
Atomic structure calculations in neutral and singly-ionized thorium

Maxime Brasseur

University of Mons

Atomic physics and Astrophysics unit

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1. Introduction

2. Numerical methods

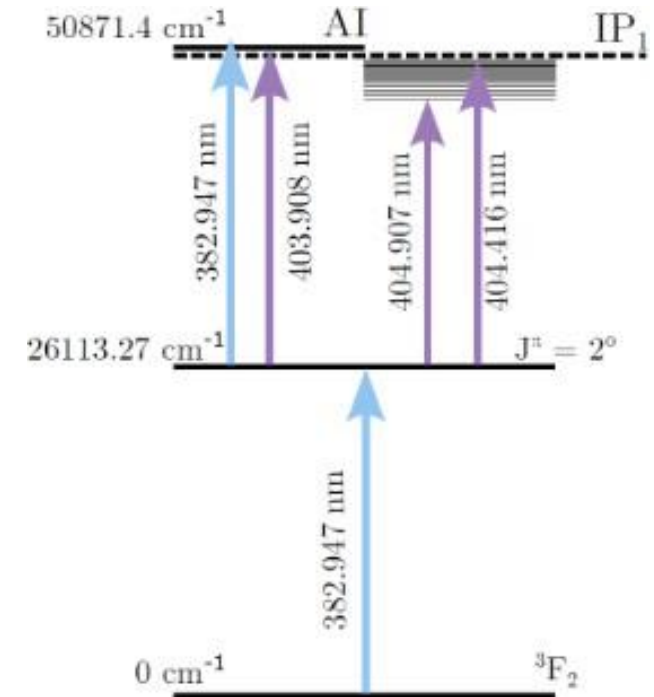
- Pseudo-relativistic Hartree-Fock method with the core polarization corrections
- Multiconfigurational Dirac-Hartree-Fock method

3. Results

- Designation of the level of interest
- First ionization potential

- Measure two first ionization potentials (IP) with a technique in-gas laser ionization
- To measure first ionization potential, second step excites the level with a measured energy of $26\,113.27\text{ cm}^{-1}$ (KUL)

➡ Designation is not known → HFR+CPOL method



- Measure first ionization potential : $50\,867(2)\text{ cm}^{-1}$ and $50\,868.41(2)\text{ cm}^{-1}$ ($50\,868.139\text{ cm}^{-1}$ NIST)
- Calculations with other methods (Weigand. A. et al., 2014) : $50\,572.127\text{ cm}^{-1}$, $50\,814.099\text{ cm}^{-1}$ and $50\,491.47\text{ cm}^{-1}$
- Calculations with MCDHF method

General procedure

- Solve $H\Psi = E\Psi$ where $H = \sum_{i=1}^N \left(-\frac{1}{2} \Delta_i + V(r_i) \right)$ (central field approximation)
- $H_i \varphi_i = E_i \varphi_i \rightarrow \varphi_i(r_i, \theta_i, \phi_i, s_i) = \frac{1}{r_i} P_{n_i l_i}(r_i) Y_{l_i}^{m_i}(\theta_i, \phi_i) \sigma_{m_{s_i}}(s_i)$
- Slater determinant: $\Psi(q_1, \dots, q_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \varphi_1(q_1) & \dots & \varphi_N(q_N) \\ \dots & \dots & \dots \\ \varphi_N(q_1) & \dots & \varphi_N(q_N) \end{vmatrix}$
- $P_{n_i l_i}(r_i) ? \rightarrow$ solve Hartree-Fock equations (Self-Consistent Field method)
- HF equations obtained by variational principle on the average energy of a configuration

Core polarization correction

- Valence electron correlations represented by **configuration interactions** (CI) and other correlations by **core-polarization potential**
- Quinet et al (1999, 2002): pseudo potential have **one-body** and **two-body** part :

$$\text{➤ } V_{P1} = -\frac{1}{2} \alpha_D \sum_{i=1}^N \frac{r_i^2}{(r_i^2 + r_c^2)^3} \text{ and } V_{P2} = -\alpha_D \sum_{i>j} \frac{\vec{r}_i \cdot \vec{r}_j}{[(r_i^2 + r_c^2)(r_j^2 + r_c^2)]^{3/2}}$$

➤ α_D : dipole polarizability; r_c : ionic core radius

Slater-Condon method

- Consider CI: $\Psi_k = \sum_b y_k^b \psi_b$, where $\sum_b (y_k^b)^2 = 1$

General procedure

- $H_{DC} = \sum_{i=1}^N h_{D_i}$ 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: $h_D \varphi = E \varphi \rightarrow \varphi(r, \theta, \phi) = \frac{1}{r} \begin{pmatrix} P_{n,\kappa}(r) \chi_{\kappa,m}(\theta, \phi) \\ i Q_{n,\kappa}(r) \chi_{\kappa,m}(\theta, \phi) \end{pmatrix}$ where $P_{n,\kappa}(r)$ and $Q_{n,\kappa}(r)$ are **large** and **small radial part**, respectively.
- $P_{n,\kappa}(r), Q_{n,\kappa}(r) ? \rightarrow$ solve MCDHF equations (Self-Consistent Field method)
- CI: $\Psi(P, J, M) = \sum_{r=1}^{n_c} c_r \Phi(\gamma_r, P, J, M)$

Designation of the level of interest

Wavelength (nm)	Intensity	Lower level (even parity)			Upper level (odd parity)	
		$E(\text{cm}^{-1})$	Designation	J	$E(\text{cm}^{-1})$	J
382.838	14000	0	$6d^2 7s^2 \ ^3F$	2	26113.269	2
445.80	4000	3687.987	$6d^2 7s^2$	2	26113.269	2
506.166	600	6362.396	$6d^3 7s \ ^5F$	2	26113.269	2
449.357	330	3865.474	$6d^2 7s^2 \ ^3P$	1	26113.269	2
698.603	220	11802.932	$6d^3 7s \ ^5P$	2	26113.269	2
1321.715	220	18549.405	$6d^3 7s$	2	26113.269	2
688.883	160	11601.030	$6d^3 7s \ ^5P$	1	26113.269	2
530.831	120	7280.123	$6d^2 7s^2$	2	26113.269	2
822.768	120	13962.520	$6d^3 7s$	1	26113.269	2
975.401	61	15863.888	$6d^3 7s$	2	26113.269	2
1348.495	35	18699.623	$5f 7s^2 7p \ ^3F$	2	26113.269	2
1562.015	35	19713.031	$6d^3 7s \ ^3F$	3	26113.269	2
486.479	18	5563.142	$6d^3 7s \ ^5F$	1	26113.269	2
430.098	16	2869.259	$6d^2 7s^2 \ ^3F$	3	26113.269	2
537.168	14	7502.288	$6d^3 7s \ ^5F$	3	26113.269	2
1326.133	11	18574.610	$6d^3 7s$	1	26113.269	2
1461.591	11	19273.281	$6d^3 7s$	2	26113.269	2
1650.123	9	20054.771	$6d^3 7s \ ^3F$	2	26113.269	2
2203.502	3	21575.037	$6d^3 7s$	2	26113.269	2
2213.077	1	21594.673	$6d^3 7s \ ^1F$	3	26113.269	2

Transitions in NIST which depopulate and populate level $26\ 113.269\ \text{cm}^{-1}$

→ some lack of data

→ cannot identify clearly a designation

Comparisons between the **highest transitions which depopulate** the level $26\ 113.27\ \text{cm}^{-1}$ available in NIST with the corresponding HFR+CPOL transitions

Wavelength (nm)	Intensity	Lower level (odd parity)		Upper level (even parity)	
		$E(\text{cm}^{-1})$	J	$E(\text{cm}^{-1})$	J
685.487	20	26113.269	2	40697.412	2 or 3
1199.960	19	26113.269	2	34444.598	2
1765.889	11	26113.269	2	31774.594	3
649.706	7	26113.269	2	41500.618	3

Designation of the level of interest

- Consider 4 configurations in each parity, $\langle r_{6p} \rangle = 1.884 a_0$ and $\alpha = 10.26 a_0^3$ (Fraga. S. et al., 1976)
- Optimize energy level ($J^\pi = 2^o$) with the experimental value $26\,113.27\text{ cm}^{-1}$ and $26\,113.268\text{ cm}^{-1}$ ($g_J = 0.980$) in NIST
- We did it for 7 levels optimizing average energies of $6d^2 7s 7p$ and $5f 6d^2 7s$:

Even parity	Odd parity
$6d^2 7s^2$	$6d^2 7s 7p$
$6d^3 7s$	$6d^3 7p$
$6d^4$	$6d 7s^2 7p$
$5f 6d^2 7p$	$5f 6d^2 7s$

Energy (cm^{-1})	24850.0	25080.9	26154.2	26431.4	27288.3	27440.1	27948.8	26113.27 (exp)
Landé g-factor	1.238	1.026	1.231	1.078	1.103	0.973	1.050	0.980

Energy (cm^{-1})	Ab initio composition in LS coupling						Presence (%)	
							$6d^2 7s 7p$	$5f 6d^2 7s$
24850.0	15.1%	$6d^2 7s 7p(^1D)^3D$	7.9%	$5f 6d^2 7s(^3F)^5P$	6.7%	$5f 6d^2 7s(^3F)^3P$	48.8	30.5
25080.9	19.7%	$6d^2 7s 7p(^3F)^3F$	10.9%	$6d^3 7p(^4F)^3F$	8.2%	$6d^2 7s 7p(^3F)^3F$	43.5	31.3
26154.2	11.9%	$5f 6d^2 7s(^3F)^3P$	10.1%	$6d^3 7p(^4F)^3D$	8.4%	$5f 6d^2 7s(^1D)^3D$	38.8	38.2
26431.4	28.2%	$6d^2 7s 7p(^1D)^3F$	4.8%	$6d^2 7s 7p(^3F)^3D$	4.5%	$6d^3 7p(^4P)^5D$	48.9	24.8
27288.3	16.1%	$5f 6d^2 7s(^3F)^3P$	13.2%	$5f 6d^2 7s(^3P)^5F$	7.1%	$6d^3 7p(^4F)^3D$	28.6	51.9
27440.1	36.5%	$5f 6d^2 7s(^3F)^5P$	19.9%	$6d^2 7s 7p(^3P)^5P$	7.9%	$6d^3 7p(^4P)^5P$	41.5	42.9
27948.8	13.8%	$6d^2 7s 7p(^1D)^3F$	13.6%	$5f 6d^2 7s(^3P)^5F$	4.7%	$6d^2 7s 7p(^1D)^3P$	33.9	43.9

⇒ Important mixing

Designation of the level of interest

Most intense transitions (NIST)

25 080.9 → 26 113.27

Wavelength (nm)	Intensity	$E(\text{cm}^{-1})$	Designation	J
382.83	14000	0	$6d^27s^2\ ^3F$	2
445.80	4000	3687.987	$6d^27s^2$	2
506.16	600	6362.396	$6d^37s\ ^5F$	2
449.35	330	3865.474	$6d^27s^2\ ^3P$	1
698.60	220	11802.932	$6d^37s\ ^5P$	2
1321.71	220	18549.405	$6d^37s$	2
688.88	160	11601.030	$6d^37s\ ^5P$	1
530.83	120	7280.123	$6d^27s^2$	2
822.76	120	13962.520	$6d^37s$	1

Wavelength (nm)	A (s^{-1})	E (cm^{-1})	CF	Expected
382.94	4.74E+07	0	0.3522	0
792.34	4.62E+06	13492.4	0.0792	3440.2
459.01	1.29E+06	4327.1	0.0238	4327.1
552.62	7.30E+05	8017.6	0.014	3720.5
630.26	4.99E+05	10246.8	0.0619	10923.1
446.57	5.70E+04	3720.5	0.0011	17847.7
658.32	4.02E+04	10923.1	0.0005	10246.8
1209.86	1.87E+04	17847.7	0.013	8017.6
441.05	1.15E+03	3440.2	0	13492.4

26 431.4 → 26 113.27

Wavelength (nm)	A (s^{-1})	E (cm^{-1})	CF	Expected
382.94	1.65E+07	0	0.2358	0
432.17	4.63E+06	3440.2	0.0983	3440.2
446.58	2.03E+06	3720.5	0.0387	4327.1
552.62	1.61E+06	8017.6	0.045	3720.5
459.01	8.98E+05	4327.1	0.0189	10923.1
630.26	3.21E+05	10246.8	0.0263	17847.7
792.34	2.16E+05	13492.4	0.0158	10246.8
658.33	1.80E+05	10923.1	0.008	8017.6
1209.86	9.43E+04	17847.7	0.0323	13492.4

Designation of the level of interest

27 288.3 → 26 113.27

Wavelength (nm)	A (s^{-1})	E (cm^{-1})	CF	Expected
382.94	8.02E+06	0	0.1153	0
441.05	4.28E+06	3440.2	0.0381	3440.2
446.57	3.14E+06	3720.5	0.0573	4327.1
459.01	2.03E+06	4327.1	0.0461	3720.5
552.62	7.62E+05	8017.6	0.0205	10923.1
1209.86	9.48E+04	17847.7	0.0368	17847.7
792.34	8.41E+04	13492.4	0.0061	10246.8
658.33	7.60E+04	10923.1	0.0051	8017.6
630.26	3.12E+04	10246.8	0.0056	13492.4

27 440.1 → 26 113.27

Wavelength (nm)	A (s^{-1})	E (cm^{-1})	CF	Expected
382.94	3.58E+06	0	0.0835	0
446.57	1.82E+06	3720.5	0.0621	3440.2
459.01	8.16E+05	4327.1	0.0224	4327.1
441.05	5.78E+05	3440.2	0.0074	3720.5
792.34	4.07E+05	13492.4	0.0618	10923.1
630.26	1.77E+05	10246.8	0.0583	17847.7
658.33	4.12E+04	10923.1	0.0037	10246.8
552.62	2.95E+03	8017.6	0.0001	8017.6
1209.86	1.52E+03	17847.7	0.0015	13492.4

27 948.8 → 26 113.27

Wavelength (nm)	A (s^{-1})	E (cm^{-1})	CF	Expected
446.57	1.15E+07	3720.5	0.2268	0
459.00	4.14E+06	4327.1	0.0694	3440.2
382.94	3.81E+06	0	0.0464	4327.1
552.62	6.52E+05	8017.6	0.019	3720.5
441.05	7.30E+04	3440.2	0.0007	10923.1
792.33	5.50E+04	13492.4	0.0042	17847.7
658.32	4.13E+04	10923.1	0.0022	10246.8
630.06	2.01E+04	10246.8	0.0024	8017.6
1209.83	3.99E+03	17847.7	0.0015	13492.4

Designation of the level of interest

Level of interest computed in our method at energy $26\,431.4\text{ cm}^{-1}$ ($J^\pi = 2^\circ$)

Other confirmations :

1. Ratio between the two most intense transitions from NIST : 3.5

2. Ratio between the two most probable transitions from our calculations : 3.56

3. Designation : $27.4\% \text{ } 6d^27s7p(^1D)^3F + 4.8\% \text{ } 5f6d27s(^1D)^3D + 4.8\% \text{ } 6d^27s7p(^3F)^3D$

$6d^27s7p$	$5f6d^27s$	$6d^37p$	$6d7s^27p$
44.50%	33.56%	18.24%	0.04%

4. Designation of ground state ($J=2^e$): $77.1\% \text{ } 6d^27s^2(^3F)^3F + 13.1\% \text{ } 6d^27s^2(^1D)^1D + 2.7\% \text{ } 6d^37s(^2F)^3F$

Model A

Th I :

- ❖ MR : $6d^2 7s^2, 6d^3 7s, 6d^4 \Rightarrow 21$ CSFs;
- ❖ VV1: SD {MR} $\rightarrow \{7s, 6p, 6d, 5f, 5g\} \Rightarrow 291$ CSFs;
- ❖ VV2: SD {MR} $\rightarrow \{7s, 6p, 6d, 6f, 6g\} \Rightarrow 971$ CSFs;
- ❖ VV3: SD {MR} $\rightarrow \{7s, 7p, 7d, 7f, 7g\} \Rightarrow 3102$ CSFs;
- ❖ VV4: SD {MR} $\rightarrow \{8s, 8p, 8d, 8f, 8g\} \Rightarrow 6730$ CSFs;
- ❖ CV: S {6s, 6p} $\rightarrow$ MR $\Rightarrow 6756$ CSFs;
- ❖ CC: SD {6s, 6p} $\rightarrow$ MR $\Rightarrow 6858$ CSFs

Th II :

- ❖ MR : $6d 7s^2, 6d^2 7s, 6d^3 \Rightarrow 10$ CSFs;
- ❖ VV1: SD {MR} $\rightarrow \{7s, 6p, 6d, 5f, 5g\} \Rightarrow 61$ CSFs;
- ❖ VV2: SD {MR} $\rightarrow \{7s, 6p, 6d, 6f, 6g\} \Rightarrow 188$ CSFs;
- ❖ VV3: SD {MR} $\rightarrow \{7s, 7p, 7d, 7f, 7g\} \Rightarrow 584$ CSFs;
- ❖ VV4: SD {MR} $\rightarrow \{8s, 8p, 8d, 8f, 8g\} \Rightarrow 1258$ CSFs;
- ❖ CV: S {6s, 6p} $\rightarrow$ MR $\Rightarrow 1275$ CSFs;
- ❖ CC: SD {6s, 6p} $\rightarrow$ MR $\Rightarrow 1332$ CSFs

IP1 MR	IP1(1)	IP1(2)	IP1(3)	IP1(4)	IP1(CV)	IP1(CC)	Exp	NIST	Weigand
40 498.4	41 484.8	41 704.9	47 808.1	48 260.6	48 253.2	47 831.6	50 868.4	50 868.1	50 814.1

First ionization potential

Model B

Th I :

- ❖ MR: $6d^2 7s^2, 6d^3 7s, 6d^4, 5f^2 6d 7s, 5f^2 6d^2, 5f^2 7s^2 \Rightarrow 128$ CSFs;
- ❖ Same active set

Th II :

- ❖ MR: $6d 7s^2, 6d^2 7s, 6d^3, 5f^2 7s, 5f^2 6d \Rightarrow 29$ CSFs;
- ❖ Same active set

IP1 MR	IP1(1)	IP1(2)	IP1(3)	IP1(4)	IP1(CV)	IP1(CC)	Exp	NIST	Weigand
41 553.0	42 017.2	42 157.0	48 281.3	48 907.6	47 923.4	46 860.0	50 868.4	50 868.1	50 814.1

Model C

Th I :

- ❖ MR: $6d^2 7s^2, 6d^3 7s, 6d^4, 5f^2 6d 7s, 5f^2 6d^2, 5f^2 7s^2, 5f 6d^2 7p, 5f 6d 7s 7p, 5f 7s^2 7p \Rightarrow 254$ CSFs;
- ❖ Same active set

Th II :

- ❖ MR: $6d 7s^2, 6d^2 7s, 6d^3, 5f^2 7s, 5f^2 6d, 5f 6d 7p, 5f 7s 7p \Rightarrow 52$ CSFs;
- ❖ Same active set

IP1 MR	IP1(1)	IP1(2)	IP1(3)	IP1(4)	IP1(CV)	IP1(CC)	Exp	NIST	Weigand
44 592.3	48 010.8	48 093.7	48 424.6	49 236.2	47 330.7	45 591.0	50 868.4	50 868.1	50 814.1

Model D

Th I :

- ❖ MR: $6d^2 7s^2, 6d^3 7s, 6d^4, 5f^2 6d 7s, 5f^2 6d^2, 5f^2 7s^2, 5f 6d^2 7p, 5f 6d 7s 7p, 5f 7s^2 7p \Rightarrow 254$ CSFs;
- ❖ VV1: SD {MR} $\rightarrow \{7s, 7p, 6d, 5f, 5g\}$;
- ❖ VV2: SD {MR} $\rightarrow \{7s, 7p, 6d, 6f, 6g, 6h\}$;
- ❖ VV3: SD {MR} $\rightarrow \{7s, 7p, 7d, 7f, 7g, 7h\}$;
- ❖ VV4: SD {MR} $\rightarrow \{8s, 8p, 8d, 8f, 8g, 8h\}$;
- ❖ VV5: SD {MR} $\rightarrow \{9s, 9p, 9d, 9f, 9g, 9h\}$;
- ❖ VV6: SD {MR} $\rightarrow \{10s, 10p, 10d, 10f, 10g, 10h\}$;
- ❖ CV: S {6s, 6p} $\rightarrow$ MR
- ❖ CC: SD {6s, 6p} $\rightarrow$ MR $\Rightarrow 210\,849$ CSFs

Th II :

- ❖ MR: $6d 7s^2, 6d^2 7s, 6d^3, 5f^2 7s, 5f^2 6d, 5f 6d 7p, 5f 7s 7p \Rightarrow 52$ CSFs;
- ❖ VV1: SD {MR} $\rightarrow \{7s, 7p, 6d, 5f, 5g\}$;
- ❖ VV2: SD {MR} $\rightarrow \{7s, 7p, 6d, 6f, 6g, 6h\}$;
- ❖ VV3: SD {MR} $\rightarrow \{7s, 7p, 7d, 7f, 7g, 7h\}$;
- ❖ VV4: SD {MR} $\rightarrow \{8s, 8p, 8d, 8f, 8g, 8h\}$;
- ❖ VV5: SD {MR} $\rightarrow \{9s, 9p, 9d, 9f, 9g, 9h\}$;
- ❖ VV6: SD {MR} $\rightarrow \{10s, 10p, 10d, 10f, 10g, 10h\}$;
- ❖ CV: S {6s, 6p} $\rightarrow$ MR
- ❖ CC: SD {6s, 6p} $\rightarrow$ MR $\Rightarrow 27\,890$ CSFs

IP1 MR	IP1(1)	IP1(2)	IP1(3)	IP1(4)	IP1(5)	IP1(6)	IP1(CV)	IP1(CC)	Exp
44 592.3	48 010.8	48 202.9	48 519.0	49 327.3	49 394.2	49 406.2	47 789.8	46 306.4	50 868.4

First ionization potential

Model E

Th I :

- ❖ MR: $6d^2 7s^2, 6d^3 7s, 6d^4, 5f^2 6d 7s, 5f^2 6d^2, 5f^2 7s^2, 5f 6d^2 7p, 5f 6d 7s 7p, 5f 7s^2 7p \Rightarrow 254$ CSFs;
- ❖ VV1-VV6: SDTQ {MR} $\rightarrow$ active set ($n_{\max} l_{\max} = 10h$)
- ❖ CV: S {6s,6p} $\rightarrow$ MR $\Rightarrow 2\,939\,952$ CSFs reducing to 157 258 CSFs

Th II :

- ❖ MR: $6d 7s^2, 6d^2 7s, 6d^3, 5f^2 7s, 5f^2 6d, 5f 6d 7p, 5f 7s 7p \Rightarrow 52$ CSFs;
- ❖ VV1-VV6: SDTQ {MR} $\rightarrow$ active set ($n_{\max} l_{\max} = 10h$)
- ❖ CV: S {6s,6p} $\rightarrow$ MR $\Rightarrow 28\,424$ CSFs

IP1 MR	IP1(1)	IP1(2)	IP1(3)	IP1(4)	IP1(5)	IP1(6)	IP1(CV)	Exp	NIST
44 592.3	48 017.6	48 210.5	48 538.8	49 324.3	49 390.4	49 402.4	47 786.7	50 868.4	50 868.1

Model F

Th I :

- ❖ CV: SrD {MR} $\rightarrow \{8s, 8p, 8d, 8f, 8g, 8h\} \Rightarrow 2\,490\,400$ CSFs
- ❖ CV: SrD {MR} $\rightarrow 8s, 8p, 8d, 8f, 8g, 8h \Rightarrow 324\,348$ CSFs

Th II :

IP1(4) (model E)	IP1(SrD4) (model F)	IP1(SrD5) (model F)	Exp	NIST
49 327.3	49 519.7	In progress	50 868.4	50 868.1

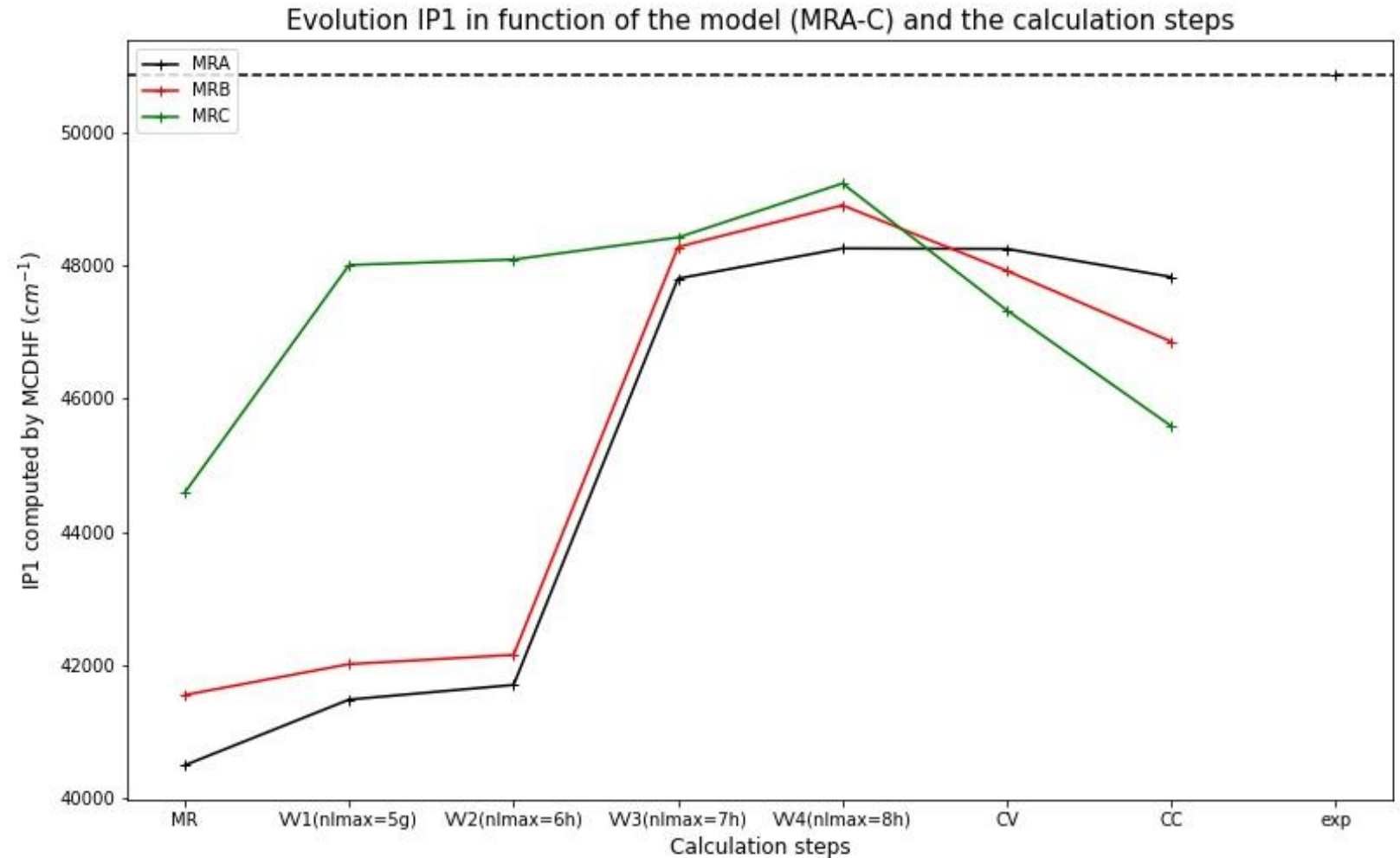
First ionization potential

Some graphs

Number of configurations

	Th I	Th II
MRA	3	3
MRB	6	5
MRC	9	7

Increase MR, tend to the experimental value until the CV and CC correlations

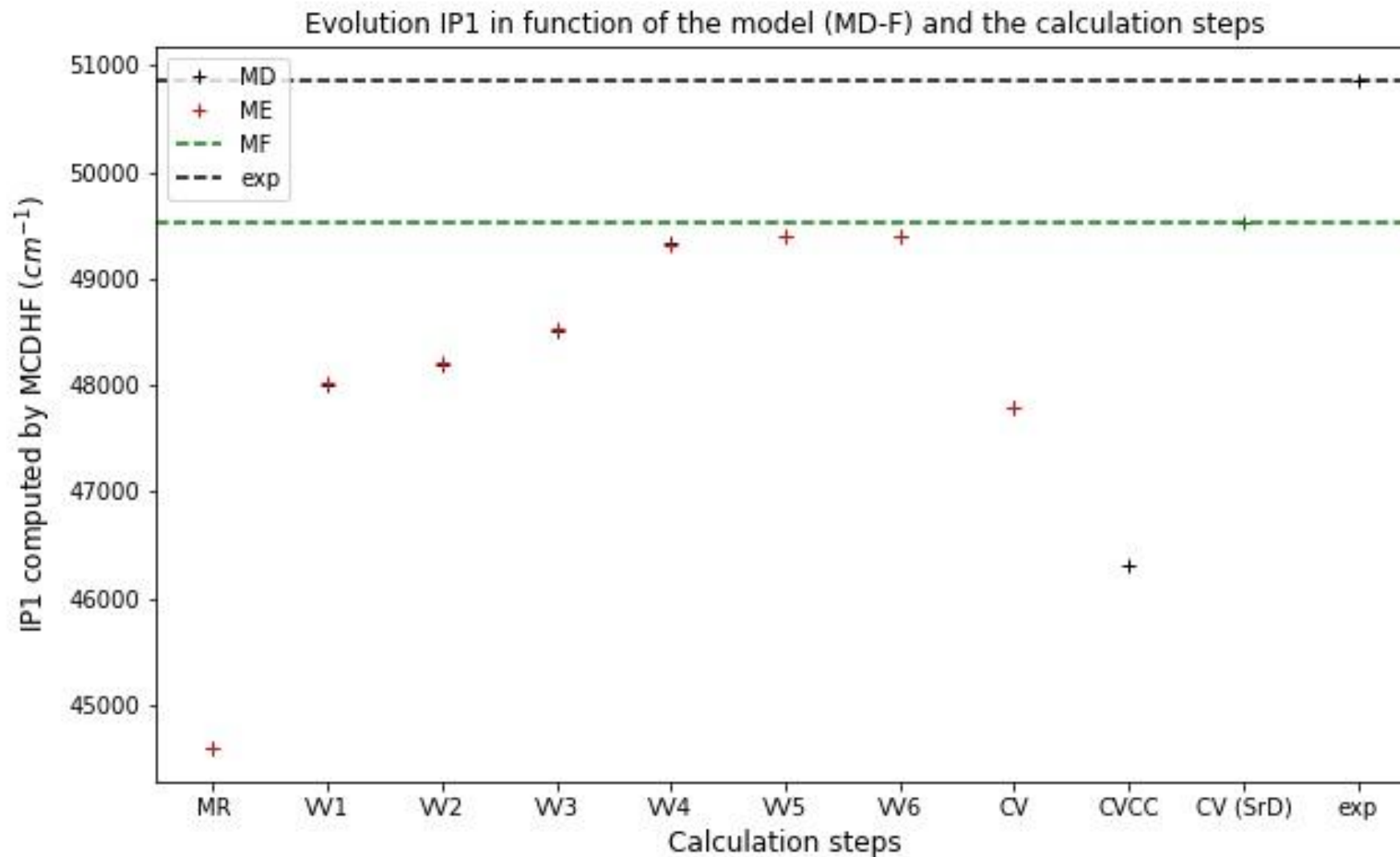


First ionization potential

MD : SD
ME : SDTQ
MF : CV (SrD)

Not significant
differences
between MD
and ME

Improvement
with SrD



Designation

- Use HFR+CPOL to identify a designation of the level 26 113.27 cm⁻¹
- Not obvious due to some lack of data and significant mixing but there are some convergence points which tend to this designation : $21.0\% \ 6d^2 7s 7p(^1D)^3F + 7.0\% \ 6d^3 7p(^4F)^3D + 4.8\% \ 6d^3 7p(^2P)^3P$
- The level of interest is computed in our method at 26 431.4 cm⁻¹

First ionization potential

- By increasing the MR, the calculated value tends to the experimental one but the CV and CC correlations cause divergence
- We decide to increase the active set in VV correlations which improve the IP1 value but not enough and complicate to reproduce CV and CC correlations
- CV correlations with SrD to {8s, 8p, 8d, 8f, 8g, 8h} improve the IP1 value. Assume could reproduce experimental value by increasing active set but calculation size becomes significant

- Atomic Spectra Database *NIST*, 2009. Available at: <https://www.nist.gov/pml/atomic-spectra-database> (Accessed: 03 April 2024).
- Cowan. R. D. The Theory of Atomic Structure and Spectra. *University of California Press*, California, 731 p, 1981.
- Grant. I. P. Relativistic Quantum Theory of Atoms and Molecules. *Springer*, New-York, 799 p, 2007.
- Fraga. S, Karwowski. J, and Saxena. K. M. S. Handbook of atomic data. Elsevier, Amsterdam, 1976.
- Quinet. P, Palmeri. P , Biémont. E , McCurdy. M. M , Rieger. G , Pinnington. E. H , Wickliffe. M. E, and Lawler. J. E. Experimental and theoretical radiative lifetimes, branching fractions and oscillator strengths in Lu ii. *Monthly Notices of the Royal Astronomical Society*, 307(4):934–940, 1999.
- Quinet. P, Palmeri. P, Biémont. E, Li. Z. S, Zhang. Z. G, and Svanberg. S. Radiative lifetime measurements and transition probability calculations in lanthanide ions. *Journal of Alloys and Compounds*, 344(1):255–259, 2002.
- Weigand. A. et al. Relativistic Small-Core Pseudopotentials for Actinium, Thorium, and Protactinium, *The Journal of Physical Chemistry A*, 118(13), pp. 2519–2530.

$$CF_{ij} = \left(\frac{|\sum_b \sum_c y_j^b y_i^c \langle \psi_c | \mathbf{P}^{(1)} | \psi_b \rangle|}{\sum_b \sum_c |y_j^b y_i^c \langle \psi_c | \mathbf{P}^{(1)} | \psi_b \rangle|} \right)^2 \quad \text{Where } S_{ij} = |\langle \Psi_i | P^{(1)} | \Psi_j \rangle|^2$$

Model A

Th I :

- ❖ MR: $6d^2 7s^2, 6d^3 7s, 6d^4 \Rightarrow 21$ CSFs;
- ❖ VV1: SD {MR} $\rightarrow \{7s, 6p, 6d, 5f, 5g\} \Rightarrow 291$ CSF
- ❖ VV2: SD {MR} $\rightarrow \{7s, 6p, 6d, 6f, 6g\} \Rightarrow 971$ CSFs;
- ❖ VV3: SD {MR} $\rightarrow \{7s, 7p, 7d, 7f, 7g\} \Rightarrow 3102$ CSFs;
- ❖ VV4: SD {MR} $\rightarrow \{8s, 8p, 8d, 8f, 8g\} \Rightarrow 6730$ CSFs;
- ❖ CV: S {6s, 6p} $\rightarrow$ MR $\Rightarrow 6756$ CSFs
- ❖ CC: SD {6s, 6p} $\rightarrow$ MR $\Rightarrow 6858$ CSFs

Th II :

- ❖ MR: $6d 7s^2, 6d^2 7s, 6d^3 \Rightarrow 10$ CSFs;
- ❖ VV1: SD {MR} $\rightarrow \{7s, 6p, 6d, 5f, 5g\} \Rightarrow 61$ CSF
- ❖ VV2: SD {MR} $\rightarrow \{7s, 6p, 6d, 6f, 6g\} \Rightarrow 188$ CSFs;
- ❖ VV3: SD {MR} $\rightarrow \{7s, 7p, 7d, 7f, 7g\} \Rightarrow 584$ CSFs;
- ❖ VV4: SD {MR} $\rightarrow \{8s, 8p, 8d, 8f, 8g\} \Rightarrow 1258$ CSFs;
- ❖ CV: S {6s, 6p} $\rightarrow$ MR $\Rightarrow 1275$ CSFs
- ❖ CC: SD {6s, 6p} $\rightarrow$ MR $\Rightarrow 1332$ CSFs

IP1 MR	IP1(1)	IP1(2)	IP1(3)	IP1(4)	IP1(CV)	IP1(CC)	Exp	NIST	Weigand
40 498.4	41 484.8	41 704.9	47 808.1	48 260.6	48 253.2	47 831.6	50 868.4	50 868.1	50 814.1

First ionization potential

Model B

Th I :

- ❖ MR: $6d^2 7s^2, 6d^3 7s, 6d^4, 5f^2 6d 7s, 5f^2 6d^2, 5f^2 7s^2 \Rightarrow 128$ CSFs;
- ❖ Same active set

Th II :

- ❖ MR: $6d 7s^2, 6d^2 7s, 6d^3, 5f^2 7s, 5f^2 6d \Rightarrow 29$ CSFs;
- ❖ Same active set

IP1 MR	IP1(1)	IP1(2)	IP1(3)	IP1(4)	IP1(CV)	IP1(CC)	Exp	NIST	Weigand
41 553.0	42 017.2	42 157.0	48 281.3	48 907.6	47 923.4	46 860.0	50 868.4	50 868.1	50 814.1

Model C

Th I :

- ❖ MR: $6d^2 7s^2, 6d^3 7s, 6d^4, 5f^2 6d 7s, 5f^2 6d^2, 5f^2 7s^2, 5f 6d^2 7p, 5f 6d 7s 7p, 5f 7s^2 7p \Rightarrow 254$ CSFs;
- ❖ Same active set

Th II :

- ❖ MR: $6d 7s^2, 6d^2 7s, 6d^3, 5f^2 7s, 5f^2 6d, 5f 6d 7p, 5f 7s 7p \Rightarrow 52$ CSFs;
- ❖ Same active set

IP1 MR	IP1(1)	IP1(2)	IP1(3)	IP1(4)	IP1(CV)	IP1(CC)	Exp	NIST	Weigand
44 592.3	48 010.8	48 093.7	48 424.6	49 236.2	47 330.7	45 591.0	50 868.4	50 868.1	50 814.1

Model D

Th I :

- ❖ MR: $6d^2 7s^2, 6d^3 7s, 6d^4, 5f^2 6d 7s, 5f^2 6d^2, 5f^2 7s^2, 5f 6d^2 7p, 5f 6d 7s 7p, 5f 7s^2 7p \Rightarrow 254$ CSFs;
- ❖ VV1: SD {MR} $\rightarrow \{7s, 7p, 6d, 5f, 5g\} \Rightarrow 1242$ CSF
- ❖ VV2: SD {MR} $\rightarrow \{7s, 7p, 6d, 6f, 6g, 6h\} \Rightarrow 7366$ CSFs;
- ❖ VV3: SD {MR} $\rightarrow \{7s, 7p, 7d, 7f, 7g, 7h\} \Rightarrow 23\,085$ CSFs;
- ❖ VV4: SD {MR} $\rightarrow \{8s, 8p, 8d, 8f, 8g, 8h\} \Rightarrow 53\,545$ CSFs;
- ❖ VV5: SD {MR} $\rightarrow \{9s, 9p, 9d, 9f, 9g, 9h\} \Rightarrow 96\,812$ CSFs;
- ❖ VV6: SD {MR} $\rightarrow \{10s, 10p, 10d, 10f, 10g, 10h\} \Rightarrow 152\,886$ CSFs;
- ❖ CV: S {6s,6p} $\rightarrow$ MR $\Rightarrow 157\,930$ CSFs
- ❖ CC: SD {6s,6p} $\rightarrow$ MR $\Rightarrow 210\,849$ CSFs

Th II :

- ❖ MR: $6d 7s^2, 6d^2 7s, 6d^3, 5f^2 7s, 5f^2 6d, 5f 6d 7p, 5f 7s 7p \Rightarrow 52$ CSFs;
- ❖ VV1: SD {MR} $\rightarrow \{7s, 7p, 6d, 5f, 5g\} \Rightarrow 131$ CSF
- ❖ VV2: SD {MR} $\rightarrow \{7s, 7p, 6d, 6f, 6g, 6h\} \Rightarrow 589$ CSFs;
- ❖ VV3: SD {MR} $\rightarrow \{7s, 7p, 7d, 7f, 7g, 7h\} \Rightarrow 1712$ CSFs;
- ❖ VV4: SD {MR} $\rightarrow \{8s, 8p, 8d, 8f, 8g, 8h\} \Rightarrow 3859$ CSFs;
- ❖ VV5: SD {MR} $\rightarrow \{9s, 9p, 9d, 9f, 9g, 9h\} \Rightarrow 6892$ CSFs;
- ❖ VV6: SD {MR} $\rightarrow \{10s, 10p, 10d, 10f, 10g, 10h\} \Rightarrow 10\,881$ CSFs;
- ❖ CV: S {6s,6p} $\rightarrow$ MR $\Rightarrow 12\,085$ CSFs
- ❖ CC: SD {6s,6p} $\rightarrow$ MR $\Rightarrow 27\,890$ CSFs

IP1 MR	IP1(1)	IP1(2)	IP1(3)	IP1(4)	IP1(5)	IP1(6)	IP1(CV)	IP1(CC)	Exp
44 592.3	48 010.8	48 202.9	48 519.0	49 327.3	49 394.2	49 406.2	47 789.8	46 306.4	50 868.4

First ionization potential

Model E

Th I :

- ❖ MR: $6d^2 7s^2, 6d^3 7s, 6d^4, 5f^2 6d 7s, 5f^2 6d^2, 5f^2 7s^2, 5f 6d^2 7p, 5f 6d 7s 7p, 5f 7s^2 7p \Rightarrow 254$ CSFs;

❖ VV1-VV6: SDTQ {MR} $\rightarrow$ active set ($n_{\max} l_{\max} = 10h$)

- ❖ CV: S {6s,6p} $\rightarrow$ MR $\Rightarrow 2\,939\,952$ CSFs
reducing to 157 258 CSF

Th II :

- ❖ MR: $6d 7s^2, 6d^2 7s, 6d^3, 5f^2 7s, 5f^2 6d, 5f 6d 7p, 5f 7s 7p \Rightarrow 52$ CSFs;

❖ VV1-VV6: SDTQ {MR} $\rightarrow$ active set ($n_{\max} l_{\max} = 10h$)

❖ CV: S {6s,6p} $\rightarrow$ MR $\Rightarrow 28\,424$ CSFs

IP1 MR	IP1(1)	IP1(2)	IP1(3)	IP1(4)	IP1(5)	IP1(6)	IP1(CV)	Exp	NIST
44 592.3	48 017.6	48 210.5	48 538.8	49 324.3	49 390.4	49 402.4	47 786.7	50 868.4	50 868.1

Model F

Th I :

- ❖ CV: SDr {MR} $\rightarrow \{8s, 8p, 8d, 8f, 8g, 8h\} \Rightarrow 2\,490\,400$ CSFs

Th II :

- ❖ CV: SDr {MR} $\rightarrow 8s, 8p, 8d, 8f, 8g, 8h \Rightarrow 324\,348$ CSFs

IP1(4) (model E)	IP1(SDr4) (model F)	IP1(SDr5) (model F)	Exp	NIST
49 324.3	49 519.7	In progress	50 868.4	50 868.1