	24.305 $_{12}$Mg											26.98 $_{13}$Al	28.09 $_{14}$Si	30.974 $_{15}$P	32.06 $_{16}$S	35.453 $_{17}$Cl	39.948 $_{18}$Ar
4	39.098 $_{19}$K	40.08 $_{20}$Ca	44.96 $_{21}$Sc	47.88 $_{22}$Ti	50.94 $_{23}$V	52.00 $_{24}$Cr	54.94 $_{25}$Mn	55.85 $_{26}$Fe	58.93 $_{27}$Co	58.69 $_{28}$Ni	63.546 $_{29}$Cu	65.38 $_{30}$Zn	69.72 $_{31}$Ga	72.59 $_{32}$Ge	74.92 $_{33}$As	78.96 $_{34}$Se	79.904 $_{35}$Br	83.80 $_{36}$Kr
5	85.47 $_{37}$Rb	87.62 $_{38}$Sr	88.91 $_{39}$Y	91.22 $_{40}$Zr	92.91 $_{41}$Nb	95.94 $_{42}$Mo	(98) $_{43}$Tc	101.1 $_{44}$Ru	102.91 $_{45}$Rh	106.4 $_{46}$Pd	107.87 $_{47}$Ag	112.41 $_{48}$Cd	114.82 $_{49}$In	118.69 $_{50}$Sn	121.75 $_{51}$Sb	127.60 $_{52}$Te	126.90 $_{53}$I	131.29 $_{54}$Xe
6	132.91 $_{55}$Cs	137.33 $_{56}$Ba	138.91 $_{57}$La	178.49 $_{72}$Hf	180.95 $_{73}$Ta	183.85 $_{74}$W	186.2 $_{75}$Re	190.2 $_{76}$Os	192.2 $_{77}$Ir	195.08 $_{78}$Pt	196.97 $_{79}$Au	200.59 $_{80}$Hg	204.38 $_{81}$Tl	207.2 $_{82}$Pb	208.98 $_{83}$Bi	(244) $_{84}$Po	(210) $_{85}$At	(222) $_{86}$Rn
7	(223) $_{87}$Fr	226.03 $_{88}$Rd	227.03 $_{89}$Ac															

Lanthanide Series	140.12 $_{58}$Ce	140.9077 $_{59}$Pr	44.24 $_{60}$Nd	(145) $_{61}$Pm	150.36 $_{62}$Sm	151.96 $_{63}$Eu	157.25 $_{64}$Gd	158.93 $_{65}$Tb	162.50 $_{66}$Dy	164.93 $_{67}$Ho	167.26 $_{68}$Er	168.93 $_{69}$Tm	173.04 $_{70}$Yb	174.97 $_{71}$Lu
Actinide Series	232.04 $_{90}$Th	[illegible] $_{91}$Pa	238.03 $_{92}$U	237.05 $_{93}$Np	(244) $_{94}$Pu	(243) $_{95}$Am	(247) $_{96}$Cm	(247) $_{97}$Bk	(251) $_{98}$Cf	(254) $_{99}$Es	(257) $_{100}$Fm	(258) $_{101}$Md	(259) $_{102}$No	(260) $_{103}$Lr

Pr IV: HFR+CPOL Model

Similar model as in the isoelectronic ion Ce III (Biémont et al 2002, MNRAS 336, 1155) which gave a good agreement (within 5%) with the TR-LIF lifetime measurements.

→ Accuracy of ~5% is expected in Pr IV

Intravalence Correlation:

$4f^2 + 4fnp\ (n=6\text{-}7) + 5d^2 + 5dns\ (n=6\text{-}7) + 6s^2 + 5d6d + 4fnf\ (n=5\text{-}7) + 6p^2$ (even parity)

4fnd (n=5-7) + 4fns (n=6-8) + 5d6p + 4fng (n=5-6) + 6s6p (odd parity)

Pr IV: HFR+CPOL Model

Core-Polarization Potential:

Xe-like Pr^{5+} $5p^6$ ionic core: $\alpha_d = 5.40\ a_0^3$ (Fraga et al, 1976)

$r_c = \langle r \rangle_{5p} = 1.60\ a_0$

Semi-Empirical Optimization:

Even parity: 50 $4f^2+5d^2+4f6p+4f5f$ experimental levels (NIST database). Average deviation = 34 cm^{-1}.

Odd parity: 36 $4f^2+5d^2+4f6p+4f5f$ experimental levels (NIST database). Average deviation = 95 cm^{-1}.

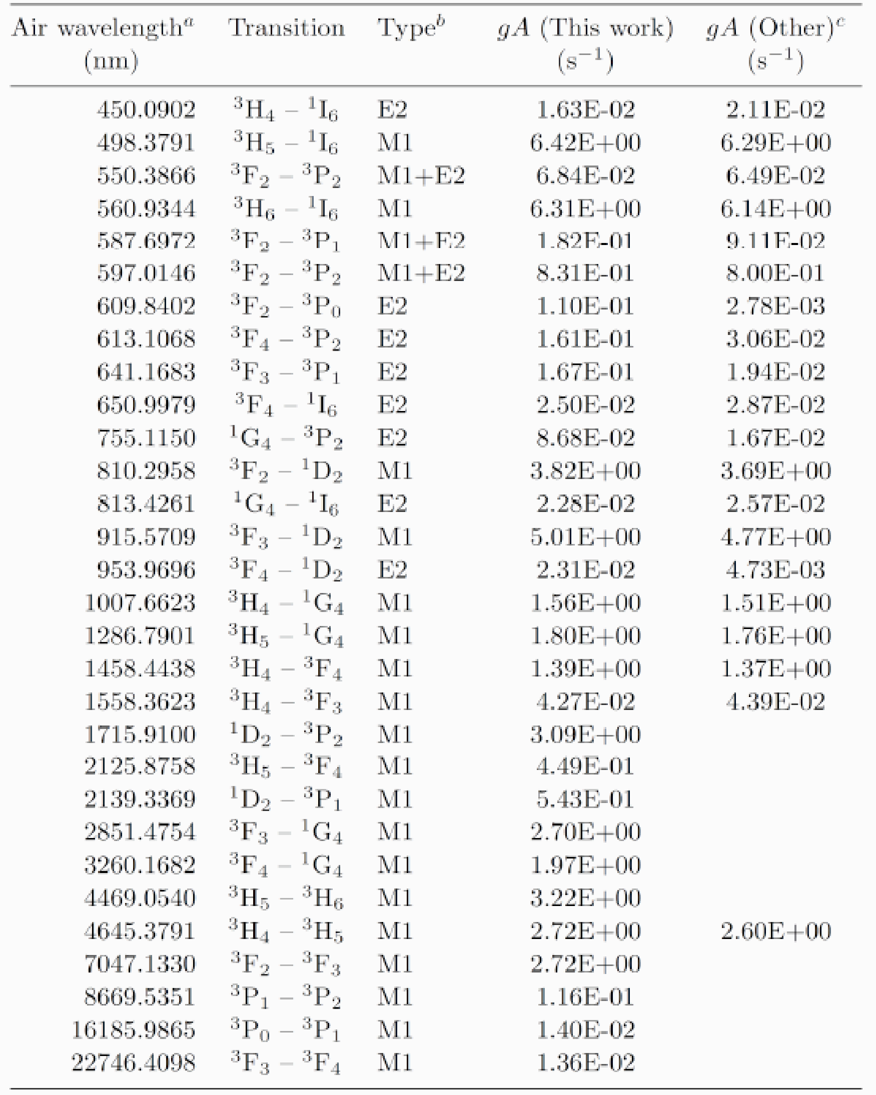
Pr IV: Radiative Rates

The transition probabilities and oscillator strengths have been calculated for :

- 199 strong (log gf $\geq$ -2) E1 transitions in the spectral region 118 - 302 nm.

- 30 forbidden (M1+E2) transitions (gA > 0.01 s^{-1}) within the $4f^2$ configuration in the spectral region 450 - 22,800 nm.

Pr IV: Forbidden transitions within $4f^2$



Air wavelength[a] (nm)	Transition	Type[b]	gA (This work) (s^{-1})	gA (Other)[c] (s^{-1})
450.0902	$^3H_4 - {}^1I_6$	E2	1.63E-02	2.11E-02
498.3791	$^3H_5 - {}^1I_6$	M1	6.42E+00	6.29E+00
550.3866	$^3F_2 - {}^3P_2$	M1+E2	6.84E-02	6.49E-02
560.9344	$^3H_6 - {}^1I_6$	M1	6.31E+00	6.14E+00
587.6972	$^3F_2 - {}^3P_1$	M1+E2	1.82E-01	9.11E-02
597.0146	$^3F_2 - {}^3P_2$	M1+E2	8.31E-01	8.00E-01
609.8402	$^3F_2 - {}^3P_0$	E2	1.10E-01	2.78E-03
613.1068	$^3F_4 - {}^3P_2$	E2	1.61E-01	3.06E-02
641.1683	$^3F_3 - {}^3P_1$	E2	1.67E-01	1.94E-02
650.9979	$^3F_4 - {}^1I_6$	E2	2.50E-02	2.87E-02
755.1150	$^1G_4 - {}^3P_2$	E2	8.68E-02	1.67E-02
810.2958	$^3F_2 - {}^1D_2$	M1	3.82E+00	3.69E+00
813.4261	$^1G_4 - {}^1I_6$	E2	2.28E-02	2.57E-02
915.5709	$^3F_3 - {}^1D_2$	M1	5.01E+00	4.77E+00
953.9696	$^3F_4 - {}^1D_2$	E2	2.31E-02	4.73E-03
1007.6623	$^3H_4 - {}^1G_4$	M1	1.56E+00	1.51E+00
1286.7901	$^3H_5 - {}^1G_4$	M1	1.80E+00	1.76E+00
1458.4438	$^3H_4 - {}^3F_4$	M1	1.39E+00	1.37E+00
1558.3623	$^3H_4 - {}^3F_3$	M1	4.27E-02	4.39E-02
1715.9100	$^1D_2 - {}^3P_2$	M1	3.09E+00	
2125.8758	$^3H_5 - {}^3F_4$	M1	4.49E-01	
2139.3369	$^1D_2 - {}^3P_1$	M1	5.43E-01	
2851.4754	$^3F_3 - {}^1G_4$	M1	2.70E+00	
3260.1682	$^3F_4 - {}^1G_4$	M1	1.97E+00	
4469.0540	$^3H_5 - {}^3H_6$	M1	3.22E+00	
4645.3791	$^3H_4 - {}^3H_5$	M1	2.72E+00	2.60E+00
7047.1330	$^3F_2 - {}^3F_3$	M1	2.72E+00	
8669.5351	$^3P_1 - {}^3P_2$	M1	1.16E-01	
16185.9865	$^3P_0 - {}^3P_1$	M1	1.40E-02	
22746.4098	$^3F_3 - {}^3F_4$	M1	1.36E-02	

[a] Deduced from experimental levels compiled by Martin *et al.* (1978)

[b] Contributions larger than 1%

[c] Dodson and Zia (2012)

Conclusions & Perspectives

- New radiative data have been calculated in Te II-III, Rh III, Pd III, Ag III & Pr IV using the HFR+CPOL method
- Accuracy of ~60% has been estimated through comparisons with independent MCDHF calculations in Te II-III
- Use of similar experimentally benchmarked models in isoelectronic ions for Rh III, Pd III, Ag III & Pr IV: expected accuracy of a few %
- Lifetime & branching fraction measurements are needed!
- Publications: Zhang et al (2013, A&A 551, A136); Zhang et al (2013, Phys Scr, to be published); Enzonga Yoca & Quinet (2013, in preparation)

Collaborations

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Thank you for your attention!