Three-Body $Cs(H_2,\gamma)La$ Nuclear Synthesis in Cuboctahedron CsH_2Pd_{12}

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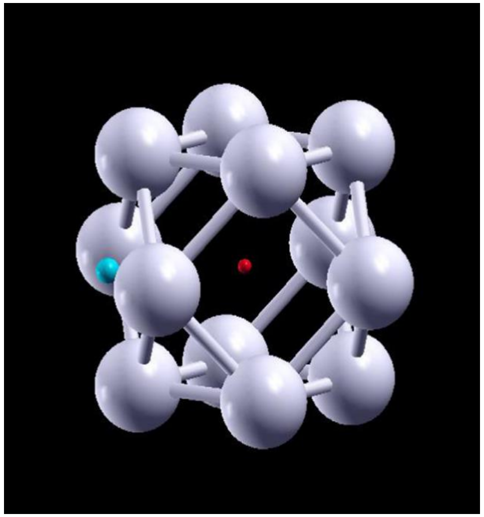
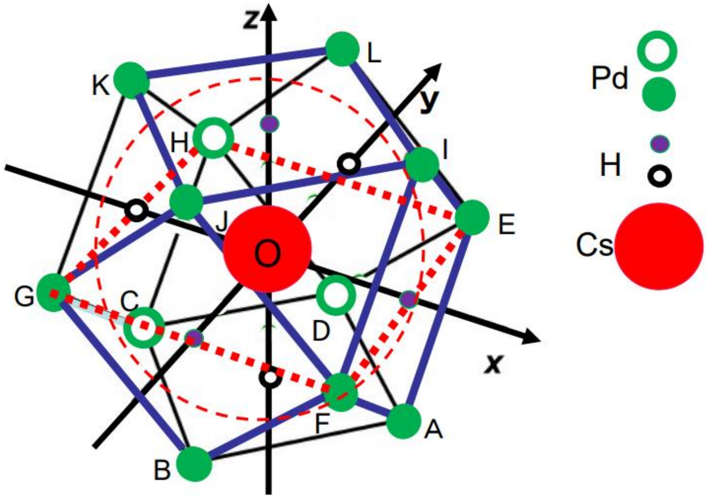
Cs+H+H three-body calculation in cuboctahedron twelve Pd cluster.





R_{pd}=2.75 Å , R_H=1.75 Å , a_{Cs}=2.65 Å ,   Z: electron number: 55+6+12x46=613

$\boxed{{}^{133}_{55}Cs} + \boxed{2T} \rightarrow \boxed{{}^{139}_{57}La}$, $\boxed{{}^{135}_{55}Cs}$ + 2D $\rightarrow \boxed{{}^{139}_{57}La}$, $\boxed{{}^{137}_{55}Cs}$ +2p $\rightarrow \boxed{{}^{139}_{57}La}$,

Life time: 12.33y 2.3×10^6y   30.07y

$$
\begin{aligned}
H &= K_{12\mathrm{Pd}} + K_{3\mathrm{N}} + V_{3\mathrm{N}}^{had} + V_t \\
&\quad + (K_{\mathrm{Zel}} + V_{3\mathrm{N}}^{C} + V_{\mathrm{PdN}}^{C} + V_{\mathrm{ZelPd}}^{M} + V_{\mathrm{ZelN}}^{M} + V_{\mathrm{el-el}}^{M}) \\
&= K_{12\mathrm{Pd}} + K_{3\mathrm{N}} + V_{3\mathrm{N}}^{had} + V_t + \boxed{H_{el}^{M}}
\end{aligned}
$$

Cs+H+H three-ion Hamiltonian:

$$
\begin{aligned}
H &\approx \boxed{K_{rel}} + V_{3\mathrm{N}}^{had} + V_t + V_{3\mathrm{N}}^{C} + V_{\mathrm{PdN}}^{C} + \boxed{V_{\mathrm{ZelN}}^{M}} \\
&\quad + (\langle \boxed{K_{\mathrm{Zel}}} \rangle + \boxed{\langle V_{\mathrm{ZelPd}}^{M} \rangle + \langle V_{\mathrm{el-el}}^{M} \rangle}), \\
&= \boxed{K_{rel}} + \underset{\textcircled{1}}{V_{3\mathrm{N}}^{had}} + \underset{\textcircled{2}}{V_t} + \underset{\textcircled{3}}{V_{3\mathrm{N}}^{C}} + \underset{\textcircled{4}}{V_{\mathrm{PdN}}^{C}} + \boxed{\underset{\textcircled{5}}{\overline{V}_{\mathrm{ZelN}}^{M}},}
\end{aligned}
$$

Cs+H+H molecular Hamiltonian:

$$
H_{el}^{M} = \boxed{K_{\mathrm{Zel}}} + V_{3\mathrm{N}}^{C} + V_{\mathrm{PdN}}^{C} + \boxed{\underset{\textcircled{5}Z_{\text{Zel-N}}}{V_{\mathrm{ZelN}}^{M}} + \underset{\textcircled{5}_{\text{Zel-Pd}}}{V_{\mathrm{ZelPd}}^{M}} + \underset{\textcircled{5}_{\text{el-el}}}{V_{\mathrm{el-el}}^{M}},}
$$

① $$V_{3N}^{had}(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3) = [\overset{\text{①R}}{V_N^{\mathrm{Csd_1}}(\boldsymbol{r}_{31})} + \overset{\text{①R}}{V_N^{\mathrm{Csd_2}}(\boldsymbol{r}_{23})} + \overset{\text{①R}}{V_N^{\mathrm{d_1d_2}}(\boldsymbol{r}_{12})}]$$

③ $$V_{3N}^{C}(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3) = [\underset{\text{③R}}{V_c^{\mathrm{Csd_1}}(\boldsymbol{r}_{31})} + \underset{\text{③R}}{V_c^{\mathrm{Csd_2}}(\boldsymbol{r}_{23})} + \underset{\text{③R}}{V_c^{\mathrm{d_1d_2}}(\boldsymbol{r}_{12})}].$$

④ $$V_{\mathrm{PdN}}^{C}(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3) = \underset{\text{④R}}{V_c^{\mathrm{PdCs}}(\boldsymbol{r}_3)} + \underset{\text{④R}}{V_c^{\mathrm{PdD_1}}(\boldsymbol{r}_1)} + \underset{\text{④R}}{V_c^{\mathrm{PdD_2}}(\boldsymbol{r}_2)},$$

Woods-Saxon potential

①R $$V_W^{\mathrm{N}_i\mathrm{N}_j}(\boldsymbol{r}_{ij}) = V_{W0}^{\mathrm{N}_i\mathrm{N}_j}\left[1 + \exp\left(\frac{r_{ij} - R_W^{\mathrm{N}_i\mathrm{N}_j}}{a_W^{\mathrm{N}_i\mathrm{N}_j}}\right)\right]^{-1},$$

$$V_{W0}^{\mathrm{CsD}} = -29.9\mathrm{MeV}, \quad R_W^{\mathrm{CsD}} = 7.6\mathrm{fm}, \quad a_W^{\mathrm{CsD}} = 0.8\mathrm{fm}$$

$$V_{W0}^{\mathrm{DD}} = -69.8\mathrm{MeV}, \quad R_W^{\mathrm{DD}} = 1.7\mathrm{fm}, \quad a_W^{\mathrm{DD}} = 0.4\mathrm{fm}.$$

TABLE II: Woods-Saxon potential was adopted A set of parameters: $V_{W0}^{\mathrm{N_iN_j}}$ [MeV], $R_{W0}^{\mathrm{N_iN_j}}$ [fm], and $a_{W0}^{\mathrm{N_iN_j}}$ [fm] are shown. A volume integral: $I(A_1, A_2) \equiv \int d^3r U_{A_1,A_2}(r)/(A_1 \times A_2) = 4\pi V_0 \int r^2 dr/\left[1 + \exp\{(r - R)/a\}\right]/(A_1 \times A_2)$ $\approx (4\pi/3)R^3 V_0\left[1 + (\pi a/R)^2\right]/(A_1 \times A_2)$ is defined by [MeV·fm^3] unit for nuclear mass numbers A_1 and A_2.

Systems	$V_0 \equiv V_{W0}^{\mathrm{N_iN_j}}$	$R \equiv R_{W0}^{\mathrm{N_iN_j}}$	$a \equiv a_{W0}^{\mathrm{N_iN_j}}$	I
^{133}Cs-^{3}H	-31.92(5)	7.6	0.8	-241.2
^{3}H-^{3}H	-41.34(0)	1.7	0.4	-328.9
^{135}Cs-^{2}H	-29.89(0)	7.6	0.8	-225.8
^{2}H -^{2}H	-69.80(0)	1.7	0.4	-554.7
^{137}Cs-^{1}H	-26.82(8)	7.6	0.8	-202.7

$$V_c^{N_iN_j}(r_{ij}) = \hbar c\alpha \frac{Z_iZ_j}{2R}\left[3-\left(\frac{r_{ij}}{R_c^{N_iN_j}}\right)^2\right] \qquad \text{for} \qquad r_{ij} \leqslant R_c^{N_iN_j}$$

$$= \hbar c\alpha \frac{Z_iZ_j}{r_{ij}} \qquad \text{for} \qquad R_c^{N_iN_j} < r_{ij}$$

where $\alpha = e^2/\hbar c = 1/137.0388$, $R_c^{\mathrm{CsD}} = 7.6\mathrm{fm} = R_W^{\mathrm{CsD}}$, and $R_c^{\mathrm{DD}} = 1.7\mathrm{fm} = R_W^{\mathrm{DD}}$ are taken.

For the N_i potential in the "electronic field", $\overline{V}^M_{\mathrm{ZelN}}$ is defined by two terms,

$$\overline{V}^M_{\mathrm{ZelN}}(r_1, r_2, r_3) = \boxed{\sum_{i=1}^{3} V_c^{\mathrm{Z_{Pd}N_i}}(r_i)} + \boxed{\sum_{i=1}^{3} V_c^{\mathrm{Z_{Cs}N}_i}(r_i),}$$

where the first term of the right hand side is the attractive potential between the effective electrons around Pd and ions (i.e., two hydrogens: $\mathrm{H}_{(1)}$,$\mathrm{H}_{(2)}$ and Cs) which is approximately defined by a Gauss type spherical shell structure,

$$\boxed{V_c^{\mathrm{Z_{Pd}N_i}}(r_i)} = Z_i v_c^{\mathrm{e(Pd)}} \exp[-a_c^{\mathrm{e(Pd)}}(r_i - r_c^{\mathrm{e(Pd)}})^2],$$

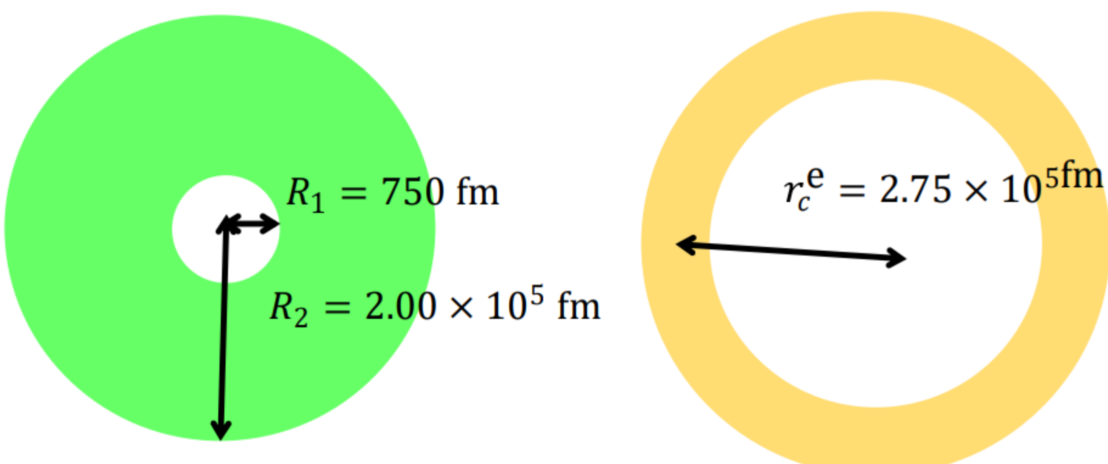
where the three parameters are fitted to reproduce the ground state energy of CsH_2 E^M_{gr}=-5.92eV and the first excited state $E^M_1 = 296.2\mathrm{eV}$. Therefore, the following parameters are selected

$$v_c^{\mathrm{e(Pd)}} = -1.204 \times 10^{-3}\mathrm{MeV}, \quad a_c^{\mathrm{e(Pd)}} = 2.415 \times 10^{-11}\mathrm{fm}^{-2}, \quad r_c^{\mathrm{e(Pd)}} = 8.19 \times 10^4\mathrm{fm}.$$

The second term is given by,

$$
\begin{aligned}
V_c^{\mathrm{Z_{Cs}N}_i}(\boldsymbol{r}_i) &= \hbar c\alpha(Z_{Cs}+2)Z_i\left[\frac{(R_1^2/2+R_1^2)}{R_2^3-R_1^3}-\frac{1}{R_2}-\frac{(R_2^2/2+R_1^3/R_2)}{R_2^3-R_1^3}\right] \\
&\qquad \text{for} \quad r_i \le R_1 \\
&= \hbar c\alpha(Z_{Cs}+2)Z_i\left[\frac{(r_i^2/2+R_1^3/r_i)}{R_2^3-R_1^3}-\frac{1}{R_2}-\frac{(R_2^2/2+R_1^3/R_2)}{R_2^3-R_1^3}\right] \\
&\qquad \text{for} \quad R_1 \le r_i \le R_2 \\
&= -\frac{\hbar c\alpha(Z_{Cs}+2)Z_i}{r_i} \qquad \text{for} \quad R_2 \le r_i,
\end{aligned}
$$

$$R_1 = 750\mathrm{fm}, \quad R_2 = 2\times 10^5\mathrm{fm}.$$



The uniform electron distribution around Cs is given on the left, while the electron distribution around 12Pd ions is portrayed by the ring of radius $R = 2.75$Å. Therefore the electron-Pd potential is given by a shallow pan type.

12 x N-Pd Coulomb potentials

$$
\begin{aligned}
V_c^{\mathrm{Pd_j N_i}}(r_i) &= \hbar c\alpha \frac{Z_i Z_{j(\mathrm{Pd})}}{2R_c^{\mathrm{Pd}}}\left[3 - \left(\frac{r_{ij}}{R_c^{\mathrm{Pd}}}\right)^2\right] && \text{for } \ r_{ij} \le R_c^{\mathrm{Pd}} \\
&= \hbar c\alpha \frac{Z_i Z_{j(\mathrm{Pd})}}{r_{ij}} && \text{for } \ R_c^{\mathrm{Pd}} < r_{ij}
\end{aligned}
$$

with R_c^{Pd}=5.561 fm,

The twelve Pd coordinates r_j for (x_j, y_j, z_j) are given by using $d = (2.75/\sqrt{2})$Å=1.94454Å.

j	1	2	3	4	5	6
(x, y, z)	$(0, d, d)$	$(0, -d, d)$	$(0, d, -d)$	$(0, -d, -d)$	$(d, 0, d)$	$(-d, 0, d)$

j	7	8	9	10	11	12
(x, y, z)	$(d, 0, -d)$	$(-d, 0, -d)$	$(d, d, 0)$	$(-d, d, 0)$	$(d, -d, 0)$	$(-d, -d, 0)$

A three-body force (potential) which can reproduce the La ground state energy.

In this paper, we adopt a $\boxed{\text{nuclear three-body potential}}$ of the form:

$$V_t(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3) = V_{t0} \exp\left[-\frac{r_{12}^2 + r_{23}^2 + r_{31}^2}{a_t{}^2} \right], \qquad V_{3BSF}$$

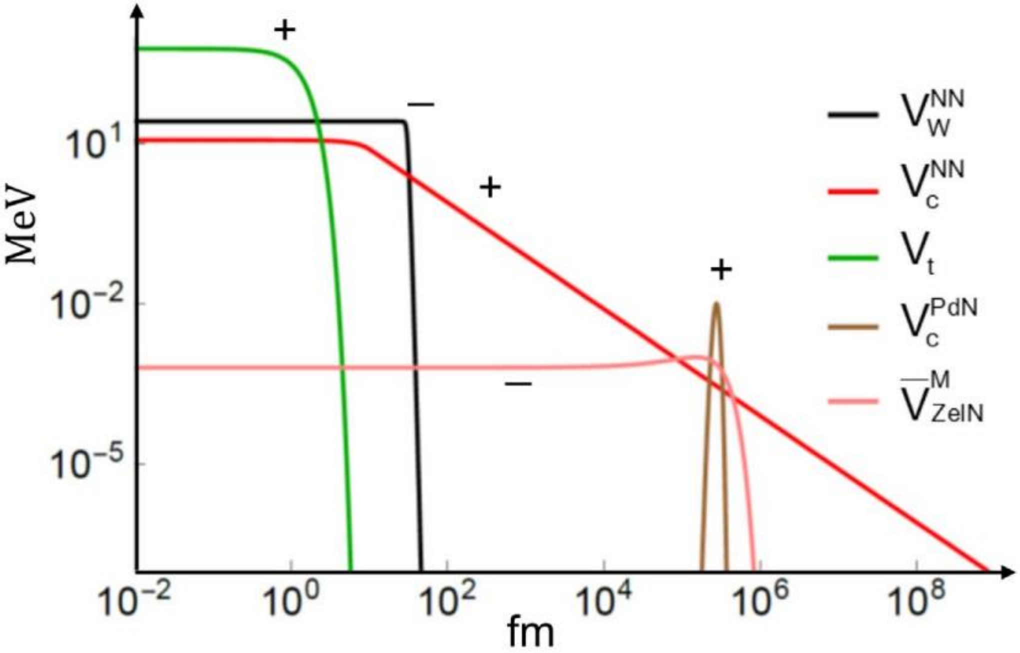
where $V_{t0} = 1720$ MeV and a_t=3.0fm are used to fit the ground state of La by adding the Coulomb force. We have obtained a very good fit to the experimental ground state energy $E_{gr}^{\mathrm{La}} = -25.92$ MeV, the root mean square (rms) radius $R_{rms}^{\mathrm{La}} = 6.388$ fm.

The sixth potential is a three-body long range hadron potential by the GPT theory,

$$V_{3\mathrm{GPT}}(r_1, r_2, r_3) \rightarrow V_{3\mathrm{BLF}}(r_1, r_2, r_3)$$

$$V_{3BLF} \qquad \approx \frac{Aa_e^2}{\left[r_{12}^2 + r_{23}^2 + r_{31}^2 + a_e^2\right]} + \frac{Ba_e^2}{\left[r_{12}^2 + r_{23}^2 + r_{31}^2 + 10a_e^2\right]}$$

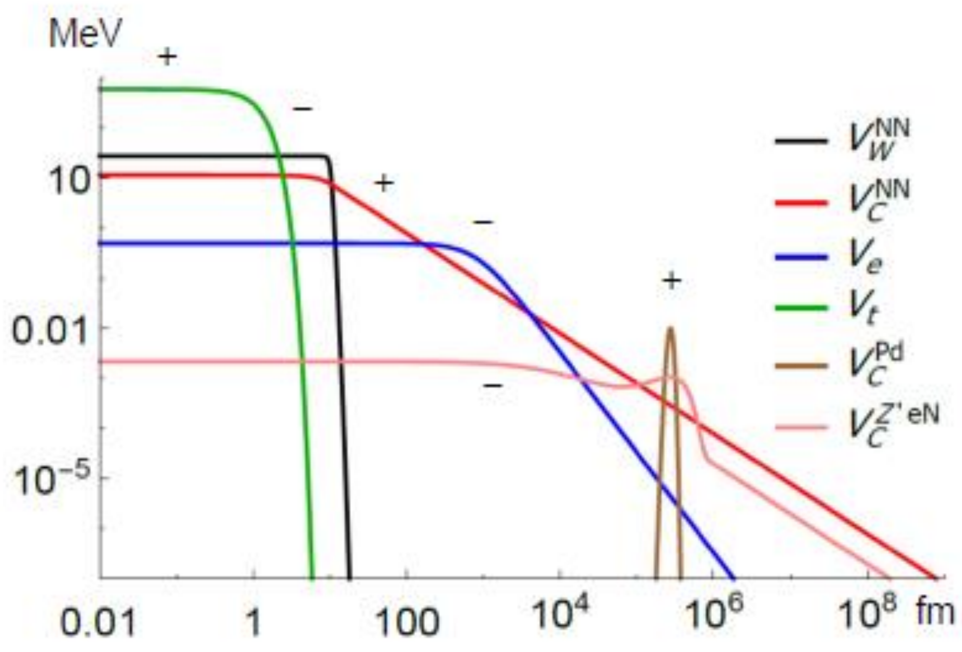
$$A = -0.5\mathrm{MeV},\ B = 0.5\mathrm{MeV},\ a_e = 2000\ \mathrm{fm},$$



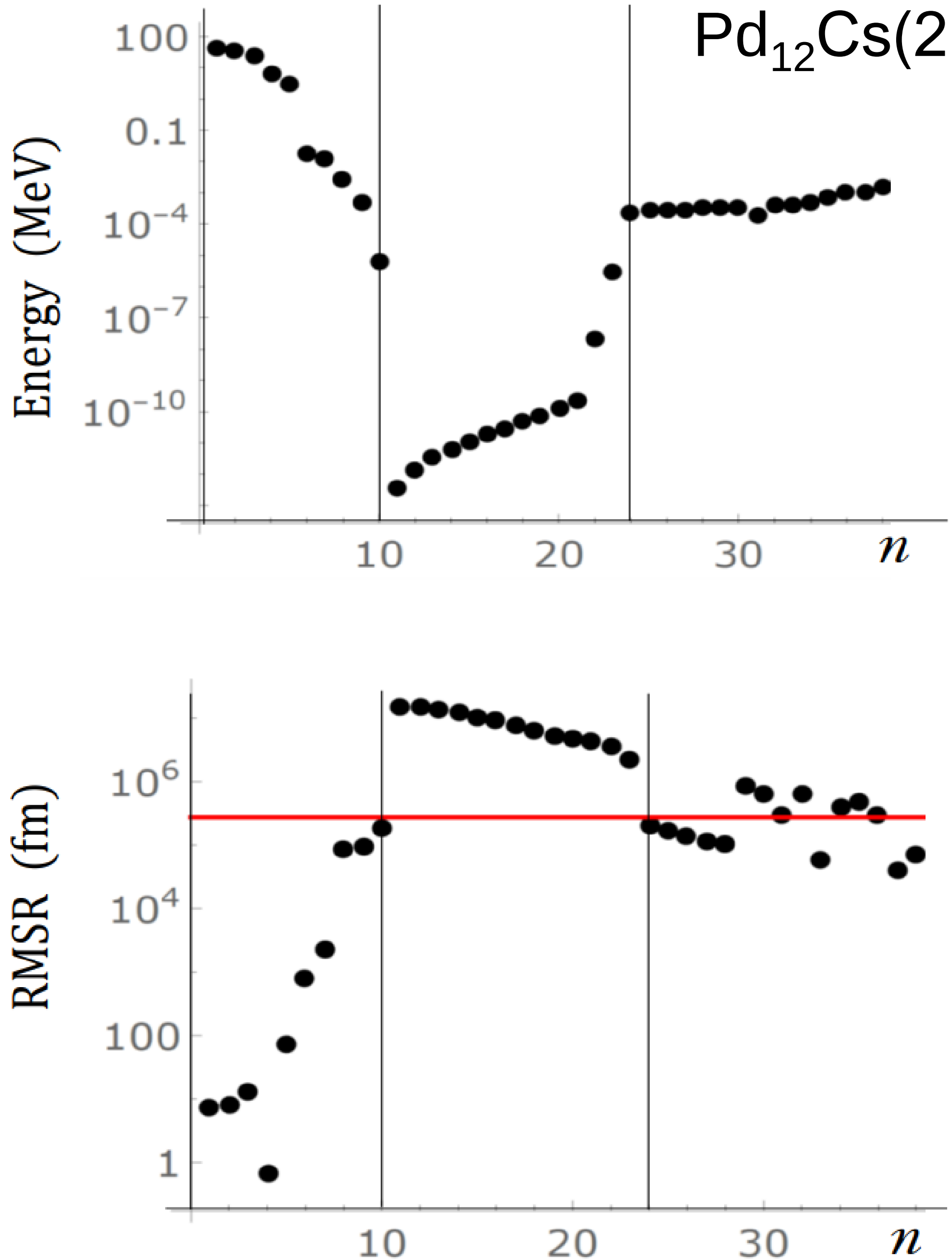
5-potentials

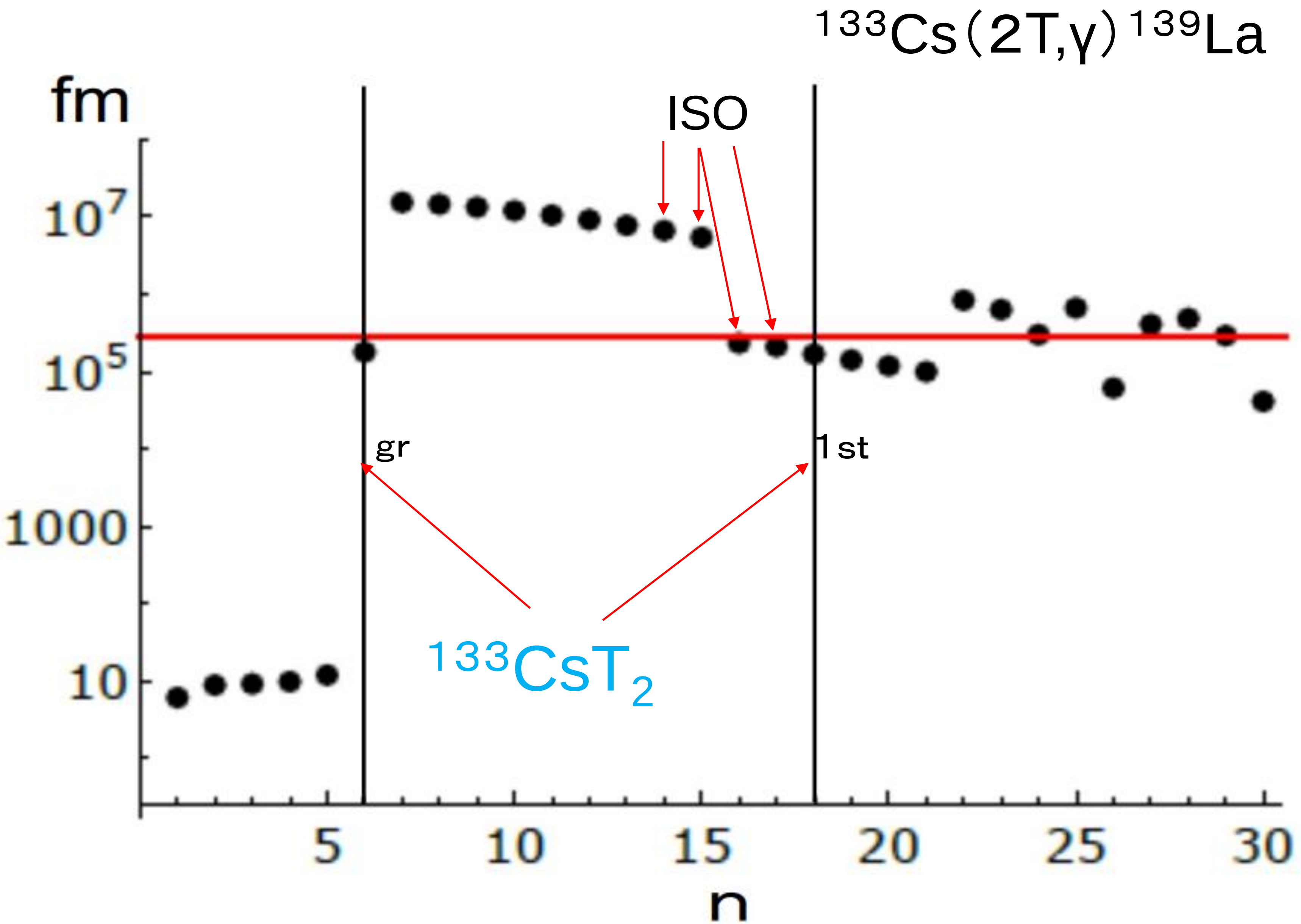
On the Cs-Pd axis

6-potentials



$Pd_{12}Cs(2D,\gamma)LaPd_{12}$





$^{133}Cs(2T,\gamma)^{139}La$
fm
ISO
10^7
10^5
1000
10
gr
1st
$^{133}CsT_2$
5
10
15
20
25
30
n

The E2 transition time $\tau_{if} = 1/W_{if}^{\mathrm{E2}}$ and the transition probability W_{if}^{E2} are defined by,

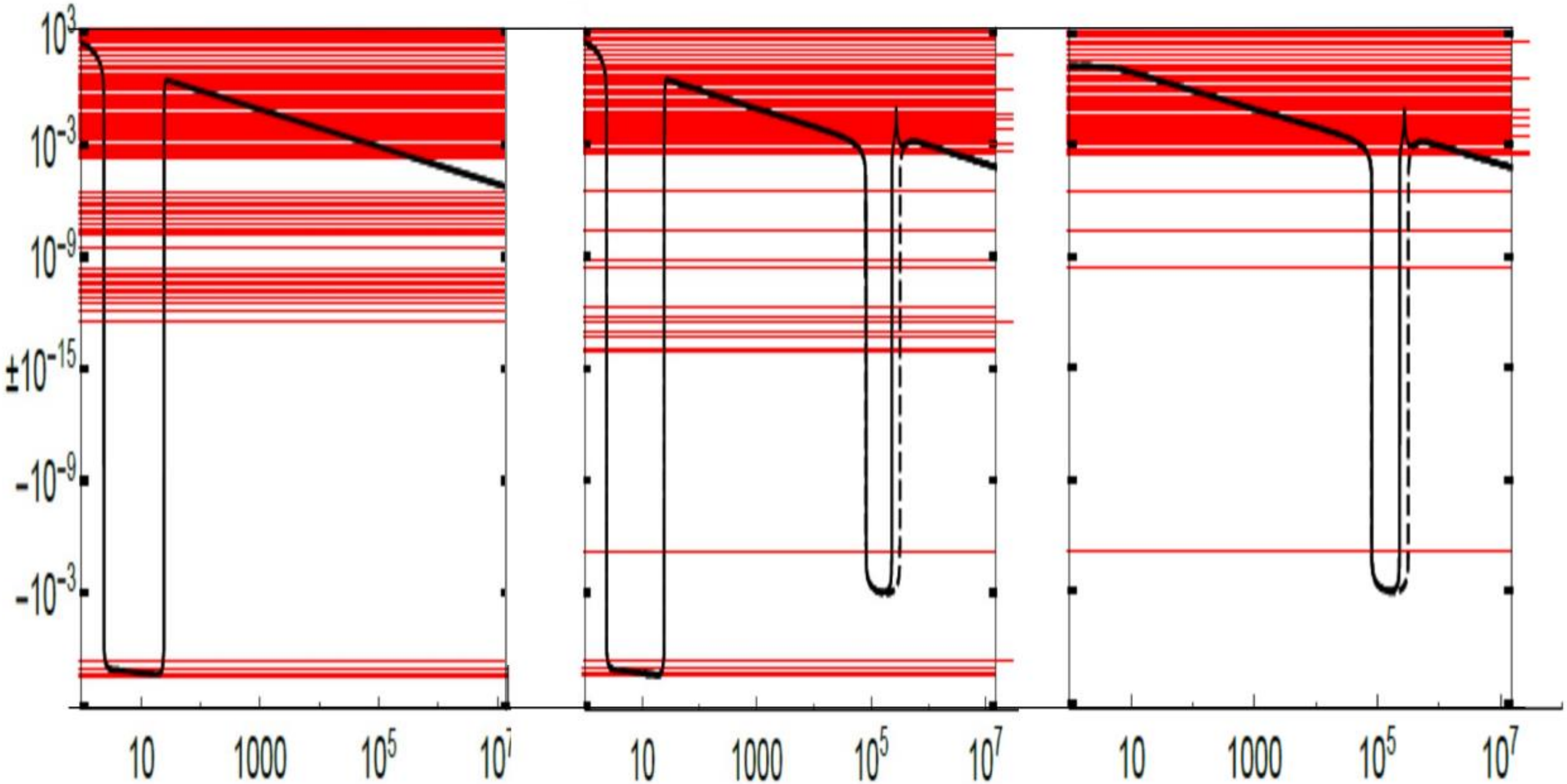
$$W_{if}^{\mathrm{E2}} = \frac{4\pi}{75\hbar}\Big(\frac{E_i - E_f}{\hbar c}\Big)^5 \sum_{\mu} | < \psi_f | \sum_{j=1}^{3} Z_j e r_j^2 Y_{2\mu}(\theta_j \phi_j) | \psi_i > |^2.$$

By using symmetry, we obtain

$$W_{if}^{\mathrm{E2}} = \frac{4\pi c}{15}\Big(\frac{E_i - E_f}{\hbar c}\Big)^5 \alpha \sum_{j=1}^{3} \Big| < \psi_f | \frac{1}{2}(2z_j^2 - x_j^2 - y_j^2) Z_j | \psi_i > \Big|^2$$

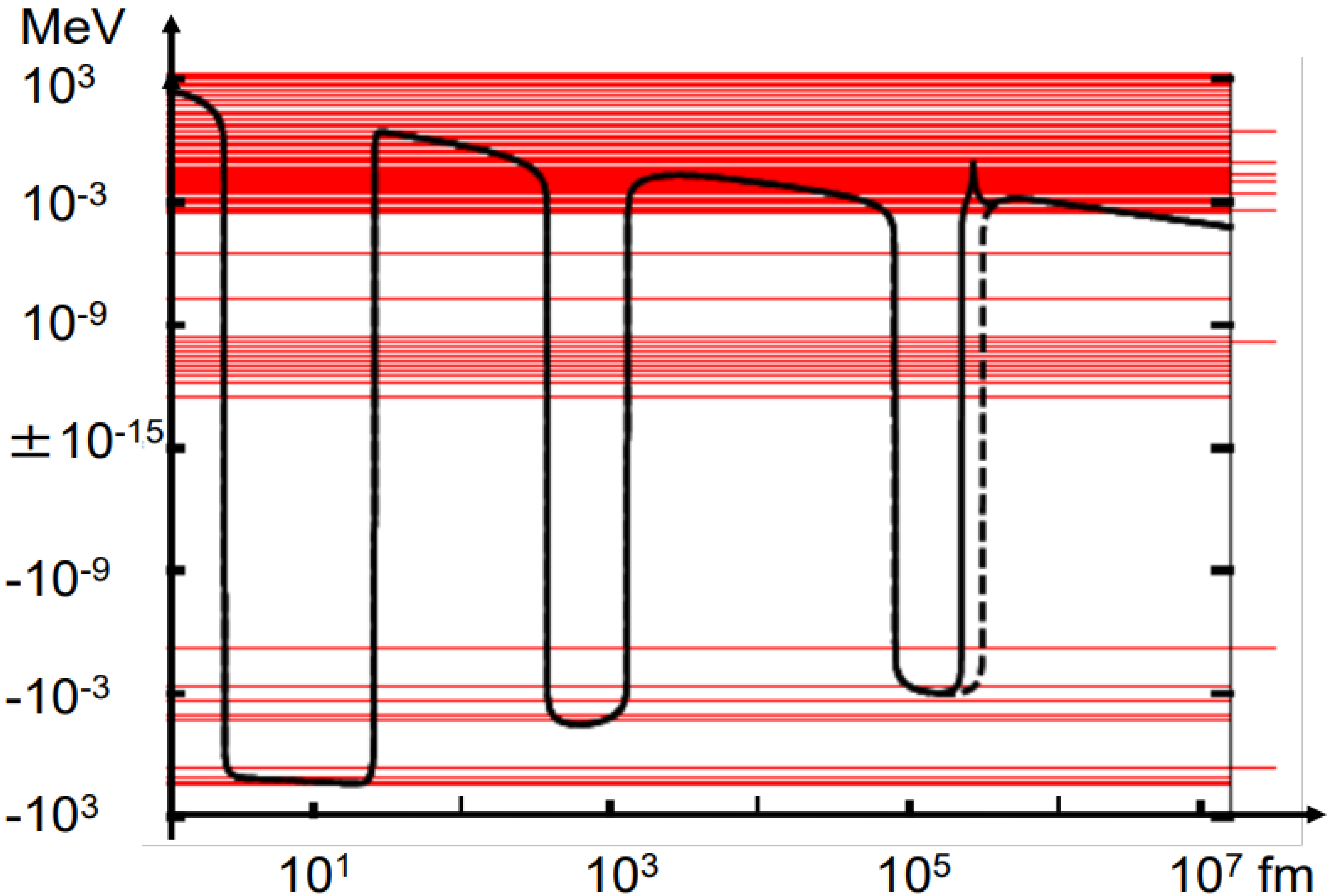
by using $(2z_j^2 - x_j^2 - y_j^2) \rightarrow r_j^2$,

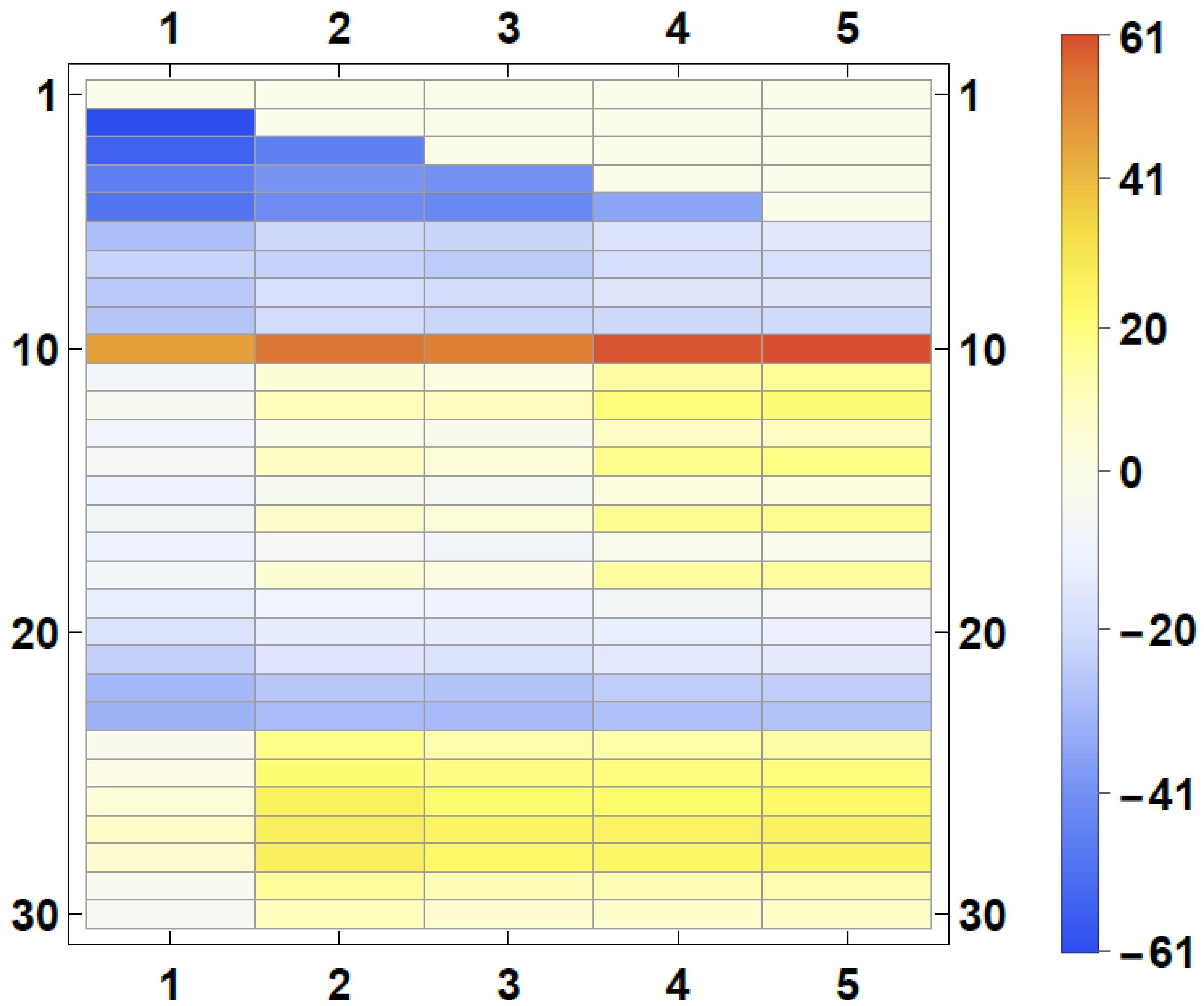
$$W_{if}^{\mathrm{E2}} \rightarrow W_{if}^{\mathrm{E2}\prime} = \frac{4\pi c}{15}\Big(\frac{E_i - E_f}{\hbar c}\Big)^5 \alpha \sum_{j=1}^{3} \Big| < \psi_f | \frac{1}{2} r_j^2 Z_j | \psi_i > \Big|^2.$$



A B C

Nu clear System Total system Molecular System


MeV
10^3
10^{-3}
10^{-9}
$\pm 10^{-15}$
-10^{-9}
-10^{-3}
-10^3
10^1
10^3
10^5
10^7 fm


1 2 3 4 5
1
10
20
30
61
41
20
0
−20
−41
−61

Critical Reaction Value:

C_{low} (in molecular system) = $t \times \rho \times T$

C_{high} (Thermo-nuclear fusion) = $t \times \rho \times T$

$C_{low}(n)$	duration time t[sec]	ρ [cm^{-3}]	T [eV]	$t\rho T$ [sec $\cdot$ eV/cm^3]	$t\rho T$ [sec$\cdot$ Pa]	transition time τ[sec]
$C_{low}(23)$	1.0	3.44×10^{22}	3.18	1.09×10^{23}	1.75×10^{10}	7.36×10^{-8}
$C_{low}(22)$	1.0	3.44×10^{22}	2.05×10^{-2}	7.05×10^{20}	1.13×10^{8}	1.02×10^{-6}
C_{high}	1.0	3.30×10^{14}	5.17×10^{4}	1.71×10^{19}	2.73×10^{7}	—
$C_{low}(21)$	1.0	3.44×10^{22}	2.40×10^{-4}	8.26×10^{18}	1.32×10^{6}	4.23×10^{-4}
$C_{low}(20)$	1.0	3.44×10^{22}	1.36×10^{-4}	4.68×10^{18}	7.50×10^{5}	1.92×10^{-2}

ρ : density

T : temperature or energy

t : duration time

Summary

1) Cs+H+H three-ion calculation in a Cuboctahedron CsH_2Pd_{12} cluster
2) Used potentials: 5 and 6
   ①Nuclear CsHH, ②Coulomb CsHH,
   ③Coulomb (Cs,H,H)-12Pd, ④Nuclear three-body short range force CsHH, ⑤ electrons-(Cs,H, Pd, and electron),

   where to freeze electron degree's of freedom fitted to gr. 1st CsH_2 molecular states by the Kohn-Sham equation or the ADF (Amsterdam density functional) package.

3) The 6th potential is the hadron three-body long range potential by the general particle transfer (GPT) method.

4) Calculation is done from 0.01fm to several ten nm region in one stretch with 100-figures accuracy.

5) Obtained 4 ion-oscillation (IOS) states
between gr and 1st states.

6) IOS states strongly interfere with the three-nuclear
resonance states of La* and go down to La ground state.

7) In order to compare the thermal nuclear fusion,
a critical value C= t x ρ x T was compered
between thermo- and ultra-low energy nuclear syntheses
(ULNS).

8) They are almost the same, because the density of
thermonuclear synthesis is $3.30\times10^{14}/cm^3$
While the cuboctahedron is $3.44\times10^{22}/cm^3$,
However, the energy is 5.17×10^4eV in the former case,
but 3.18eV in the latter case.

$C_{high}=2.73\times10^7$[sec・Pa] vs $C_{low}=1.75\times10^{10}$ [sec・Pa].

Therefore, ULNS could be easily controlled by saving energy.

Thank you very much for your attention

Molecular Hamiltonian, for 609-electrons could be solved by the Khon-Sham equation or the ADF (Amsterdam density functional) package.

$$H_{el}^{M} = K_{\mathrm{Zel}} + V_{\mathrm{3N}}^{C} + V_{\mathrm{PdN}}^{C} + V_{\mathrm{ZelN}}^{M} + V_{\mathrm{ZelPd}}^{M} + V_{\mathrm{el-el}}^{M},$$

Therefore, the ground state energy of CsH_2 in the cluster is calculated by the ADF, as

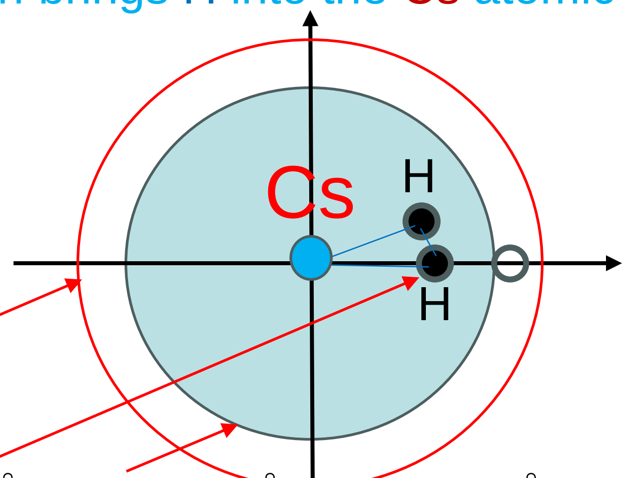
$$\boxed{E_{\mathrm{CsH_2}} = E_{\mathrm{Pd_{12}CsH_2}} - E_{\mathrm{Pd_{12}}},} \tag{A.3}$$

where the value $E_{\mathrm{CsH_2}}^{gd} = -5.9155$ eV is obtained, and the first excited state becomes 302 eV above the ground state, while the ground state energy in the free space is -4.4601eV.

Therefore, in CsH_6Pd_{12}

5.9155-4.4601=1.4554eV

deeper binding energy in the cage, which brings H into the Cs atomic radius by



In CsH_6Pd_{12} R_{pd}=2.75 Å , R_H=1.75 Å , a_{Cs}=2.65 Å , 2.65 Å - 1.75 Å =0.9 Å

Table 2. Some reaction types and separation energies by the mass relation using table 1 with [MeV] unit. The separation energies with sign (*) are used in this paper. CsD_2Pd_{12} case

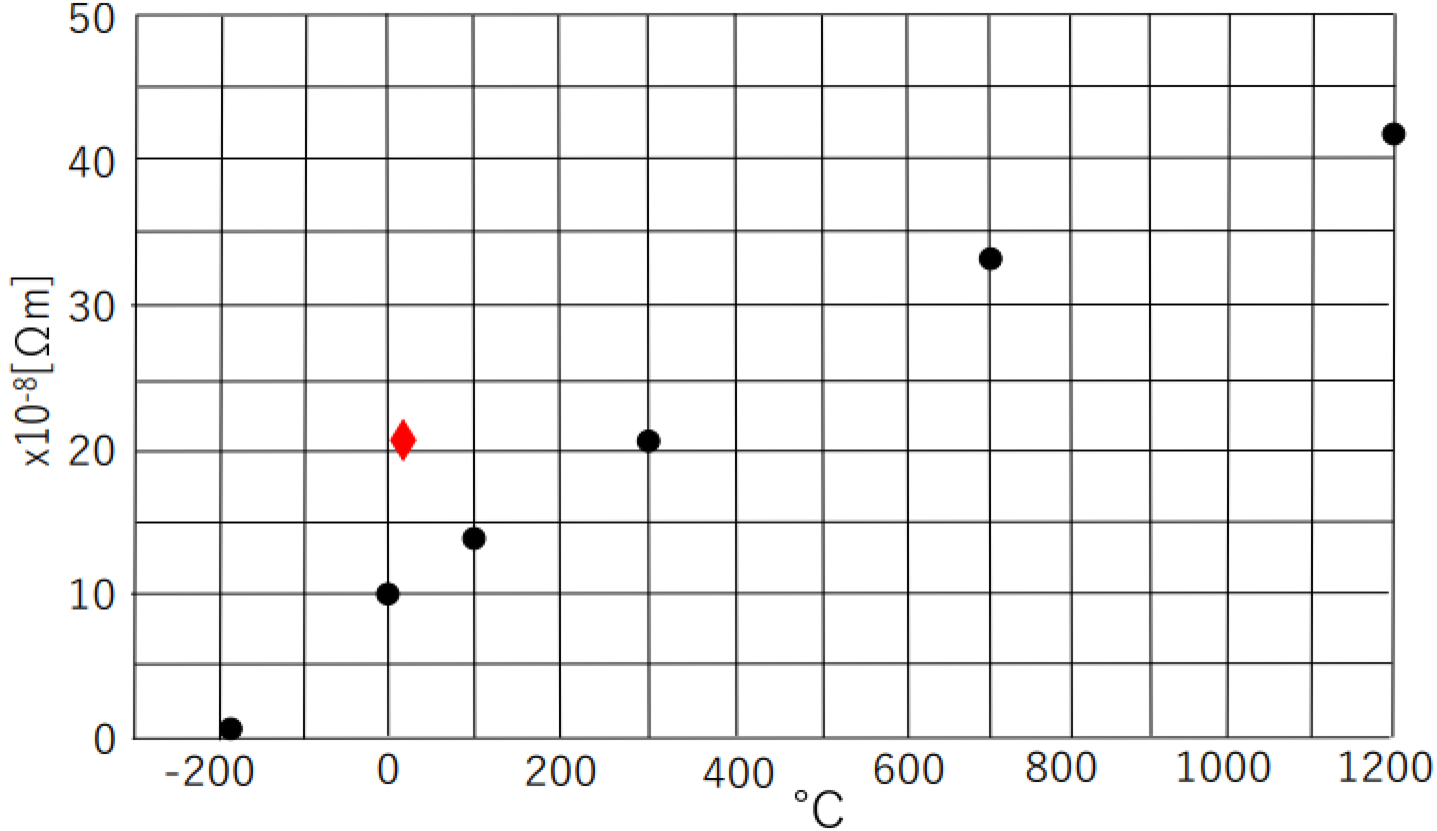
Ions	Separation type	Separation energy	[MeV]
^{2}H	p–n	$m_p + m_n - m_{^2H}$	2.224(0)
^{4}He	^{2}H-^{2}H	$2 \times m_{^2H} - m_{^4He}$	23.84(7)*
^{135}Ba	^{2}H-^{133}Cs	$m_{^2H} + m_{^{133}Cs} - m_{^{135}Ba}$	12.91(6)
^{137}La	^{2}H-^{2}H-^{133}Cs	$2 \times m_{^2H} + m_{^{133}Cs} - m_{^{137}La}$	25.32(7)
^{137}Ba	^{2}H-^{135}Cs	$m_{^2H} + m_{^{135}Cs} - m_{^{137}Ba}$	13.27(6)*
^{139}La	^{2}H-^{2}H-^{135}Cs	$2\times m_{^2H} + m_{^{135}Cs} - m_{^{139}La}$	25.92(1)*
^{139}Ba	^{2}H-^{137}Cs	$m_{^2H} + m_{^{137}Cs} - m_{^{139}Ba}$	11.50(4)
^{141}La	^{2}H-^{2}H-^{137}Cs	$2\times m_{^2H} + m_{^{137}Cs} - m_{^{141}La}$	22.66(4)

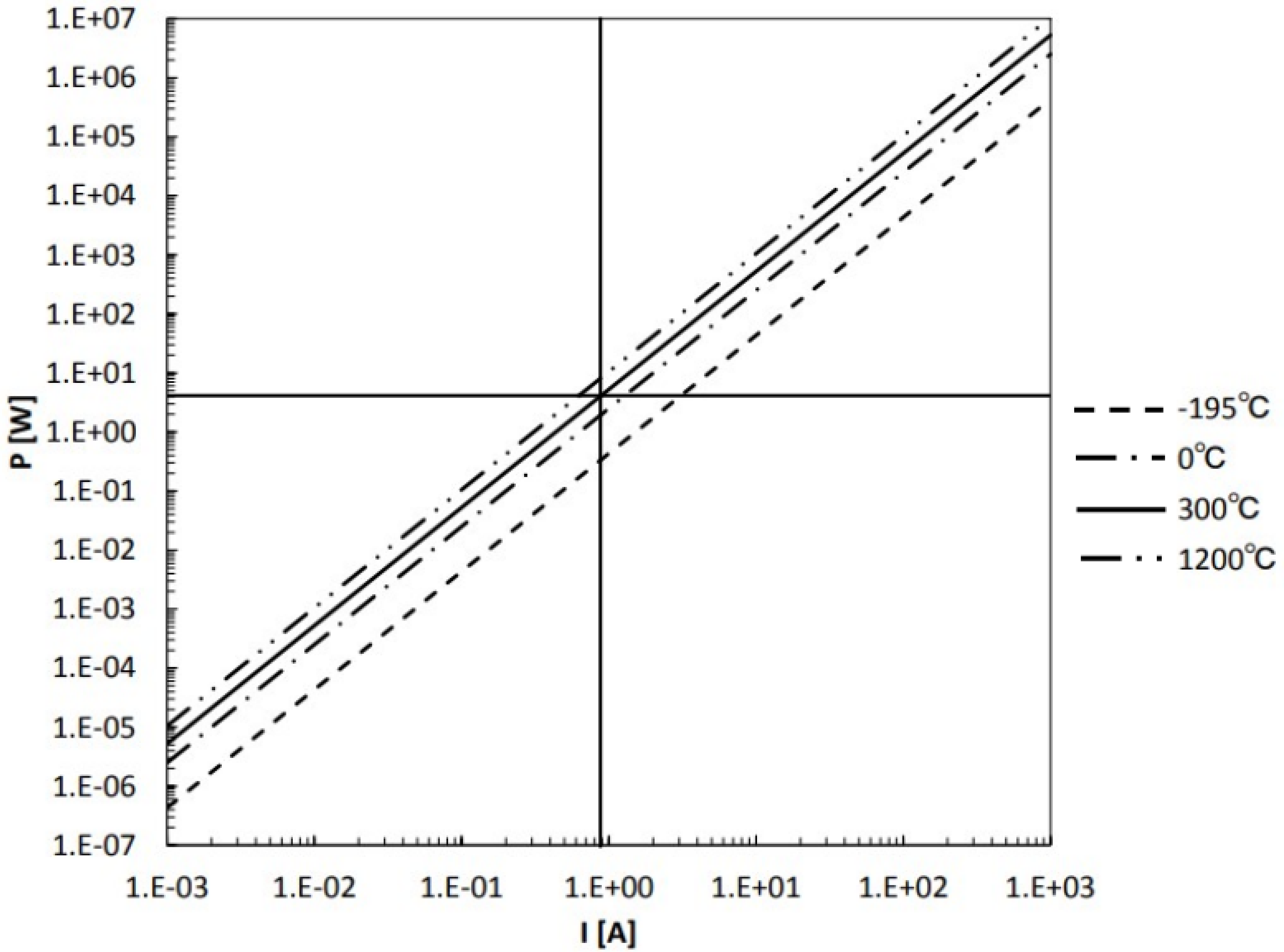
Table 3. Calculated two-body separation energies of ^{4}He and ^{137}Ba with d-d and Cs-d models are given by using the WS potentials with the above mentioned parameters and the Coulomb potentials, where the ground states are fitted with the experimental separation energies $E_1 = E_1^{exp}$ (see table 2). The ground state energy of ^{139}La by Cs-d-d separation model is calculated by above mentioned five potentials and fitted by using the three-body force. E_2, E_3, E_4 and E_5 are excited states. It should be reminded that these results are obtained only by the central force of the WS potential.

Nucleus	Separation	E_1 [MeV]	E_2 [MeV]	E_3 [MeV]	E_4 [MeV]	E_5 [MeV]
$^{4}_{2}$He	d-d	−23.85				
$^{137}_{56}$Ba	Cs-d	−13.28	−9.57	−1.98		
$^{139}_{57}$La	Cs-d-d	-25.92	-23.51	-19.02	-11.59	-3.92

n	1	2	3	4	5	6^*	7	8	9
E_n(MeV)	-29.12	-26.37	-22.03	-12.10	-4.10	-5.9×10^{-6}	1.0×10^{-15}	5.0×10^{-15}	1.0×10^{-14}
RMS(fm)	6.16	8.92	9.27	9.88	12.03	1.80×10^{5}	1.5×10^{7}	1.5×10^{7}	1.3×10^{7}
τ(sec)		1.4×10^{-18}	1.9×10^{-17}	2.5×10^{-15}	3.9×10^{-16}	3.7×10^{24}	7.3×10^{4}	2.4×10^{5}	1.8×10^{4}
n	10	11	12	13	14°	15°	16°	17°	18^{**}
E_n(MeV)	4.0×10^{-14}	1.0×10^{-13}	7.0×10^{-13}	1.8×10^{-12}	7.0×10^{-11}	2.8×10^{-10}	2.4×10^{-8}	3.1×10^{-6}	2.9×10^{-4}
RMS(fm)	1.2×10^{7}	1.1×10^{7}	9.2×10^{6}	7.8×10^{6}	6.7×10^{6}	5.4×10^{6}	2.3×10^{5}	2.1×10^{5}	1.7×10^{5}
τ(sec)	1.2×10^{5}	6.9×10^{3}	9.5×10^{4}	8.3×10^{4}	6.8×10^{-1}	1.5×10^{-2}	3.6×10^{-5}	2.6×10^{-6}	8.1×10^{5}
n	19	20	21	22	23	24	25	26	27
E_n(MeV)	3.6×10^{-4}	3.9×10^{-4}	4.0×10^{-4}	4.1×10^{-4}	4.1×10^{-4}	4.2×10^{-4}	4.5×10^{-4}	4.6×10^{-4}	5.3×10^{-4}
RMS(fm)	1.4×10^{5}	1.2×10^{5}	1.0×10^{5}	8.4×10^{5}	6.4×10^{5}	3.0×10^{5}	6.7×10^{5}	6.2×10^{4}	4.1×10^{5}
τ(sec)	2.3×10^{6}	4.7×10^{6}	7.0×10^{6}	5.5×10^{6}	5.3×10^{5}	1.7×10^{5}	4.1×10^{7}	4.7×10^{4}	7.5×10^{6}

n	1	2	3	4	5	6	7	8	9
E_n(MeV)	-29.12	-26.37	-22.03	-12.10	-4.10	-1.8×10^{-2}	-1.2×10^{-2}	-2.5×10^{-3}	-4.5×10^{-4}
RMS(fm)	6.16	8.92	9.27	9.88	12.0	8.1×10^{2}	2.1×10^{3}	8.7×10^{4}	9.0×10^{4}
τ(sec)		1.4×10^{-18}	1.9×10^{-17}	2.5×10^{-15}	3.9×10^{-16}	2.0×10^{-5}	7.6×10^{-4}	7.1×10^{-5}	3.5×10^{-5}
n	10^*	11	12	13	14	15	16	17	18
E_n(MeV)	-5.9×10^{-6}	3.3×10^{-13}	1.4×10^{-12}	3.3×10^{-12}	6.4×10^{-12}	1.1×10^{-11}	1.8×10^{-11}	3.0×10^{-11}	4.8×10^{-11}
RMS(fm)	1.8×10^{5}	1.5×10^{7}	1.5×10^{7}	1.3×10^{7}	1.2×10^{7}	1.1×10^{7}	9.2×10^{6}	7.8×10^{6}	6.7×10^{6}
τ(sec)	3.7×10^{24}	2.0×10^{3}	6.8×10^{3}	4.9×10^{2}	3.4×10^{3}	1.9×10^{2}	2.7×10^{3}	6.0×10^{1}	2.3×10^{3}
n	19	20°	21°	22°	23°	24^{**}	25	26	27
E_n(MeV)	7.7×10^{-11}	1.4×10^{-10}	2.4×10^{-10}	2.0×10^{-8}	3.2×10^{-6}	3.0×10^{-4}	3.1×10^{-4}	3.2×10^{-4}	3.3×10^{-4}
RMS(fm)	5.4×10^{6}	4.7×10^{6}	4.3×10^{6}	3.6×10^{5}	2.3×10^{5}	2.1×10^{5}	1.7×10^{5}	1.4×10^{5}	1.2×10^{5}
τ(sec)	7.2×10^{0}	1.9×10^{-2}	4.2×10^{-4}	1.0×10^{-6}	7.4×10^{-8}	2.3×10^{4}	6.5×10^{4}	1.3×10^{5}	2.0×10^{5}


50
40
30
20
10
0
x10⁻⁸[Ωm]
-200
0
200
400
600
800
1000
1200
°C


1.E+07
1.E+06
1.E+05
1.E+04
1.E+03
1.E+02
1.E+01
1.E+00
1.E-01
1.E-02
1.E-03
1.E-04
1.E-05
1.E-06
1.E-07
P [W]
1.E-03
1.E-02
1.E-01
1.E+00
1.E+01
1.E+02
1.E+03
I [A]
-195°C
0°C
300°C
1200°C

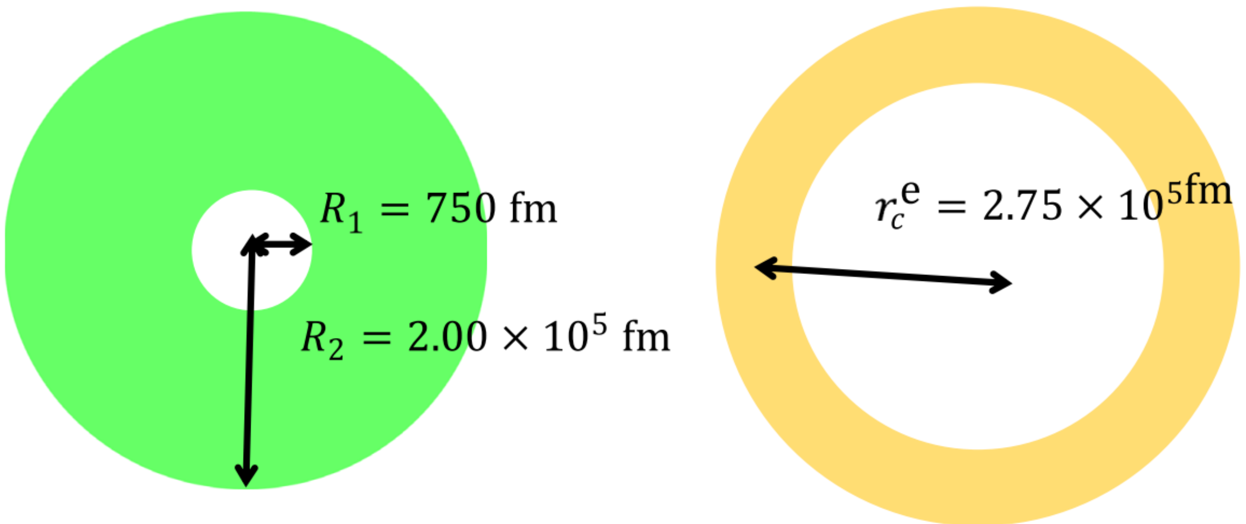
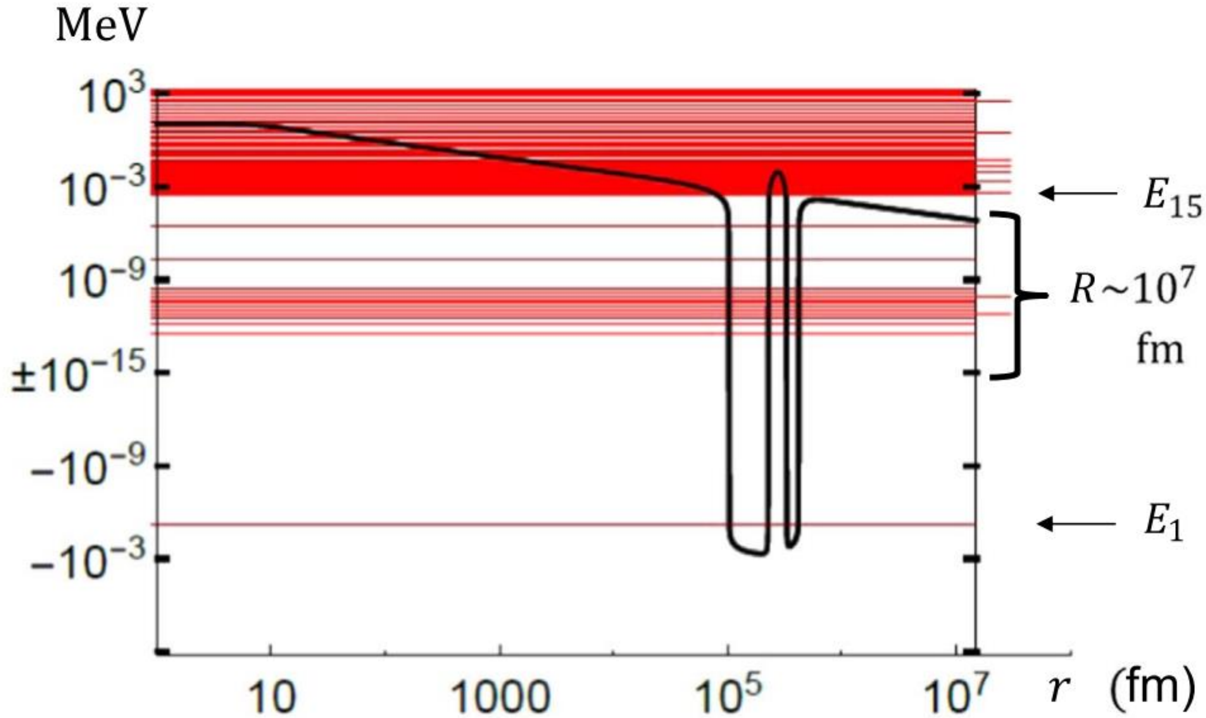
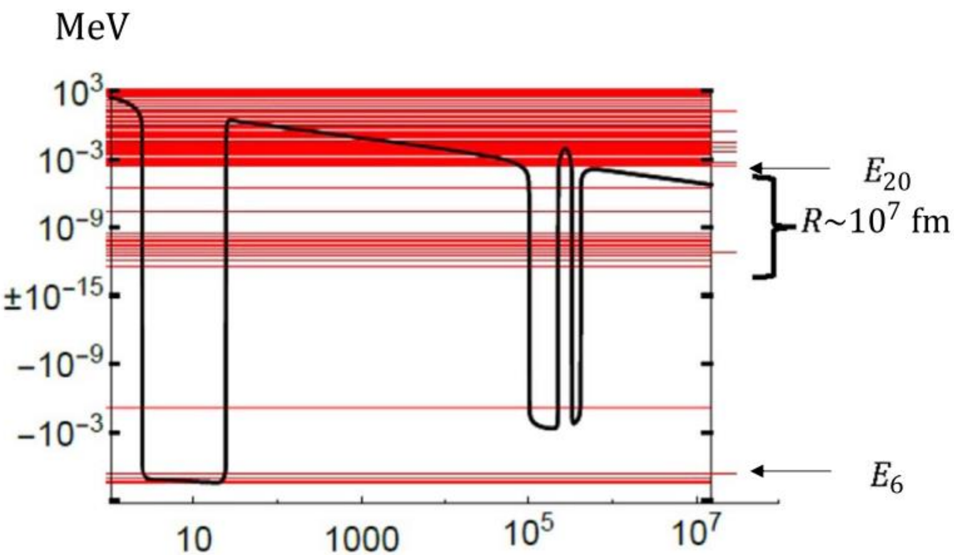


Figure 6. The uniform electron distribution around Cs is given on the left, while the electron distribution around 12Pd ions is portrayed by the ring of radius $R = 2.75\ \mathring{A}$. Therefore the electron-Pd potential is given by a shallow pan type.



$$E_1 = -5.92 \ \text{eV} \qquad E_{14} = 3.20 \ \text{eV}$$

$$E_{13} = 0.0206 \ \text{eV} \qquad E_{15} = 298 \ \text{eV}$$

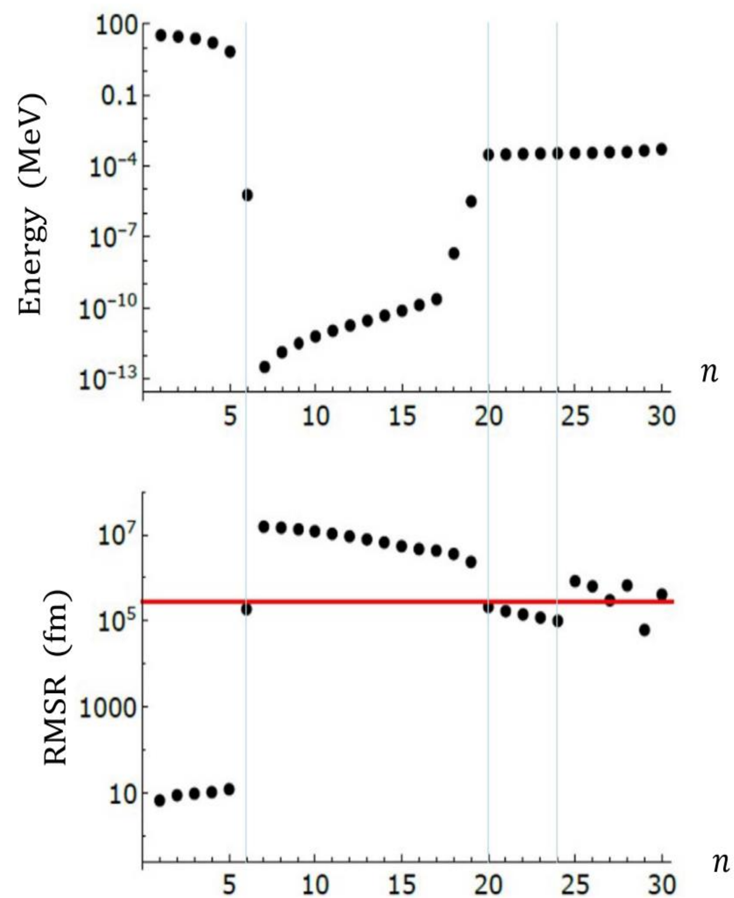


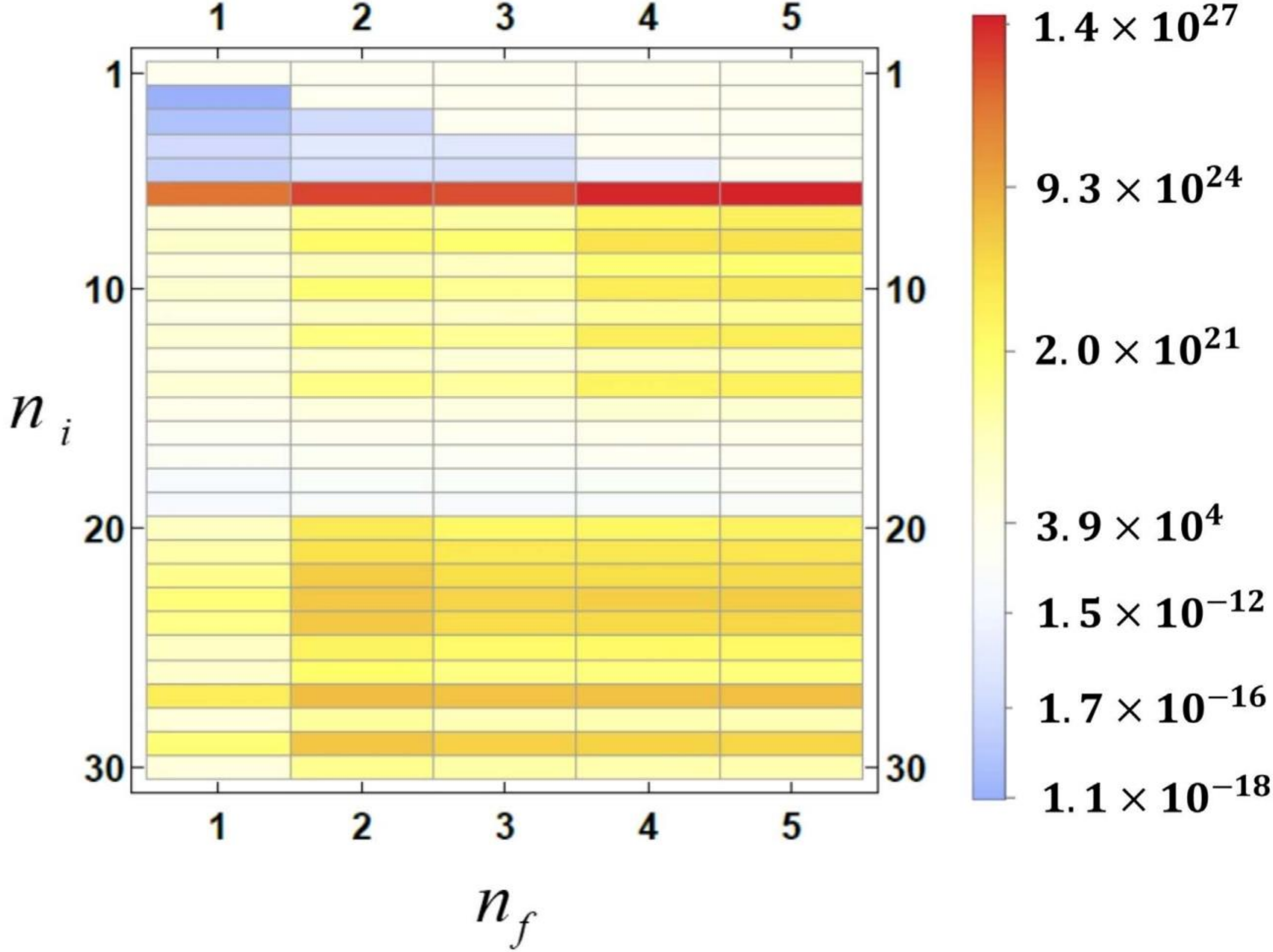
$E_6 = -5.92$ eV $\quad R_6 = 1.9 \times 10^5$ fm

$E_{20} = 296.22$ eV $\quad R_{20} = 2.1 \times 10^5$ fm

$E_{20} - E_6 = \Delta E = 302.14$ eV

$E_{18} = 2.05 \times 10^{-2}$ eV $\quad E_{19} = 3.19$ eV




1
2
3
4
5
1
10
20
30
n_i
n_f
1.4×10^{27}
9.3×10^{24}
2.0×10^{21}
3.9×10^{4}
1.5×10^{-12}
1.7×10^{-16}
1.1×10^{-18}

The second term is given by

⑤$_{\text{Zel-N}}$

$$\boxed{V_c^{\mathrm{Z_{Cs}N}_i}(\boldsymbol{r}_i)} = \hbar c\alpha Z_{Cs+1} Z_i \Big[\frac{(R_1^2/2 + R_1^2)}{R_2^3 - R_1^3} - \frac{1}{R_2} - \frac{(R_2^2/2 + R_1^3/R_2)}{R_2^3 - R_1^3}\Big] \quad \text{for} \quad r_i \le R_1 \tag{22}$$

$$= \hbar c\alpha Z_{Cs+1} Z_i \Big[\frac{(r_i^2/2 + R_1^3/r_i)}{R_2^3 - R_1^3} - \frac{1}{R_2} - \frac{(R_2^2/2 + R_1^3/R_2)}{R_2^3 - R_1^3}\Big] \quad \text{for} \quad R_1 \le r_i \le R_2 \tag{23}$$

$$= -\frac{\hbar c\alpha Z_{Cs+1} Z_i}{r_i} \quad \text{for} \quad R_2 \le r_i, \tag{24}$$

with i=D_1, D_2, Cs. Z_{Pd} and Z_{Cs+1} are effective charges around Pd- and Cs-ions with a hydrogen, and Z_i is the charge of ith-ion, respectively. In order to reproduce the binding energies of CsD_2 E^M_{gr}=-5.916eV and $E^M_1 = 296.1$eV, the following parameters are selected,

$$R_1 = 750\text{fm}, \quad R_2 = 2 \times 10^5\text{fm}.$$

⑤$_{\text{Zel-Pd}}$

$$V^M_{\mathrm{el-el}} = \sum_{k=1}^{Z} \sum_{m \ne k} V_c^{\mathrm{e}_k - \mathrm{e}_m}$$

⑤$_{\text{el-el}}$

$$V^M_{\mathrm{ZelPd}} = \sum_{j=1}^{12} V_c^{\mathrm{ZePd}_j}.$$

Therefore, these parameters are fitted with the ground state (-5.916eV) and the first excited state (296.1eV) energies by the ADF calculation.