Multi-platform atomic data calculations for Os VI spectral lines of interest to nuclear fusion research

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22 May 2025

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Osmium in the fusion plasma

- Divertor will be made of tungsten: high fluxes of heat and particles (neutrons)
- Primary transmutation products: rhenium, osmium and tantalum → impurities
- Brittleness of pure tungsten → alloying elements (tantalum, rhenium, titanium or vanadium)

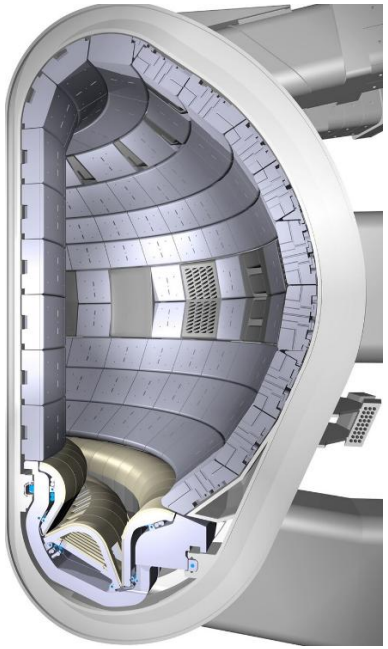
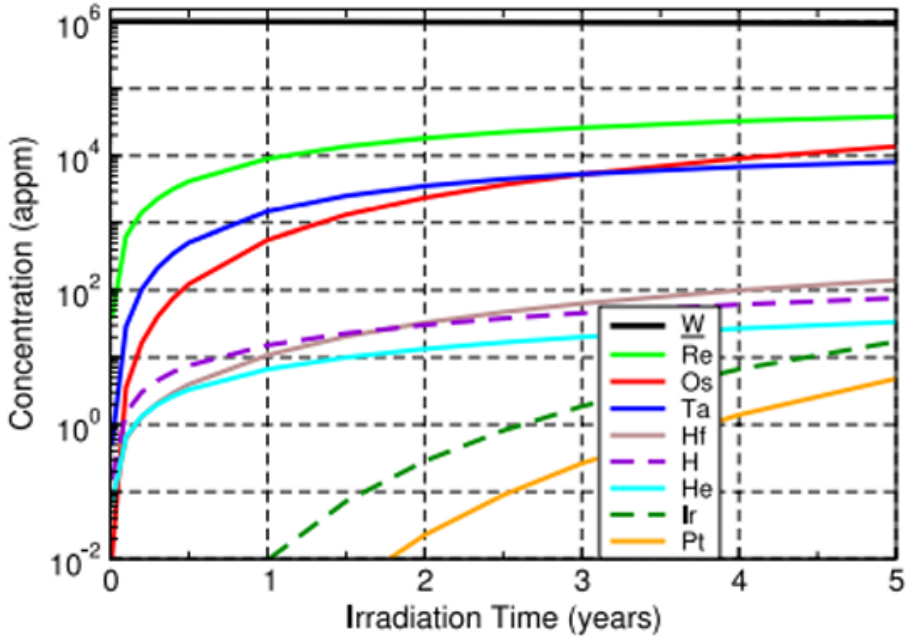


Illustration of the inside of the Tokamak. (https://encyclopedia.pub/entry/37629)



Evolution of the concentration (Atomic Part Per Millions) of all the elements produced by the transmutation of W for a five-years irradiation [Gilbert, M. R and Sublet, J.Ch , 2011]

- Ionic impurities will contribute to the radiation losses/allow to diagnose the fusion plasma

- From observed intensity ratio and radiative parameters (HJ. Kunze, 2009) :

  - $$\frac{\varepsilon_z(p\rightarrow q)}{\varepsilon_z(p'\rightarrow q')} = \frac{\lambda_{p'q'}}{\lambda_{pq}} \frac{A_z(p\rightarrow q)}{A_z(p'\rightarrow q')} \frac{A_z(p\prime\rightarrow)}{A_z(p\rightarrow)} \frac{X_z(g\rightarrow p)(T_e)}{X_z(g\rightarrow p')(T_e)} \Rightarrow T_e$$

  - $$\frac{\varepsilon_z(p\rightarrow q)}{\varepsilon_z(p'\rightarrow q')} = \frac{\lambda_{p'q'}}{\lambda_{pq}} \frac{A_z(p\rightarrow q)}{A_z(p'\rightarrow q')} \frac{A_z(p\prime\rightarrow)}{A_z(p\rightarrow)} \frac{X_z(g\rightarrow p)(T_e)}{X_z(g\rightarrow p')(T_e)} \left[1 + n_e \frac{X_z(p'\rightarrow)}{A_z(p'\rightarrow)}\right] \Rightarrow n_e$$

General procedure [Cowan, R. D. ,1981]

- Solve $H\Psi = E\Psi$ where $H = \sum_{i=1}^{N}\left(-\frac{1}{2}\Delta_i + V(r_i)\right)$ (central field approximation)

- $H_i\varphi_i = E_i\varphi_i \rightarrow \varphi_i(r_i,\theta_i,\phi_i,s_i) = \frac{1}{r_i}P_{n_il_i}(r_i)Y_{l_i}^{m_i}(\theta_i,\phi_i)\sigma_{m_{s_i}}(s_i)$

- $P_{n_il_i}(r_i)$? → solve Hartree-Fock equations (Self-Consistent Field method)

- HF equations obtained by variational principle on the average energy of each electronic configuration

- Atomic State Functions (ASFs) : $\Psi(\alpha, P, J, M_J) = \sum_{r=1}^{n_c} c_r \Phi(\alpha_r, P, L_r, S_r, J, M_J)$

Configuration State Functions (CSFs) are built thanks to Slater determinants

Core polarisation correction

- Valence electron correlations represented by configuration interactions (CI) and other correlations by core-polarization potential
- Quinet, P. et al [1999, 2002]: pseudo potential have one-body and two-body part :
  - $V_{P1} = -\frac{1}{2}\alpha_D \sum_{i=1}^{N} \frac{r_i^2}{(r_i^2+r_c^2)^3}$ and $V_{P2} = -\alpha_D \sum_{i>j} \frac{\overrightarrow{r_i}\cdot\overrightarrow{r_j}}{\left[(r_i^2+r_c^2)(r_j^2+r_c^2)\right]^{3/2}}$
  - α_D: dipole polarizability; r_c: ionic core radius

General procedure [Grant, I. P., 2007]

- $H_{DC} = \sum_{i=1}^{N} h_{D_i}$ with $h_{D_i} = c\overrightarrow{\alpha} \cdot \overrightarrow{p_i} + (\beta - 1)c^2 + V(r_i)$ ($\alpha^j = \gamma^0\gamma^j$ and $\beta = \gamma^0$)

- Each electron: $h_D\varphi = E\varphi \rightarrow \varphi(r,\theta,\phi) = \frac{1}{r}\begin{pmatrix} P_{n,\kappa}(r)\chi_{\kappa,m}(\theta,\phi) \\ iQ_{n,\kappa}(r)\chi_{\kappa,m}(\theta,\phi) \end{pmatrix}$ where $P_{n,\kappa}(r)$ and $Q_{n,\kappa}(r)$ are large and small radial part, respectively.

- $P_{n,\kappa}(r)$, $Q_{n,\kappa}(r)$? → solve MCDHF equations (Self-Consistent Field method)

- CI: (ASF) $\Psi(P,J,M) = \sum_{r=1}^{n_c} c_r\,\Phi(\gamma_r,P,J,M)$

Model for the HFR+CPOL method

Valence-Valence interactions

Even parity		Odd parity	
$5d^3$	5d5f6f	$5d^26p$	$6s^26f$
$5d^26s$	$6s^26d$	$5d^27p$	$6p^25f$
$5d^27s$	5d6p6f	$5d^25f$	$6p^26f$
$5d6s^2$	$6s6p^2$	$5d^26f$	$6p^3$
$5d^26d$	$6p^26d$	5d6s6p	$6p6d^2$
$5d6p^2$	$6s6d^2$	5d6s5f	$6d^25f$
$5d6d^2$	$6d^3$	5d6s6f	$6d^26f$
$5d5f^2$	$6s5f^2$	5d6p6d	$6p5f^2$
$5d6f^2$	$6d5f^2$	5d6d5f	$6p6f^2$
5d6s6d	$6s6f^2$	5d6d6f	$5f^26f$
5d6p5f	$6d6f^2$	$6s^26p$	$5f6f^2$
		$6s^25f$	

Core interactions

$r_c(5p) = 1.66\ a_0$ and $\alpha_D = 3.80\ a_0^3$

Least squares method

- Minimize difference between 78 computed energy levels and observed ones [A. J. J Raassen et al.(1996) and V. I Azarov (2018)] with spin-orbit and Slater parameters

- Accuracy of the fit: $\sigma = \left[\frac{\sum_k (E^k - T^k)^2}{N_k - N_p}\right]^{1/2}$, where E^k: energy eigenvalues; T^k: observed energies; N_k: number of fitted levels; N_p: number of fitted parameters

	Standard deviation (cm^{-1})	
	ab initio	**fit**
Even parity	3252	46
Odd parity	2873	150

Model for the MCDHF method

- The Atomic State Functions (ASFs) are built with the Active Set approach $(n_{max}l, n'_{max}l', \dots)$:
- Optimization of all orbitals (5s,5p,5d,4f) on the $5d^3\ {}^4F_{3/2}$ ground state
- MR : (re)optimize valence orbitals on all levels
- VV1,2 : ONLY « new » correlation orbitals are optimized on all levels of the MR (SR)
- CV,CC : Relativistic Configuration Interactions (RCI) calculations

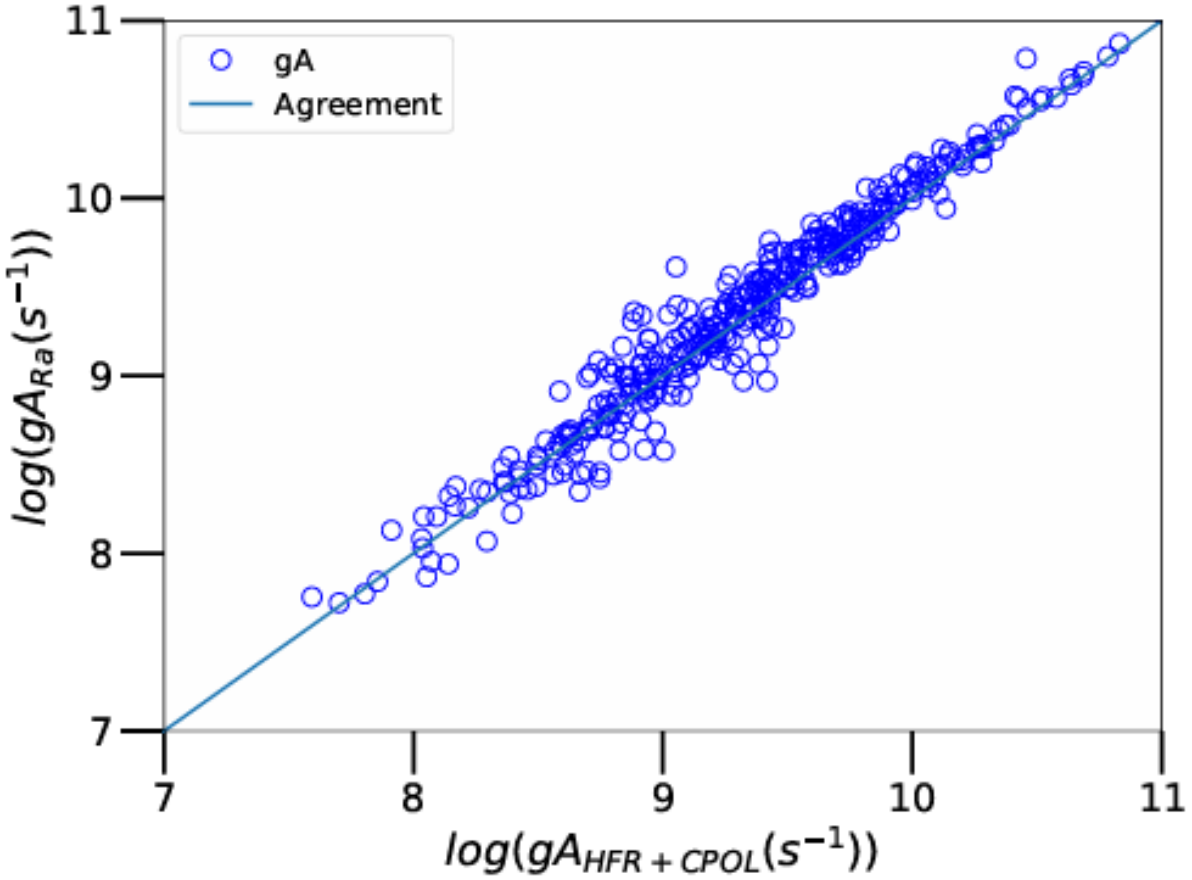
Even parity		Number of CSFs
MR ($5d^3$,$5d^2$6s)	(6s,5p,5d,4f)	35
VV1	SD(MR) → (7s,6p,6d,5f)	569
VV2	SD(MR) → (8s,7p,7d,6f)	1944
CV (RCI)	SrD (MR{4f}) → (8s,7p,7d,6f)	77 463
CC (RCI)	SD (MR{4f}) → (8s,7p,7d,6f)	515 057

Odd parity		Number of CSFs
SR ($5d^2$6p)	(5s,6p,5d,4f)	45
VV1	SD(SR) → (6s,7p,6d,5f)	875
VV2	SD(SR) → (7s,8p,7d,6f)	2790
CV (RCI)	SrD (SR{4f}) → (7s,8p,7d,6f)	132 655
CC (RCI)	SD (SR{4f}) → (7s,8p,7d,6f)	900 402

Radiative decay rates

- Compare transition probabilities from Raassen, A. J. J et al.(1996) (simple HFR calculations) with those computed by our HFR+CPOL method

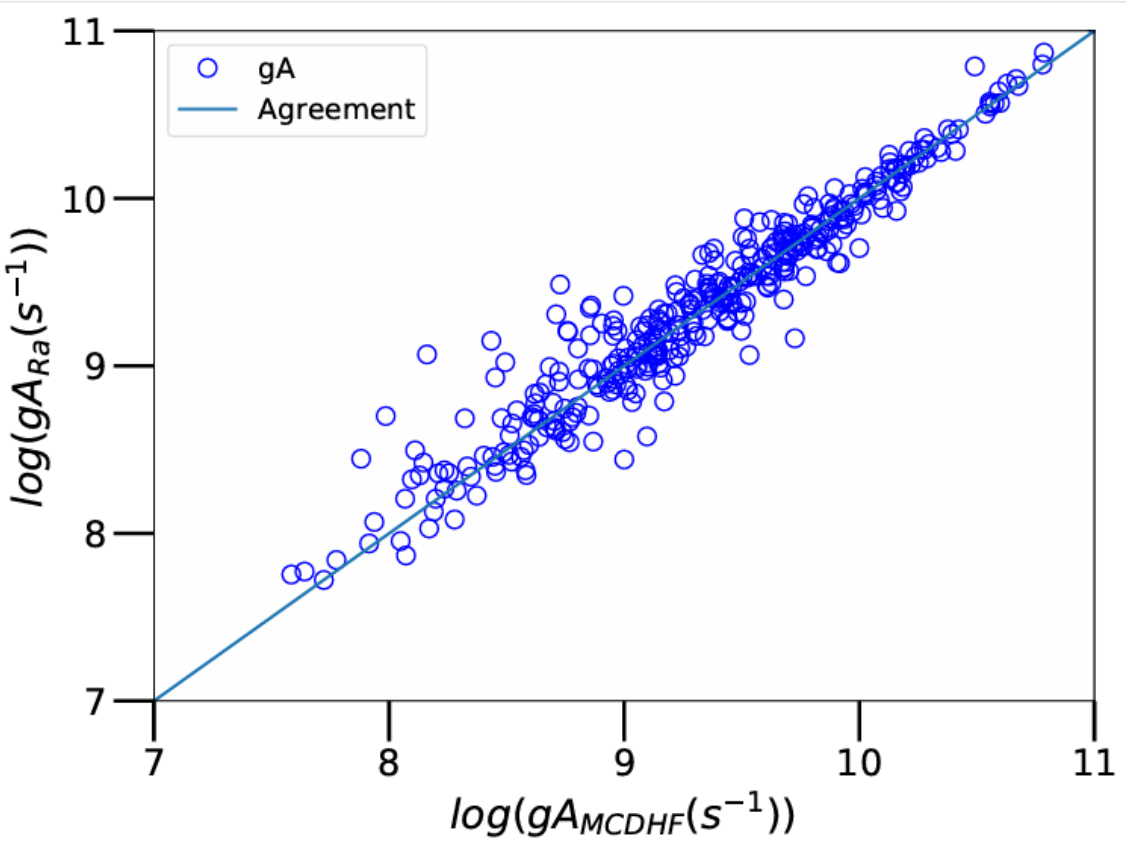
- 367 electric dipole lines between 438.720 and 1486.275 Å

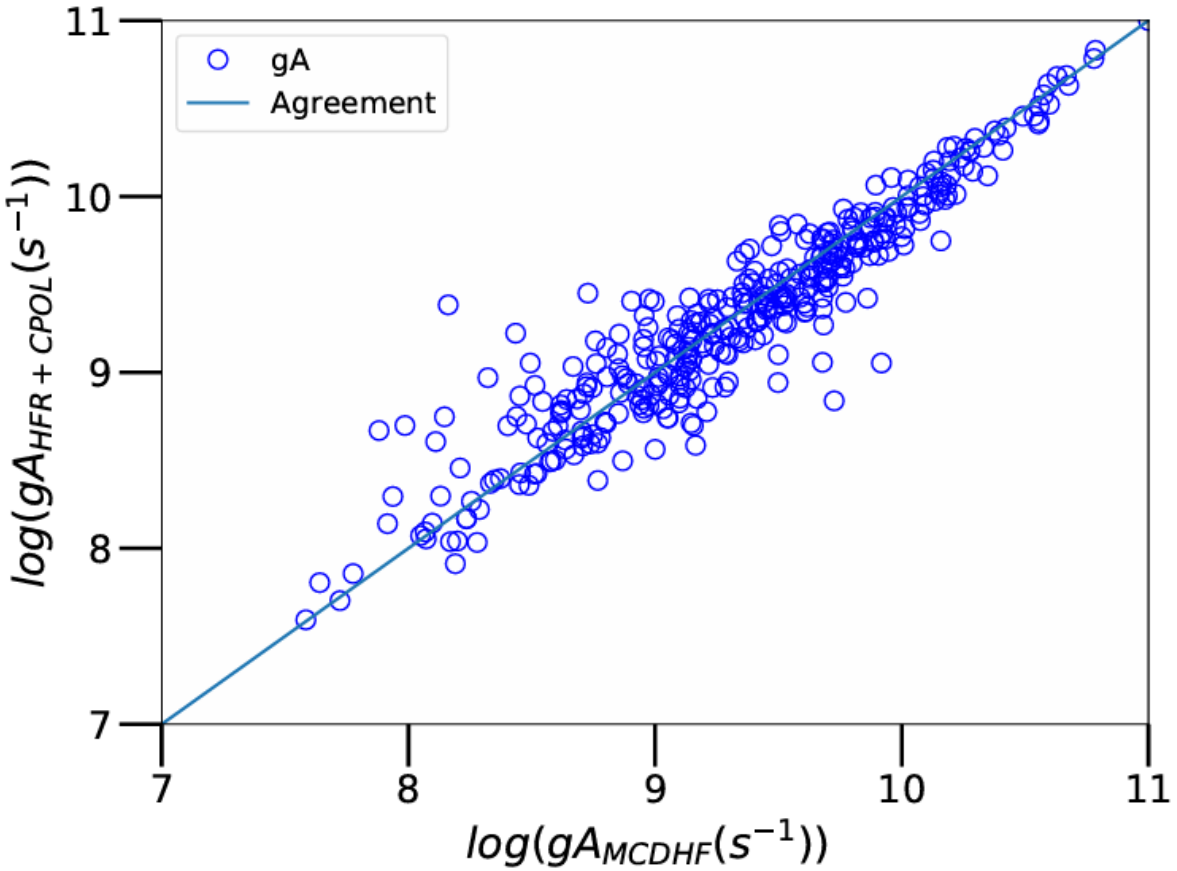


- Mean ratio $gA_{HFR+CPOL}/gA_{Ra}$ = 0.95 $\pm$ 0.21

- More complete model : more CI and CPOL corrections

Radiative decay rates





Mean ratio : gA_{MCDHF}/gA_{Ra}= 1.15 $\pm$ 0.33

Mean ratio : $gA_{HFR+CPOL}/gA_{MCDHF}$ = 1.08 $\pm$ 0.42

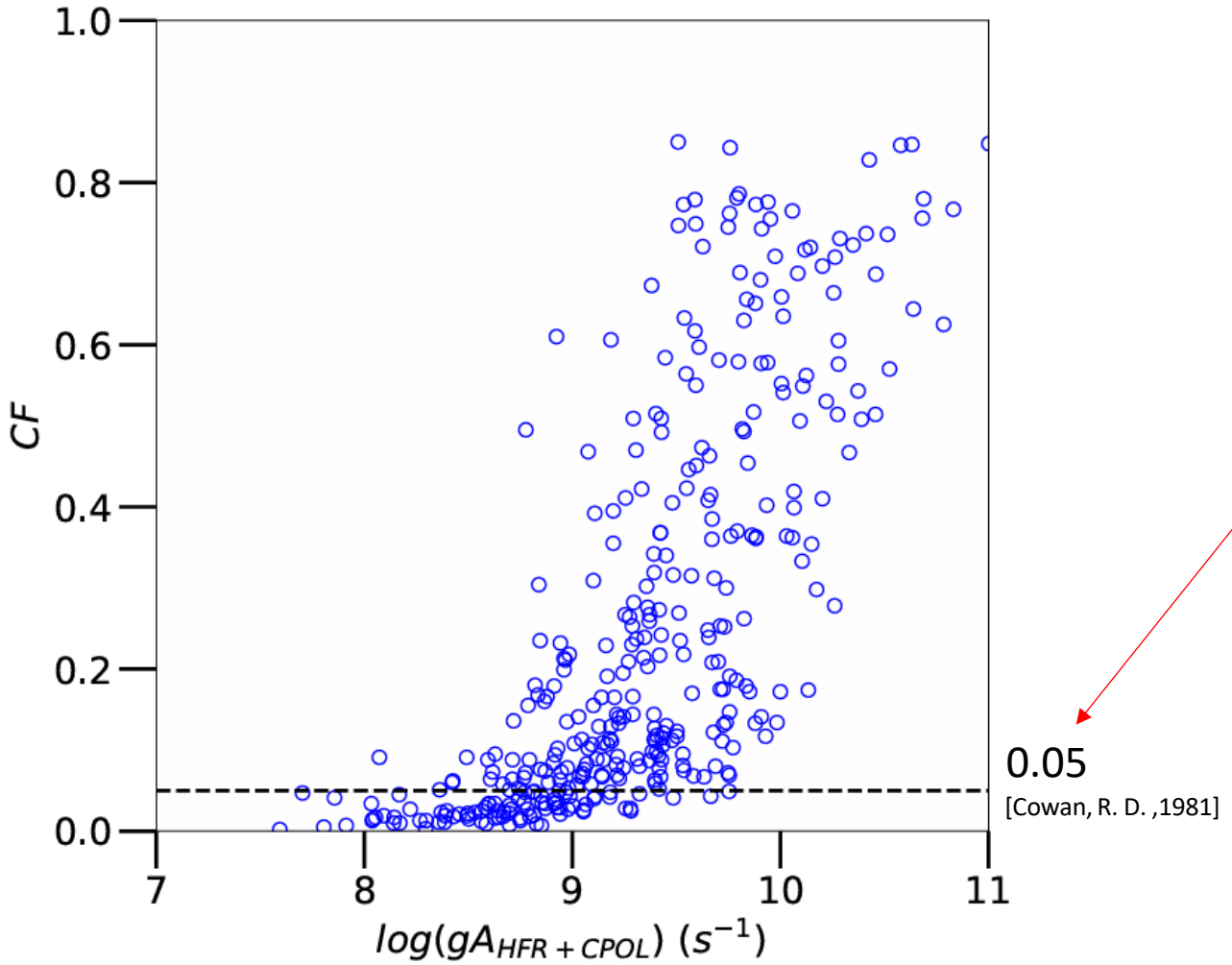
All gA (and gf) computed in both methods are not reliable

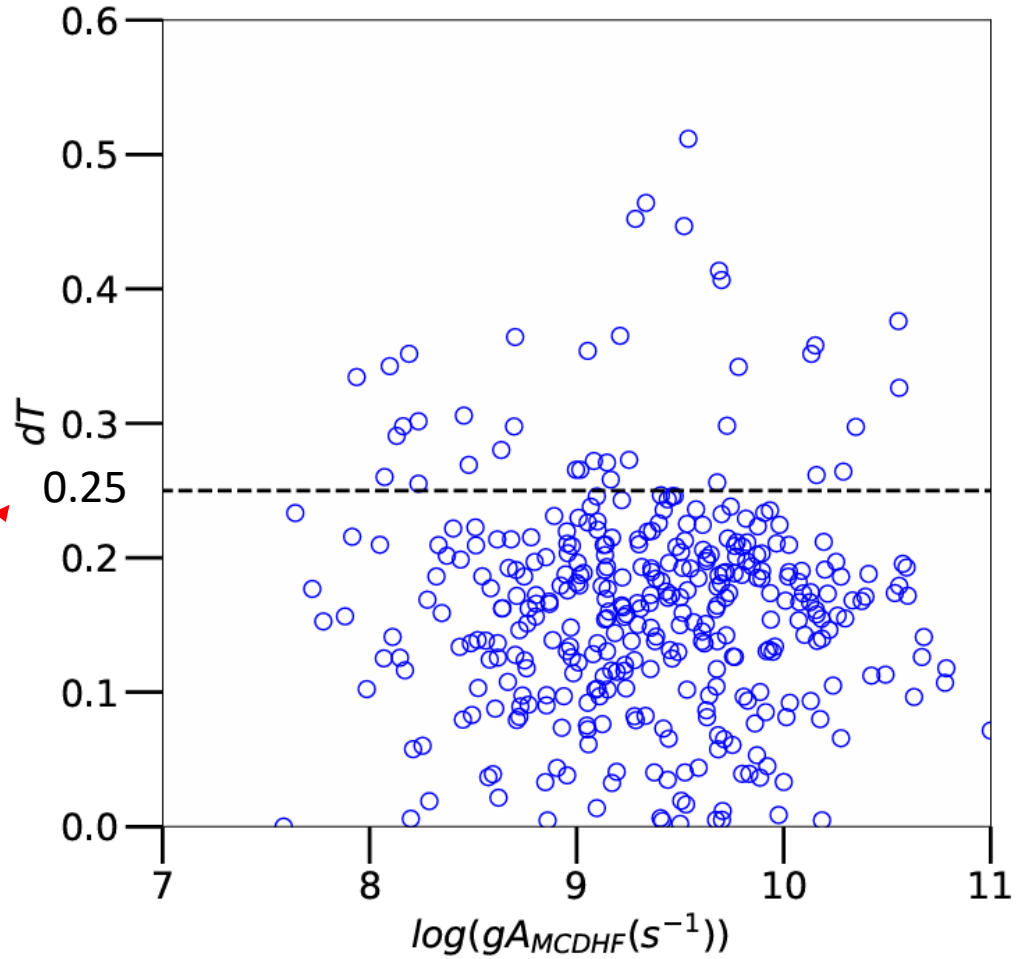
Radiative decay rates

Cancellation Factor : $CF_{ij} = \left(\frac{|\sum_b \sum_c y_j^b y_i^c \langle \psi_c | \mathbf{P}^{(1)} | \psi_b \rangle|}{\sum_b \sum_c |y_j^b y_i^c \langle \psi_c | \mathbf{P}^{(1)} | \psi_b \rangle|} \right)^2$

[Cowan, R. D. ,1981]

Uncertainty of MCDHF transition rates : $dT = \frac{|A_B - A_C|}{\max(A_B, A_C)}$





Radiative decay rates

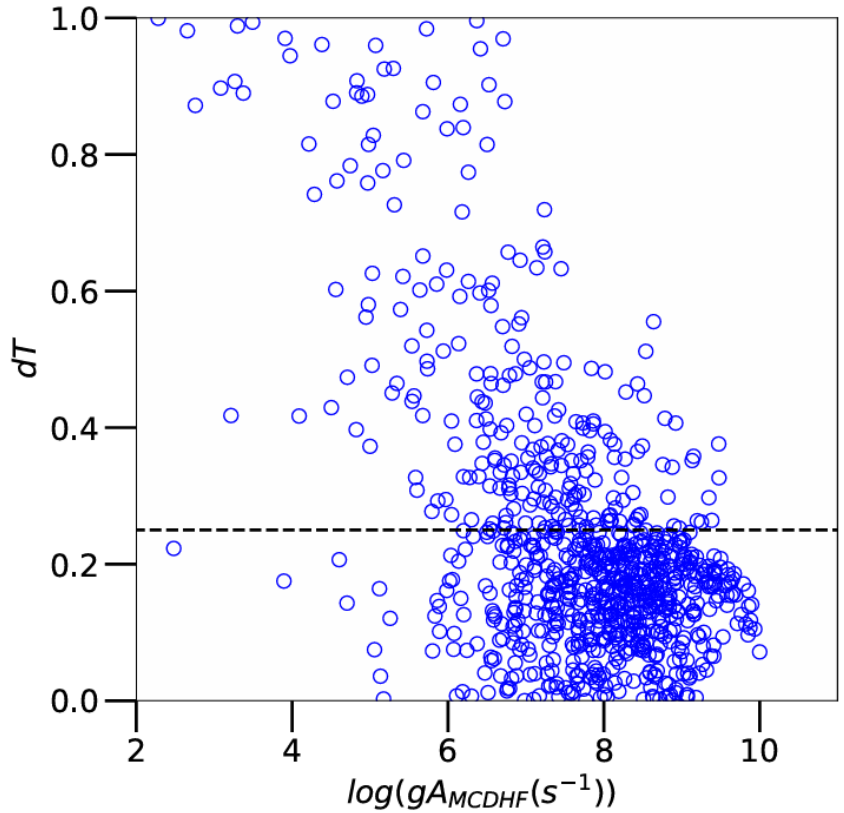
- It remains 250 transitions (among 367) with $CF > 0.05$ and $dT < 0.25$
- The uncertainty on the HFR+CPOL and MCDHF results estimated at most 30%

  $\frac{\Delta gA}{<gA>}$ where $\Delta gA = |gA_{HFR+CPOL} - gA_{MCDHF}|$ and $<gA>=(gA_{HFR+CPOL} - gA_{MCDHF})/2$

- All 867 transitions computed in the MCDHF method

  ⇒ 616 transitions have $dT < 0.25$

  ⇒ The more intense the transitions, the lower the dT value



Conclusion

- Origin of osmium (tungsten transmutation)

- Compute radiative parameters with HFR+CPOL method + least squares adjustment

- Good agreement between HFR+CPOL and MCDHF method and comparisons (250 transitions) allow to estimate uncertainty (<30%)
  - ➢ set of new atomic data for Os VI for plasma diagnosis

- Same procedure for higher ionic charge state of osmium and for other tungsten transmutation products (Ta, Os, Re, Ir, Pt)

- However, few atomic data published


THANK YOU !

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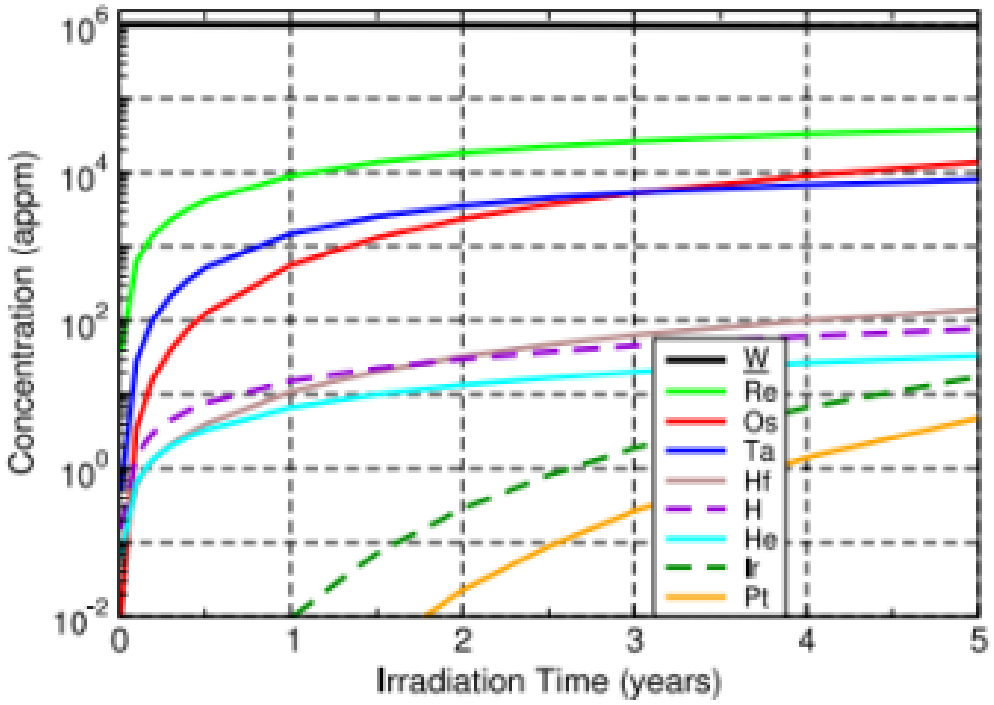
Pure tungsten



Starting composition (at%)	Transmutation products	Concentration of product in appm (in brackets, at%) after irradiating for 1 year	3 years	5 years
W (100)	W	9.89×10^5 (98.9)	9.63×10^5 (96.3)	9.40×10^5 (94.0)
	Re	9.06×10^3 (0.91)	2.59×10^4 (2.59)	3.80×10^4 (3.80)
	Os	5.58×10^2 (0.06)	5.28×10^3 (0.53)	1.38×10^4 (1.38)
	He	6.65×10^0 (<0.01)	2.00×10^1 (<0.01)	3.36×10^1 (<0.01)
	H	1.51×10^1 (<0.01)	4.56×10^1 (<0.01)	7.63×10^1 (<0.01)
Ta (100)	Ta	9.32×10^5 (93.2)	7.56×10^5 (75.6)	6.15×10^5 (61.5)
	W	6.37×10^4 (6.37)	2.32×10^5 (23.2)	3.67×10^5 (36.7)
	Hf	4.37×10^3 (0.44)	1.15×10^4 (1.15)	1.67×10^4 (1.67)
	He	2.88×10^0 (<0.01)	1.03×10^1 (<0.01)	2.00×10^1 (<0.01)
	H	1.64×10^1 (<0.01)	5.07×10^1 (<0.01)	8.68×10^1 (<0.01)
Re (100)	Re	8.73×10^5 (87.3)	6.65×10^5 (66.5)	5.08×10^5 (50.8)
	Os	1.22×10^5 (12.2)	3.20×10^5 (32.0)	4.69×10^5 (46.9)
	W	5.67×10^3 (0.57)	1.50×10^4 (1.50)	2.15×10^4 (2.15)
	He	3.58×10^0 (<0.01)	1.14×10^1 (<0.01)	1.98×10^1 (<0.01)
	H	1.89×10^1 (<0.01)	5.81×10^1 (<0.01)	9.82×10^1 (<0.01)
Ti (100)	Ti	9.99×10^5 (99.9)	9.97×10^5 (99.7)	9.95×10^5 (99.5)
	He	1.83×10^2 (0.02)	5.48×10^2 (0.05)	9.13×10^2 (0.09)
	H	5.95×10^2 (0.06)	1.79×10^3 (0.18)	2.98×10^3 (0.30)
V (100)	V	9.98×10^5 (99.8)	9.93×10^5 (99.3)	9.88×10^5 (98.8)
	He	7.26×10^1 (<0.01)	2.18×10^2 (0.02)	3.63×10^2 (0.04)
	H	5.16×10^2 (0.05)	1.55×10^3 (0.16)	2.58×10^3 (0.26)

Electrostatic interaction energy for two equivalent électrons: $E^{ii} = F^0(ii) - \frac{2l_i+1}{4l_i+1}\sum_k \begin{pmatrix} l_i & k & l_i \\ 0 & 0 & 0 \end{pmatrix}^2 F^k(ii)$

Electrostatic interaction energy for two non-equivalent électrons: $E^{ij} = F^0(ij) - \frac{1}{2}\sum_k \begin{pmatrix} l_i & k & l_j \\ 0 & 0 & 0 \end{pmatrix}^2 G^k(ij)$

Spin-angle 2-spinors: $\chi_{\kappa,m}(\theta,\phi) = \sum_{\sigma=\pm\frac{1}{2}} (l, m, -\sigma, 1/2, \sigma | l, 1/2, j, m) Y_l^{m-\sigma}(\theta,\phi)\phi_\sigma$

Where angular number: $\kappa = \begin{cases} +l & \text{if } j = l - \frac{1}{2} \\ -(l+1) & \text{if } j = l + \frac{1}{2} \end{cases}, \kappa = \pm 1, \pm 2, \pm 3, ...$

Diagonal elements of the Hamiltonian matrix: $$H_{rr} = \sum_{a=1}^{n_0} \left[q_r(a) I(aa) + \sum_{b \leq a}^{n_0} \left(\sum_{k=0,2,..}^{k_0} f_r^k(ab) F^k(ab) + \sum_{k=k_1,k_1+2,..}^{k_2} g_r^k(ab) G^k(ab) \right) \right]$$

Hamiltonian matrix elements out of the diagonal: $$H_{rs} = \sum_{a,b} t_{rs}(ab) I(ab) \delta_{\kappa_a,\kappa_b} + \sum_k \sum_{a,b,c,d} v_{rs}^k(abcd) R^k(abcd)$$

Energy functional: $$E = \sum_{r=1}^{n_c} \sum_{s=1}^{n_c} d_{rs} H_{rs} + \sum_a \sum_b (1 - \delta_{ab}) \bar{q}(a) \epsilon_{ab}(a|b)$$ where (in EOL mode) $$d_{rs} = \frac{1}{n_L} \sum_{i=1}^{n_L} c_{ri} c_{si}$$