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

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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)

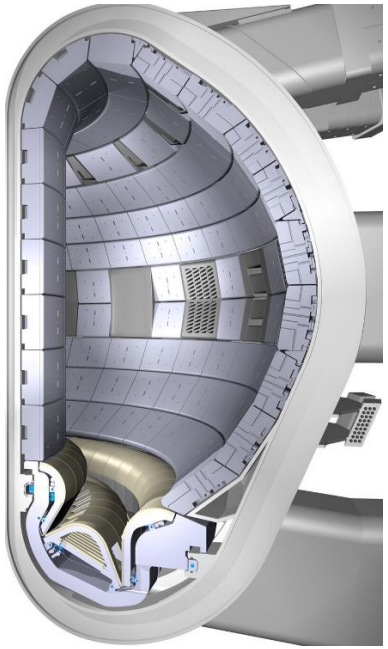
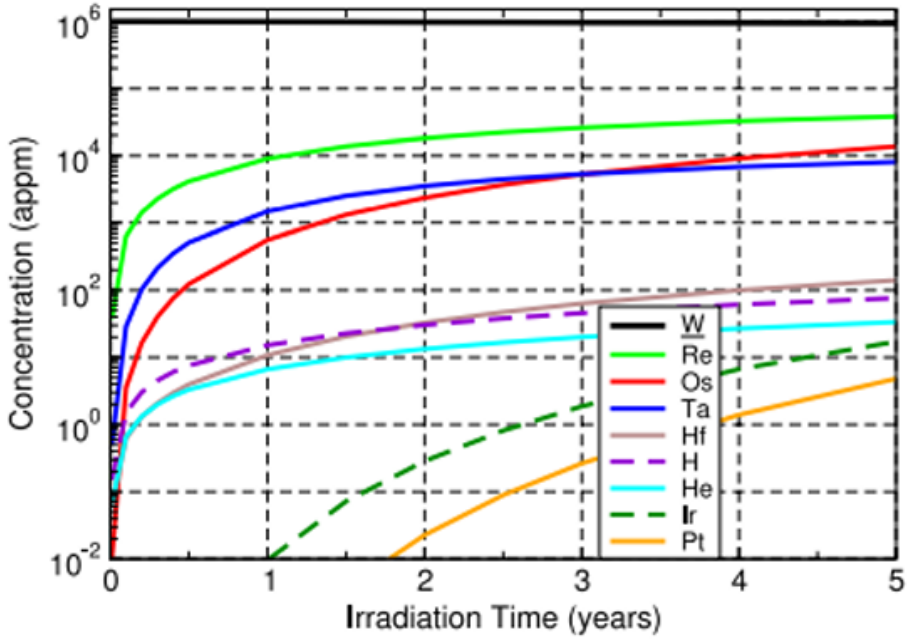


Illustration of the inside of the Tokamak. (https://encyclopedia.pub/entry/37629)



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) :

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

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

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 variationnal principle on the average energy of each eletronic 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-polarisation potential
- Quinet, P. et al [1999, 2002]: pseudo potentiel 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 polarisability; r_c: ionic core radius

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

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

- Minimise 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 $(n_{max}l, n'_{max}l', \dots)$:
- Optimisation 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

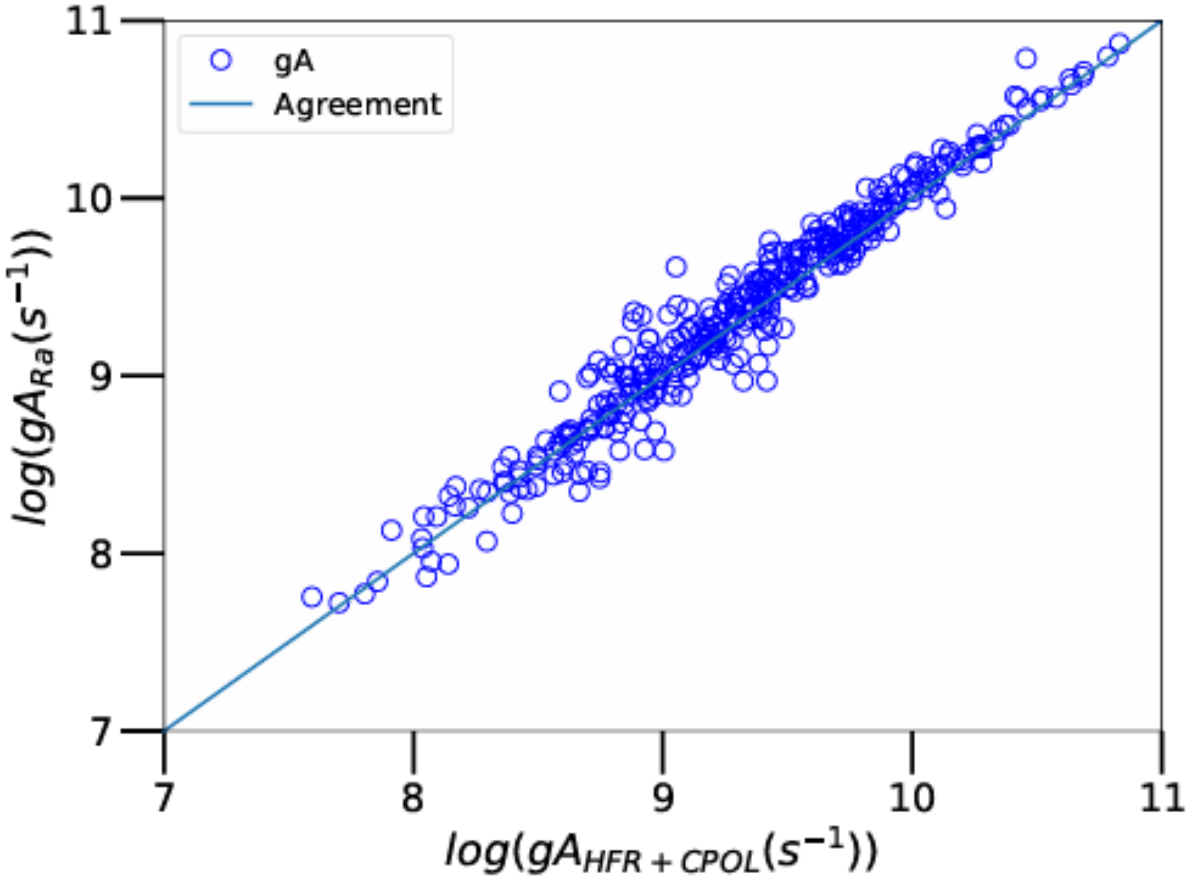
Even parity		Number of CSFs
MR ($5d^3$,$5d^2$6s)	(6s,5p,5d,4f)	35
VV1	SD(MR) → (7s,6p,6d,5f)	569
VV2	SD(MR) → (8s,7p,7d,6f)	1944
CV (RCI)	SrD (MR{4f}) → (8s,7p,7d,6f)	77 463
CC (RCI)	SD (MR{4f}) → (8s,7p,7d,6f)	515 057

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

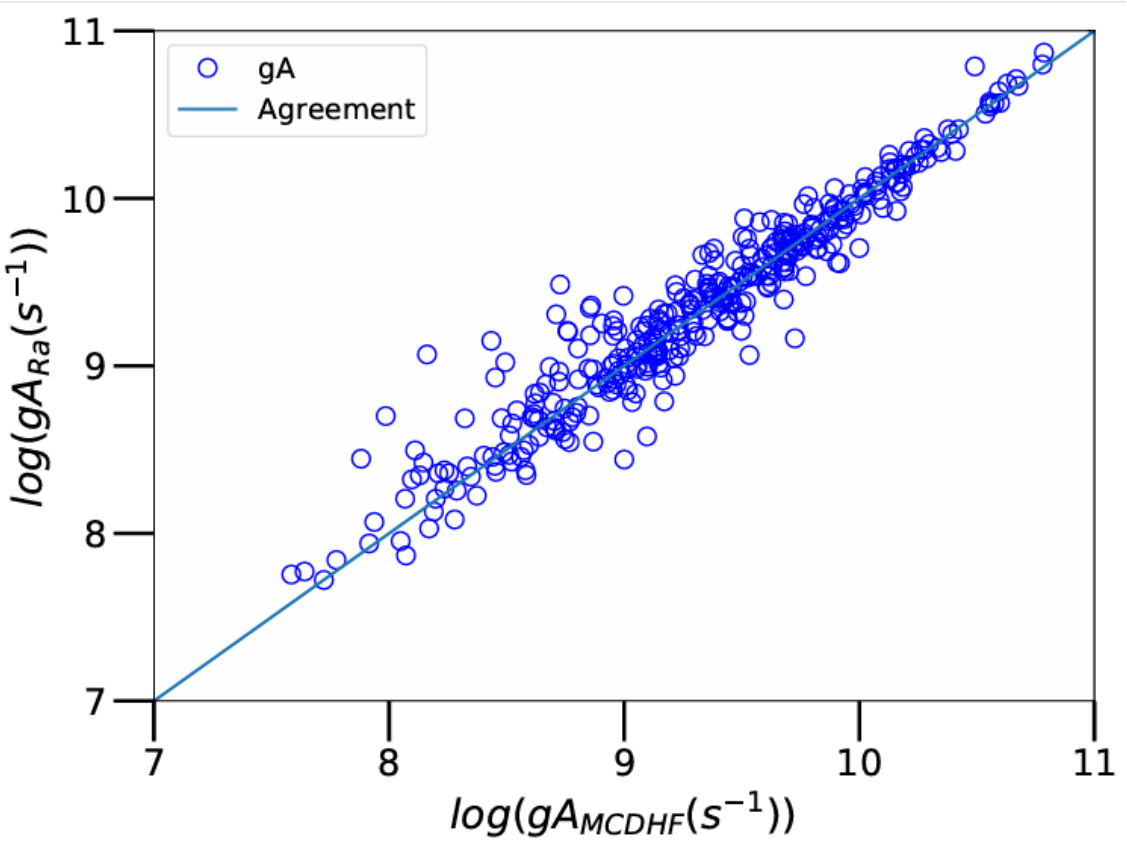
- 367 electric dipole lines between 438.720 and 1486.275 Å



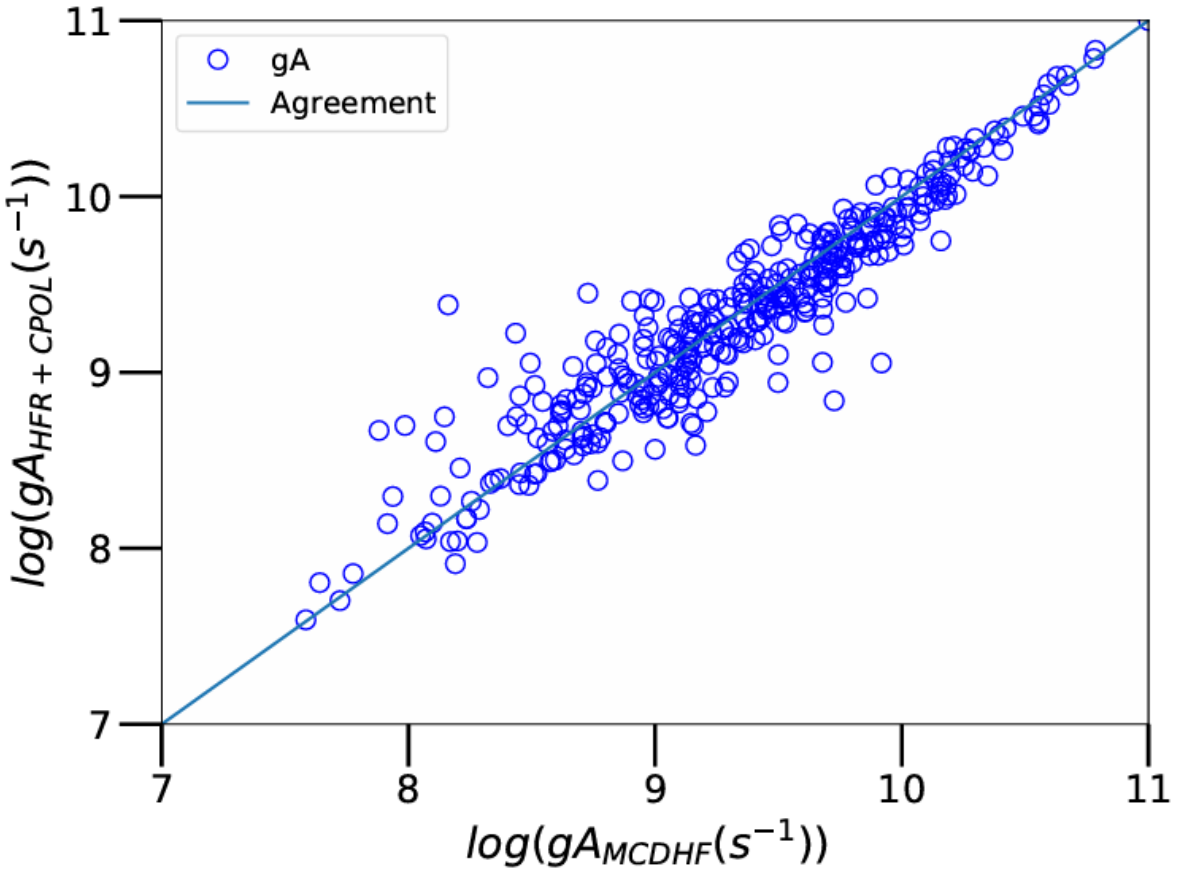
- Mean ratio $gA_{HFR+CPOL}/gA_{Ra}$ = 0.95 $\pm$ 0.21

- 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

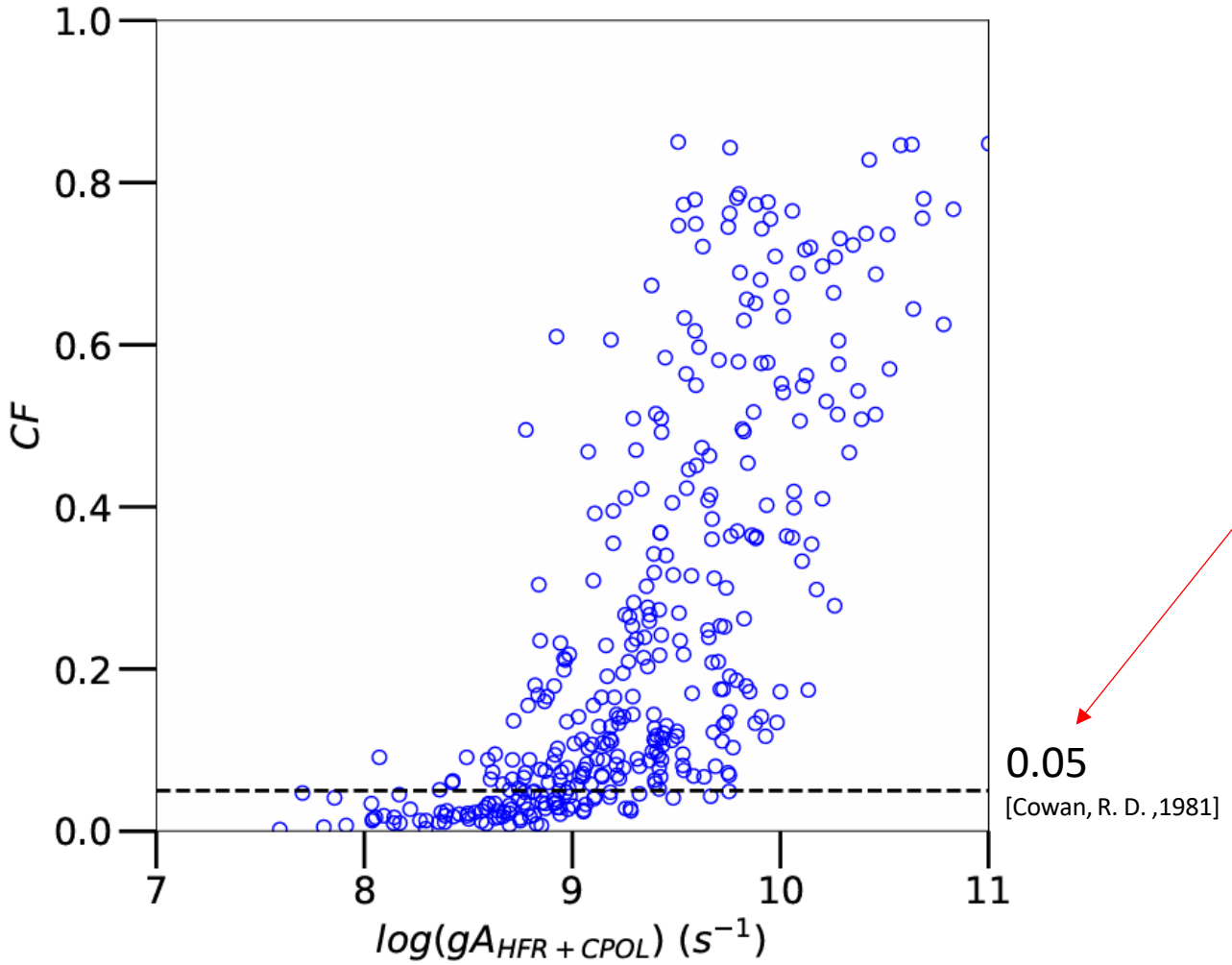
All gA (and gf) computed in both methods are not reliable

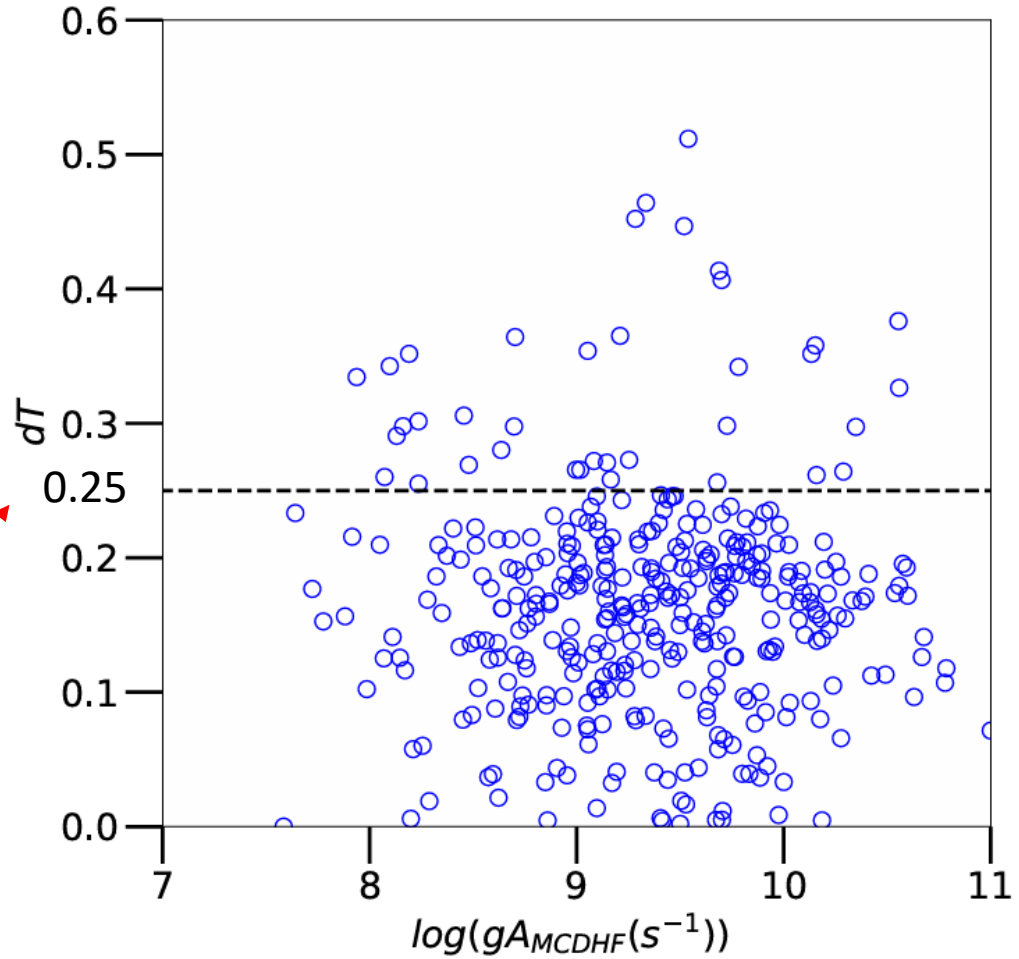
Radiative decay rates

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

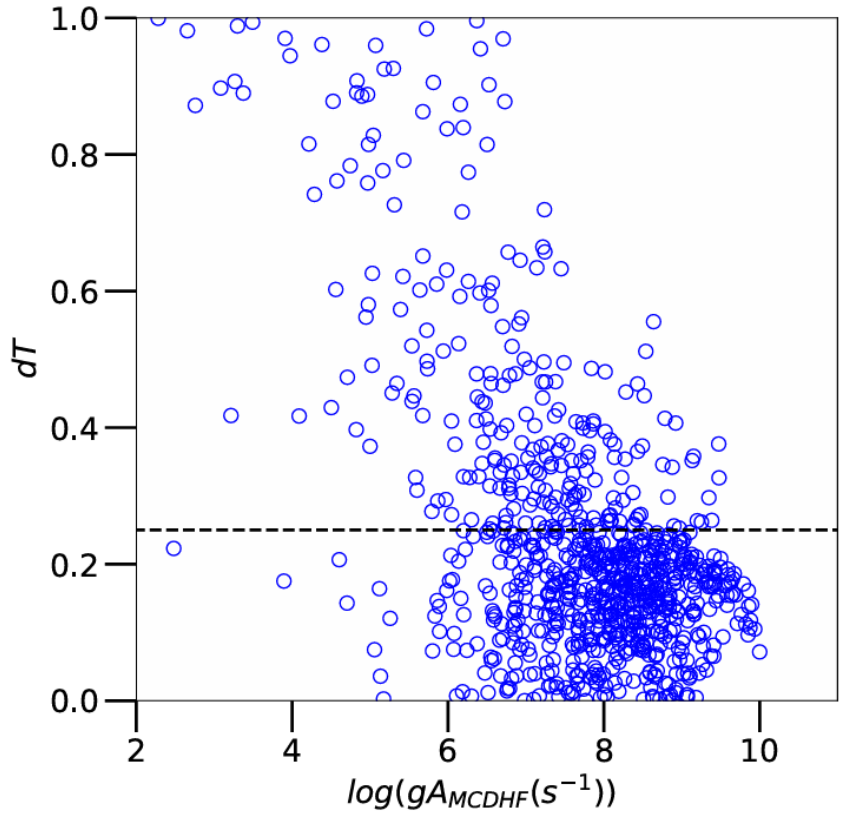
- It remains 250 transitions (among 367) with $CF > 0.05$ and $dT < 0.25$
- The uncertainty on the HFR+CPOL and MCDHF results estimated at most 30%

  → $\frac{\Delta gA}{<gA>}$ 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 adjustement

- 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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