DEPENDENCE ON THE ATOMIC NUMBER Z OF APPLICABILITY CONDITIONS OF THE QUASI-CLASSICAL APPROXIMATION ON THE EXAMPLE OF IONIZATION POTENTIALS OF ATOMS AND IONS

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Content

- Quasi-classical semi-empirical method
- Regularities in multi charged ion iso-electronic series of medium, heavy and super-heavy elements
- Approximation and replenishment of data on the ionization potentials
- Approximation of lanthanide and actinide atomic ionization potentials and homologue electronic state analysis
- Replenishment of data on heavy actinide atomic volumes
- Conclusion

Semi-classical method for representing experimental or theoretical ionization potentials $I_{Ne}(Z)$ (eV)

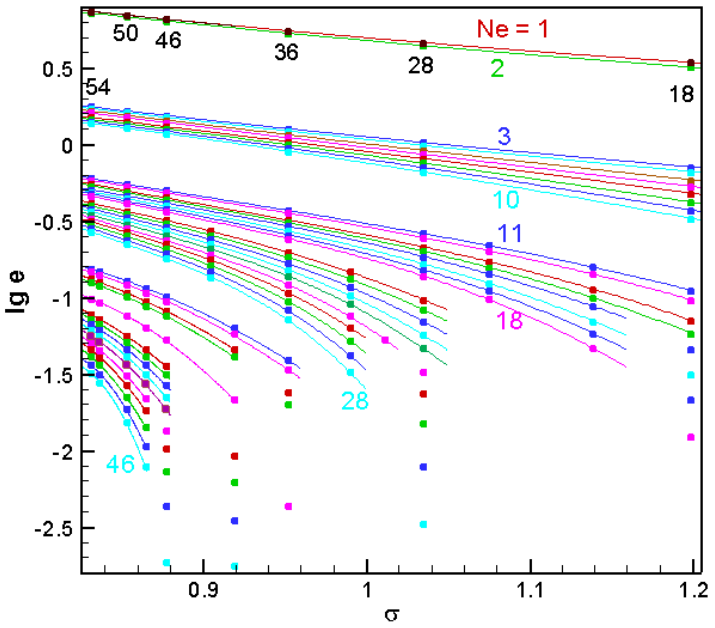
$$e_{Ne}(\sigma) = (I_{Ne}^{(Z)} / E_h) Z^{-4/3},$$

$$\sigma = \pi Z^{-1/3},$$

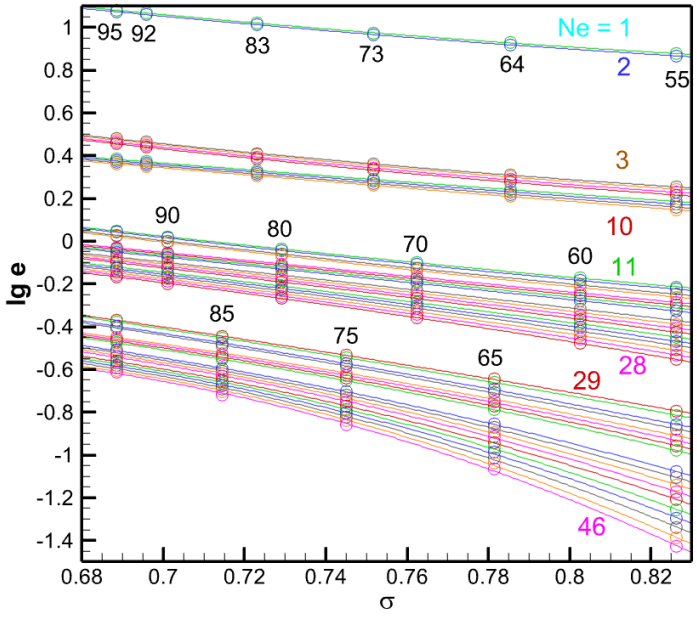
$$E_h = 27.211386\ eV.$$

Functions $e(\sigma)$ for multi-charged ions (q > 5) with N_e = 1-46 of some elements Z = 18 – 95. $\sigma \sim Z^{-1/3}$

Z = 18 – 54
[JETP, 2022]



Z = 55 – 95
[JETP Letters, 2021]



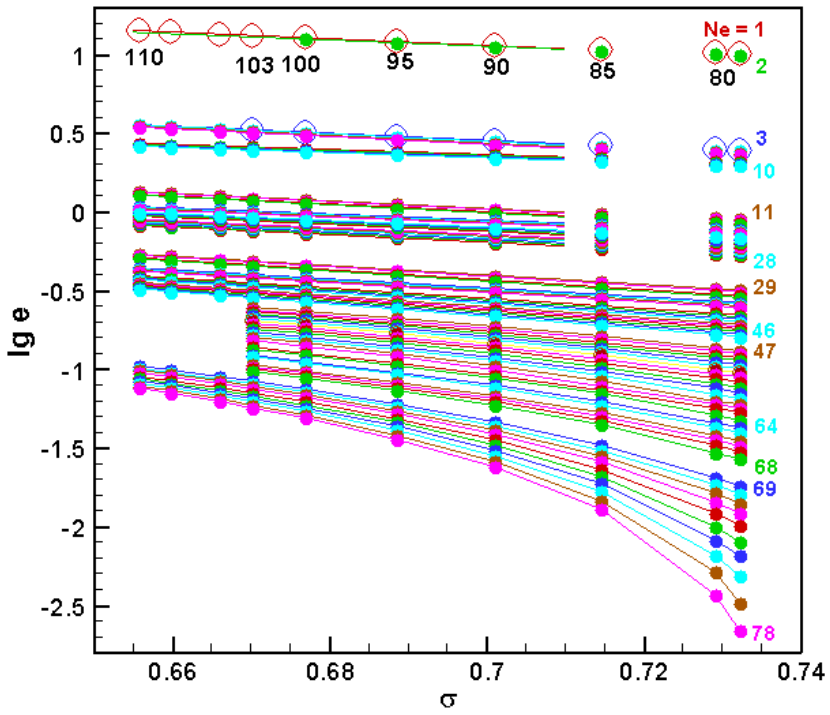
Polynomial approximation of the ionization potentials for multi-charged ions. Inaccuracy ≤ 1%.

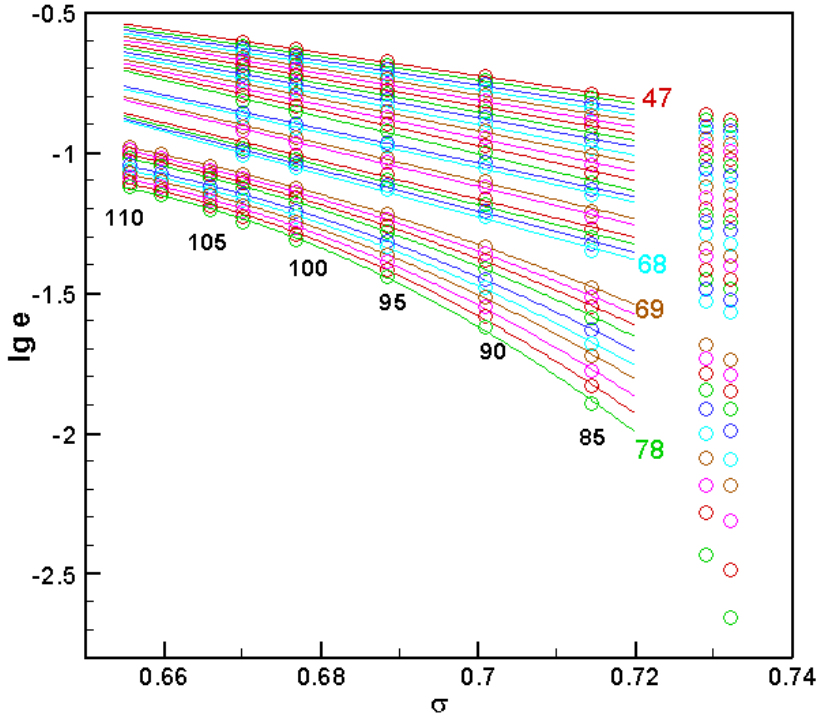
$$\lg e_{Ne} = \sum_{i=0}^{i_{\max}} a_i(N_e)\sigma^i,$$

$$\sigma = \pi Z^{-1/3},$$

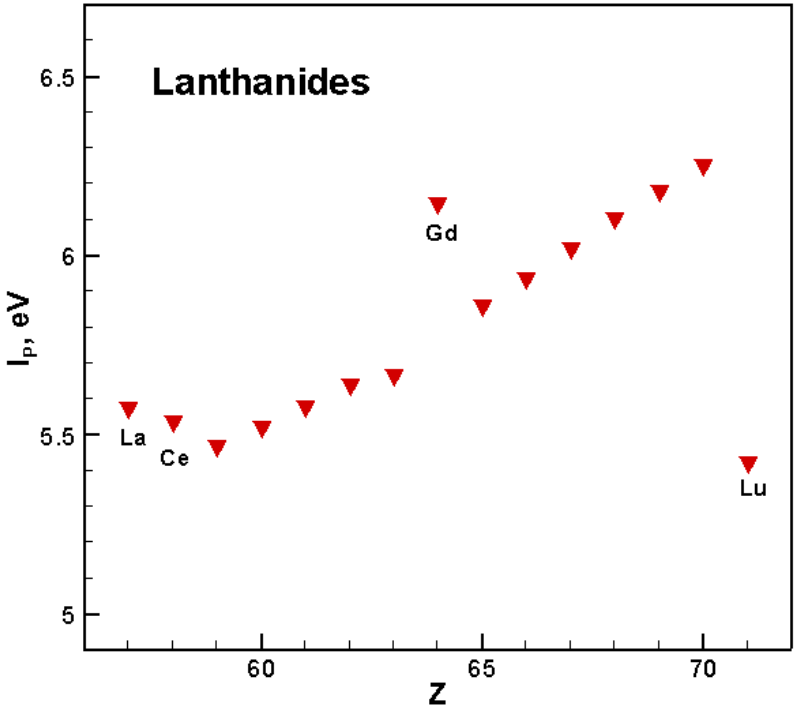
$$I_{Ne}^{(Z)} = Z^{4/3} 10^{\lg e_{Ne}(\sigma)} E_h$$

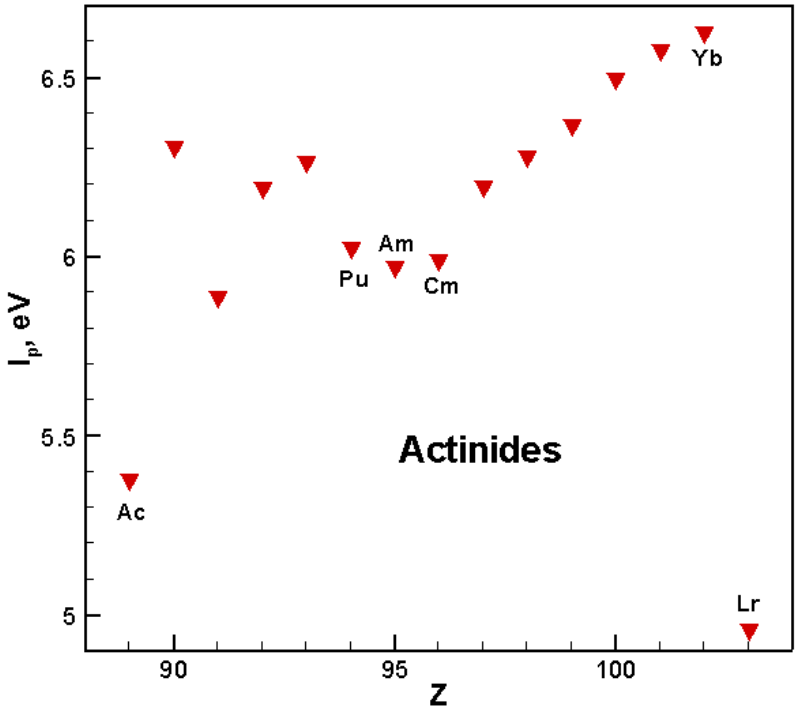
Functions $e(\sigma)$ for ions with N_e = 1 - 78 of elements 79 ≤ Z ≤ 110. H-like shell filling. Replenishment of data. [Plasma Physics Reports, 2023]





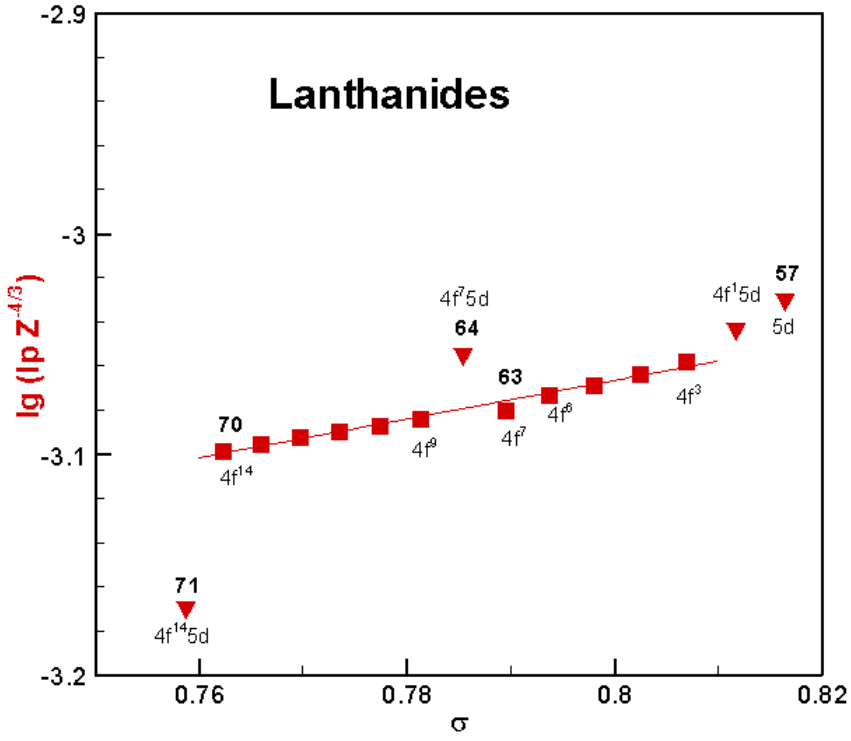
Lanthanide and Actinide Ionization Potentials. d- and f –states competition

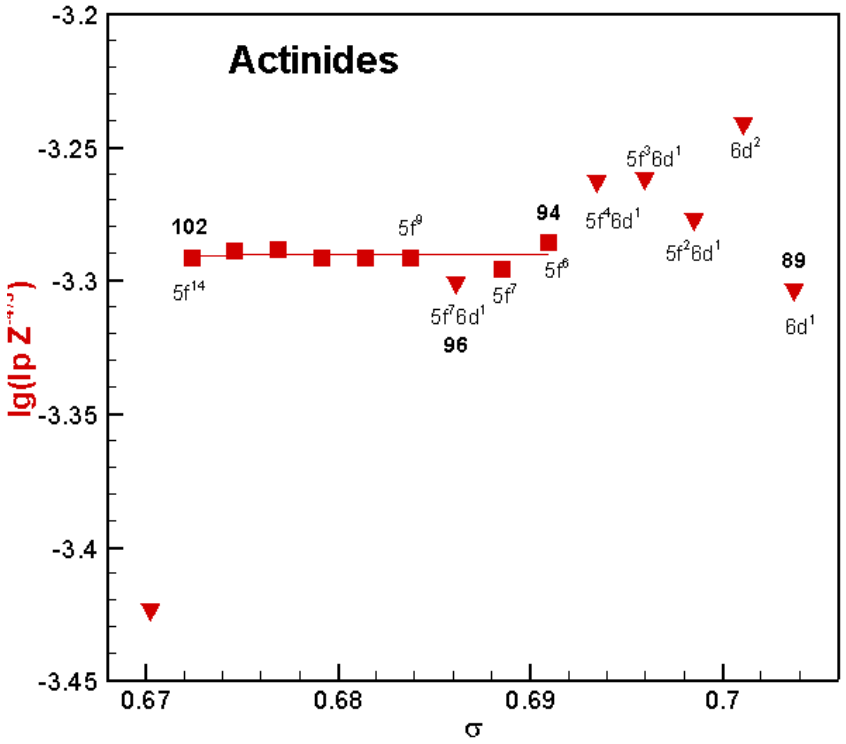




Lanthanide and Actinide Ionization Potentials I_p [a.u.] in special coordinates $\sigma=\pi Z^{-1/3}$.

[JETP Letters, 2020]





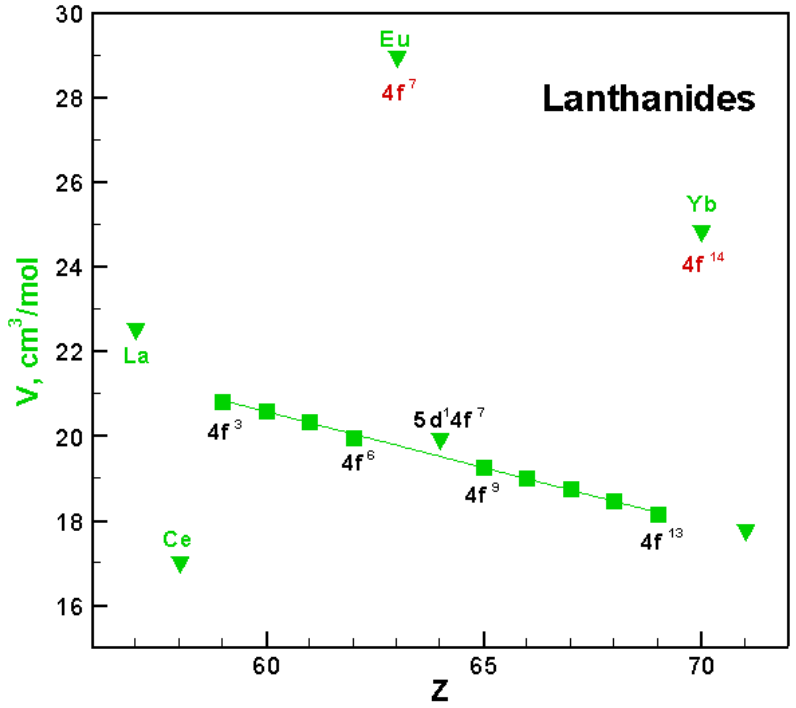
Some conclusions:

- Polynomial approximation **in special coordinates** makes it possible to **estimate with good accuracy** the NIST ion **ionization potentials** and to **extrapolate missing data.**
- In this case, the **hydrogen-like filling** of electron shells **is important.**
- General pattern **in special coordinates** becomes **simpler and more transparent with increase in Z**, which confirms the **improvement** in the conditions for using the **quasi-classical approximation.**

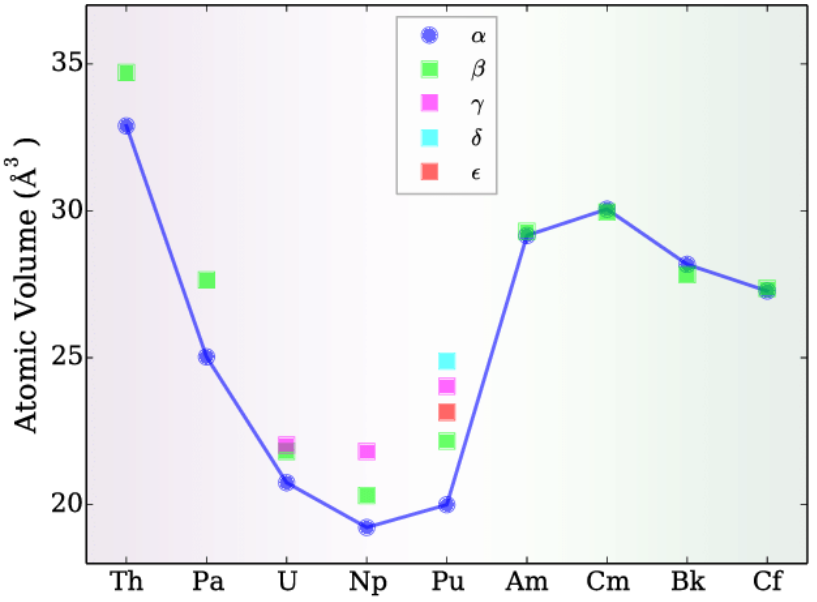
Atomic volumes of homologues V(Z).

Electronic states f^7 and f^{14} are isolated.

Lanthanoides

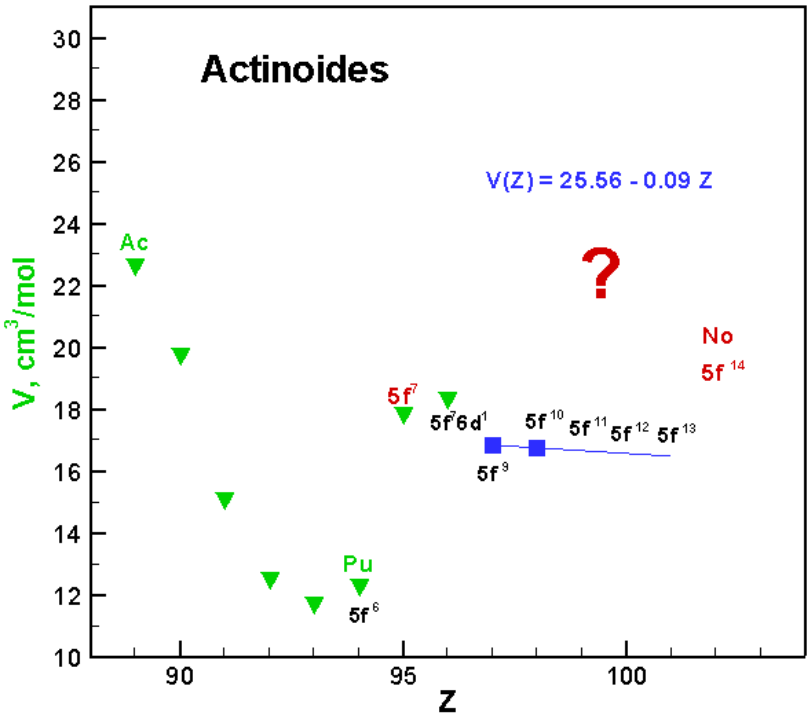


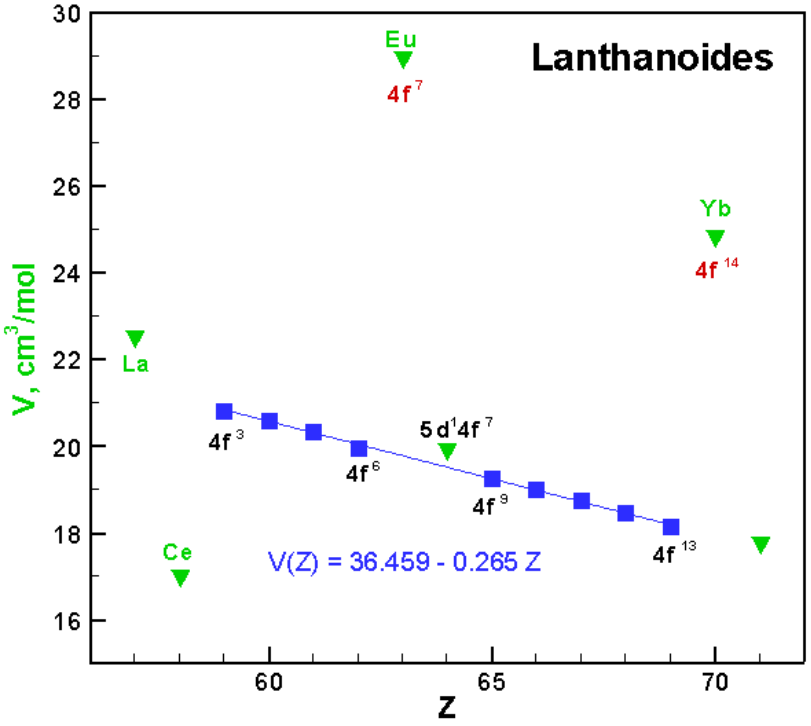
Actinoides



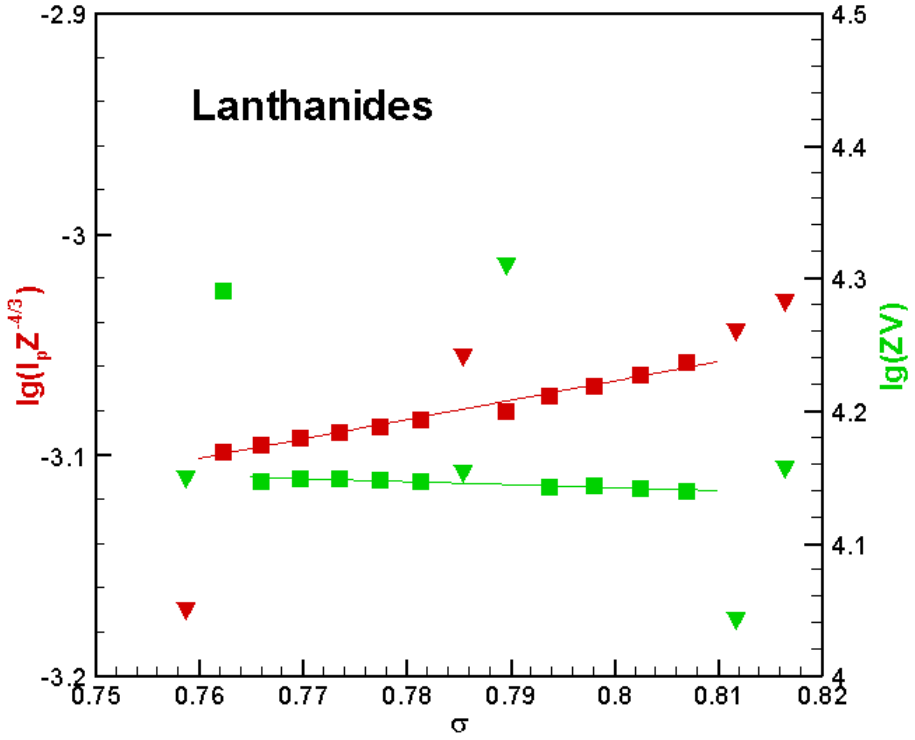
Atomic Volumes of Lanthanoides and Actinoides V(Z)

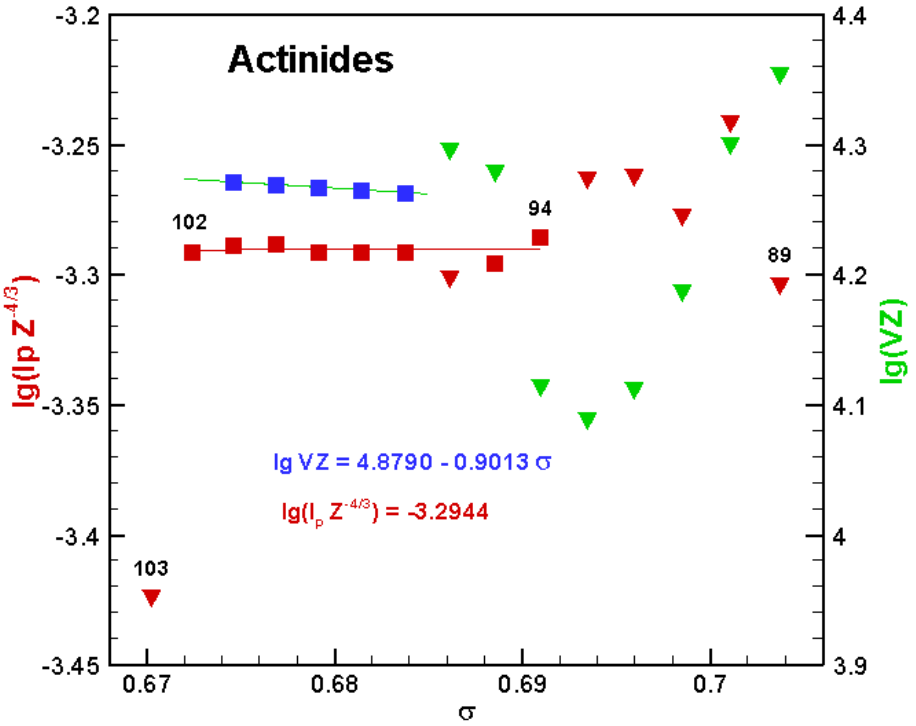
Is it correct?





Lanthanide and Actinide Ionization Potentials and Atomic volumes in special coordinates lg ZV(σ), $\sigma=\pi Z^{-1/3}$





Atomic Volumes of Heavy Actinides

Z	V_{exp}	V_{lin}	$V_{semi-class}$
97 (α)	16,83	16.83	16.83
98	16.74	16.84	16.74
99	-	16.65	16.65
100	-	16.56	16.56
101	-	16.47	16.47

Conclusions

- Quasi-classical approach reflect the **main dependence on the atomic number** of not only ionization potentials, but atomic volumes too in the case of **hydrogen-like filling** of electron shells.

- A more accurate calculation of the ionization potentials of ions with the number of electrons **47≤Ne≤68** of elements with **Z>54** is necessary.

Thank you for attention!