CHARACTERISTICS OF ATOM AND FIRST ION OF F-METALS

G.V. Shpatakovskaya

NPP-2024, December 4

Content

- F - metals
- Semi-classical relations between some characteristics of atomic system
- Results for atoms of lanthanoides and actinoides
- First positive ions of lanthanoides and actinoides and trans-actinoides
- Conclusions

F - metals

Lanthanoides

Z =57 - 71

$[Xe]4f^{0-14}5d^{0-1}6s^2$

5d: Z = 57, 58, 64, 71

Application: Batteries, Catalysts, Polishing powders, Metallurgy, Magnets, Ceramics, Glass, Phosphors

Actinoides

Z = 89 - 103

$[Rn]5f^{0-14}6d^{0-2}7s^27p^{0-1}$

6d: Z = 89-93, 96;

7p: 103

Application: Nuclear Power, Portable Batteries, Medicine (Am, Pu)

Semi-classical relations between radius r_a, volume V_a, ionization potential I_p, and scalar dipole polarizability α_0 of atomic system

Dmitrieva I.K., Plindov G.I. //Phys. Scr. **27**, 403 (1983)
Dmitrieva I.K., Plindov G.I. //J. Appl. Spectr. **44**, 4 (1986)

for atom:

$$\alpha_0(Z)\ {I_p}^{+3}(Z) = \text{const},$$

$$r_a(Z) \sim {I_p}^{-1}(Z), \quad V_a(Z) \sim {I_p}^{-3}(Z)$$

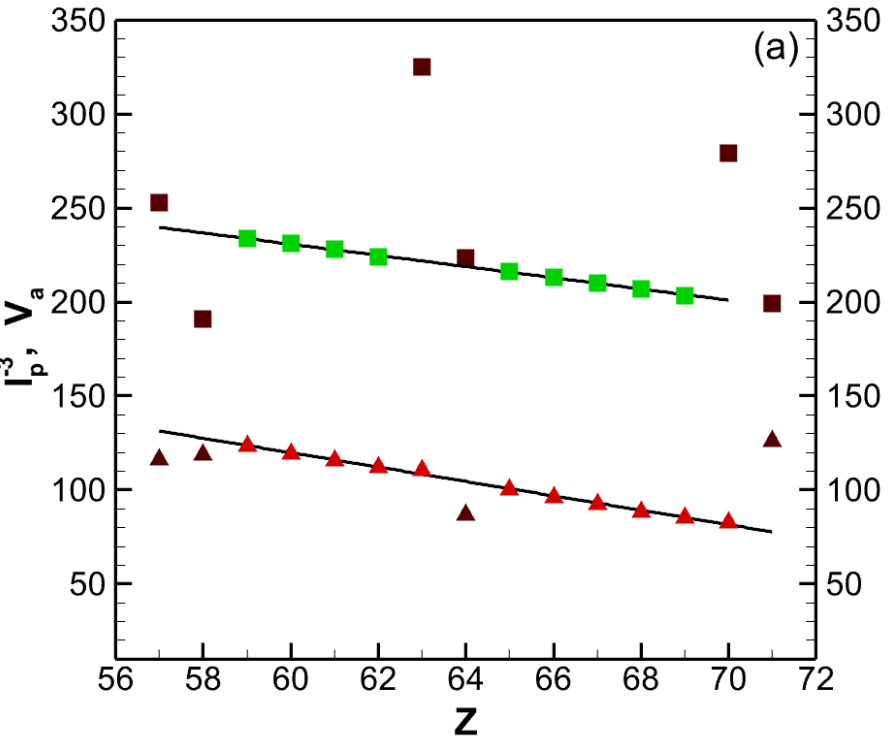
for ions:

$$r_a(N_e, Z) = (Z\text{-}N_e+1){I_p}^{-1}(N_e, Z)$$

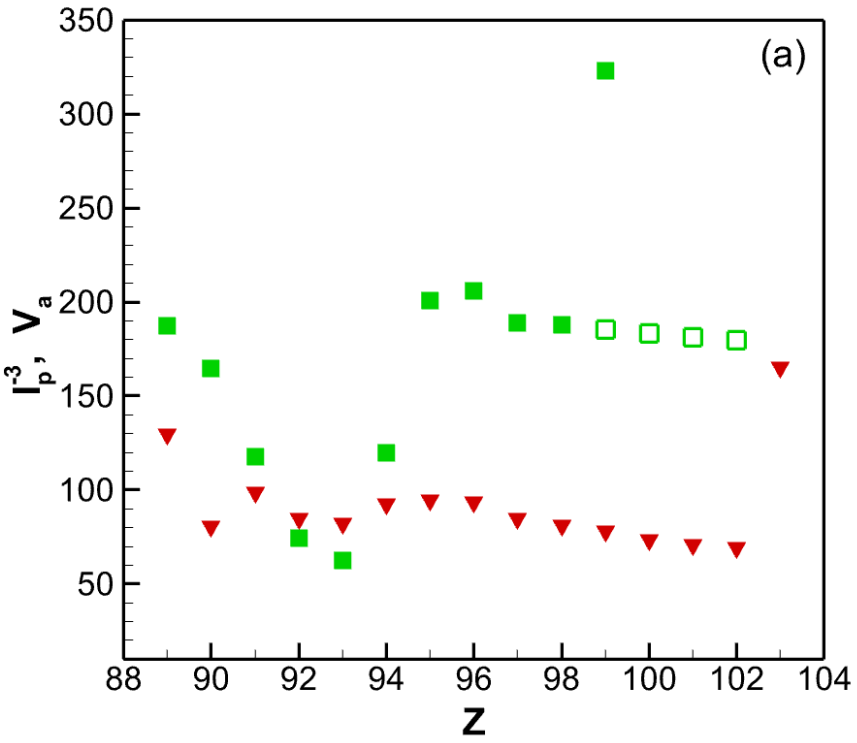
$$\alpha_0(N_e, Z)\ {I_p}^{+3}(N_e, Z) = (Z-N_e+1)^3\ f(N_e, Z)$$

Volumes $V_a(Z)$ and ionization potentials $I_p(Z)$ of homologue atoms.

Lanthanoides



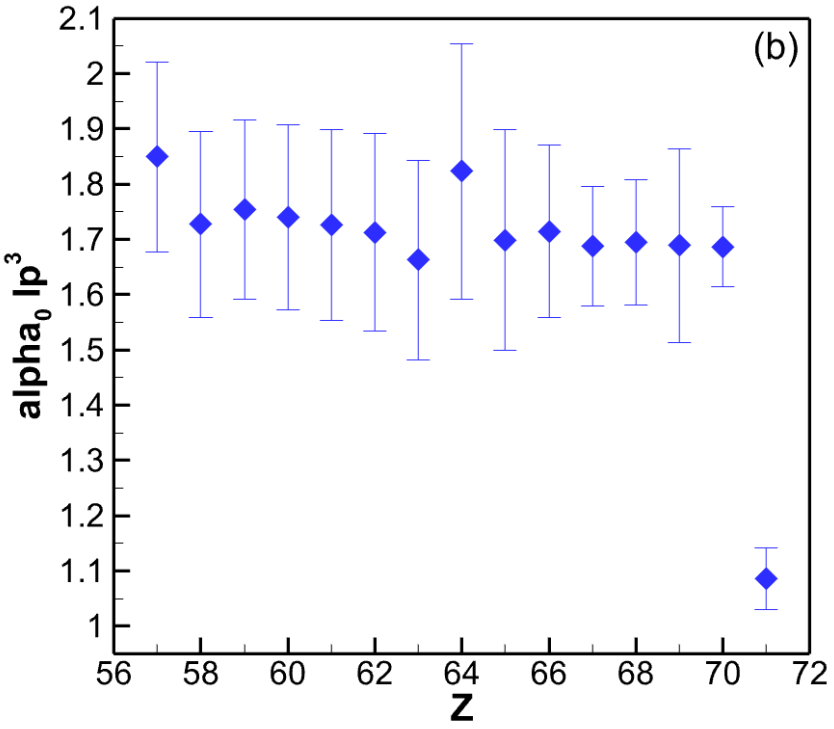
Actinoides

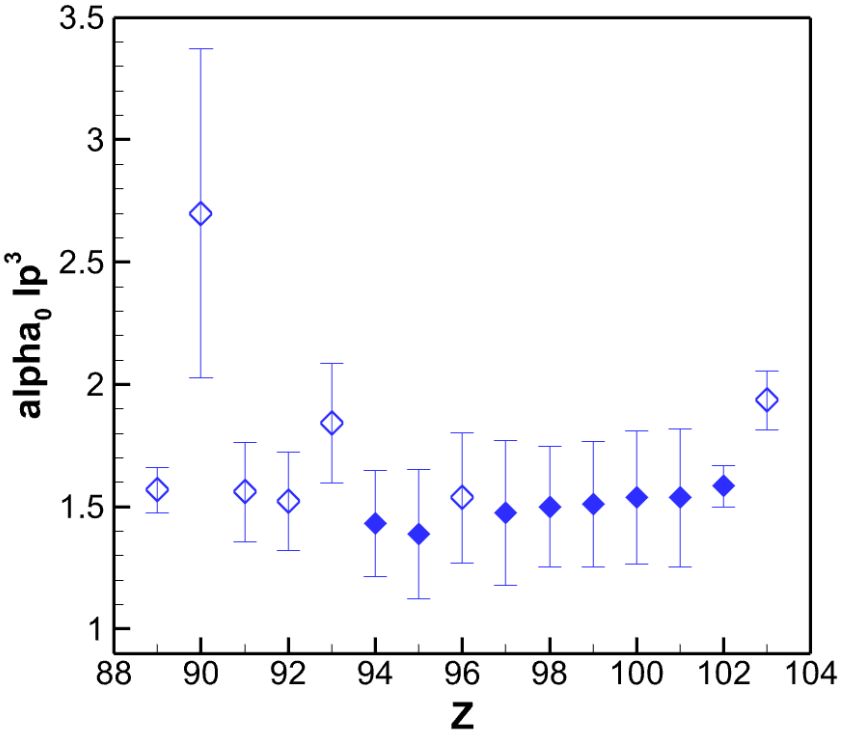


Product $\alpha_0 I_p^3 = c$ (?) for homologues.

Lanthanoides, c = 1.7

Actinoides, c = 1.5





Results for f-metal atoms

For **H-like filling f**-states:

- $\boldsymbol{\alpha_0 = c\, I_p^{-3}}$, for lanthanoides $\boldsymbol{c}$ = 1.7, for actinoides $\boldsymbol{c}$ = 1.5;
- for actinoides $\boldsymbol{\alpha_0(Z) = 1.1252 \cdot 10^{10} Z^{-4}}$;
- for the **oxidation degree +3**: $\boldsymbol{V_a = d\, Z^{-1}}$,

  for lanthanoides $\boldsymbol{d}$ = 13 932, for actinoides $Z \geq 97$ $\boldsymbol{d}$ = 18 281;
- Prediction for atomic volumes [a.u.] at **oxidation degree +3**:

$V_a(\mathbf{Fm}) = 183$, $V_a(\mathbf{Md}) = 181$. $V_a(\mathbf{No}) = 179$ [a.u.].

•what is considered the radius of an ion?

Semi-classical relations between radius r_a, ionization potentials I_p of first ions

$$r_a(Z) = 2 \cdot I_p^{-1}(Z)$$

MCDF-calculation:

Indelicato P. et al //EPJ D: Atomic, molecular, optical and plasma physics, 2007. **45**(1), 155-170

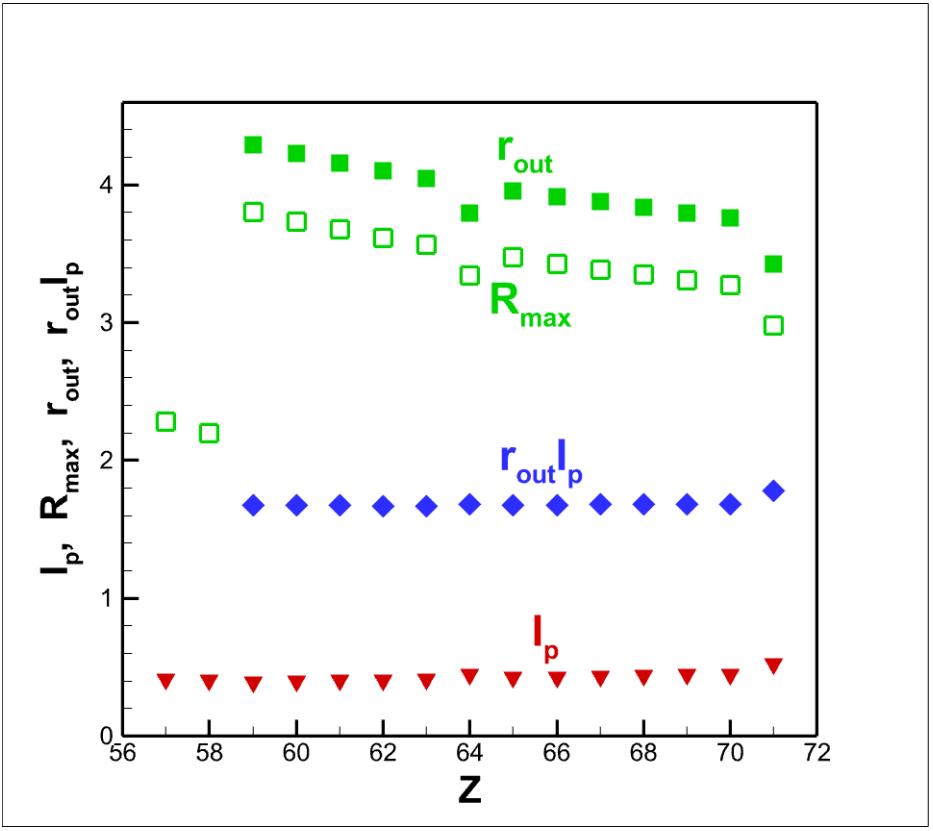
what is considered the radius of an ion?

$\boldsymbol{r_a(Z) = \mathrm{R_{max}}(Z)}$ – radius density maximum of outer orbital

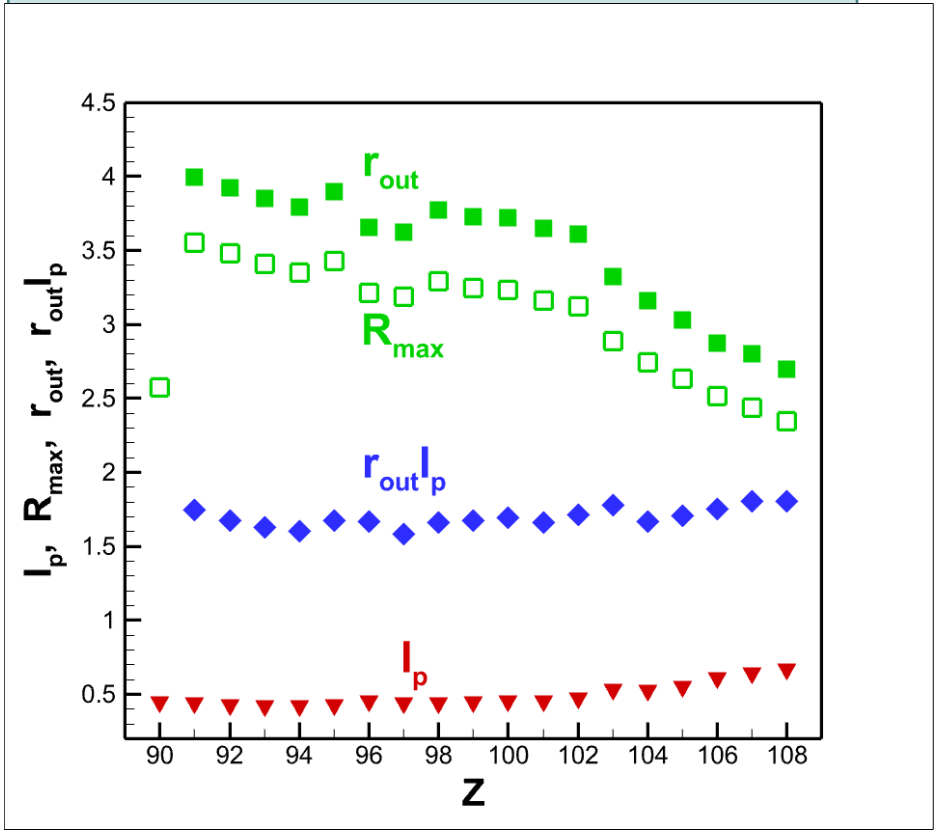
$\boldsymbol{r_a(Z) = \mathrm{r_{out}}(Z)}$ – mean radius of outmost shell

Radii R_{max}, r_{out}, ionization potential I_p, and their product for the first ions.

Lanthanoides



Actinoides and … (Z=90-108)



Results for ions, $r_a(Z) = r_{out}(Z)$

Semi-classical prediction: $r_a \cdot Ip = 2$

- for ***lanthanoides*** with **H-like** 4f-shell (Z=59-63, 65-70)

  - $r_{out} \cdot Ip = 1.677 \pm 0.007$

- for ***actinoides*** with **H-like** 5f-shell (Z=98-102)

  - $r_{out} \cdot Ip = 1.688 \pm 0.027$

- for *elements* with **H-like** 6d-shell (Z=104-108)

  - $rou_t \cdot Ip = 1.736 \pm 0.067$

- for **all H-like** *elements* $r_{out} \cdot Ip = 1.7 \pm 0.1$

Conclusions

- For the free atoms and first ions with **H-like filling** of electron shells, the **semi-classical relations are fulfilled**;
- This can be used **to approximate** the corresponding values, as well as **to estimate missing data**;
- There is a **disagreement** in the literature over the type of electronic configuration of the ground state

Thank for your attention!

NPP-2024, December 4