

COMPARISON OF EXPERIMENTAL AND THEORETICAL BINDING ENERGIES IN ELECTRONIC SHELLS OF PALLADIUM GROUP METALS

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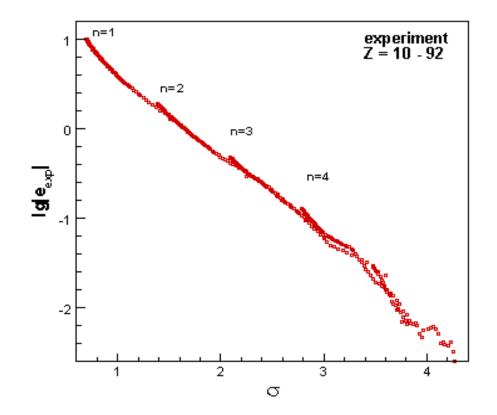
1.1 Method for representing orbital binding energies in atoms

$$e_n(\sigma) = \frac{E_{no}}{Z^{4/3}},$$

$$d_{nlj}(\sigma) = \frac{E_{nlj} - E_{no}}{(l+1/2)^2 Z^{2/3}}, \quad j = l \neq 1/2$$

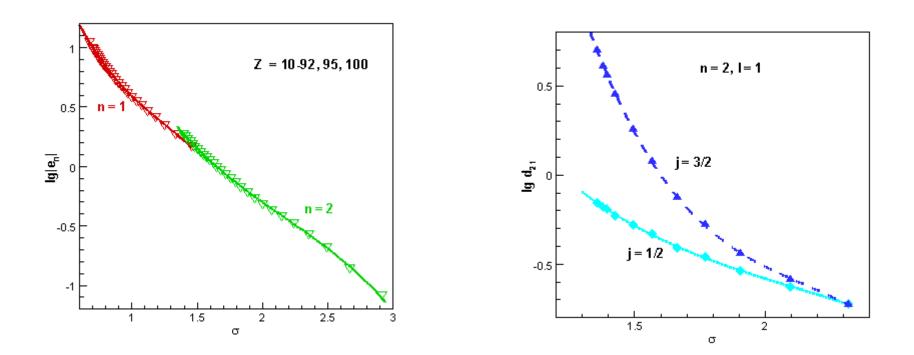


1.2 Functions $e(\sigma)$, reconstructed from the experimental s-levels E_{n0} for atoms $\mathbf{Z} = \mathbf{10} - \mathbf{92}$





2.1 Functions $e(\sigma)$ and $d(\sigma)$ from in *K* and *L* shells in free atoms. *JETP Lett.* **108** 768 (2018)





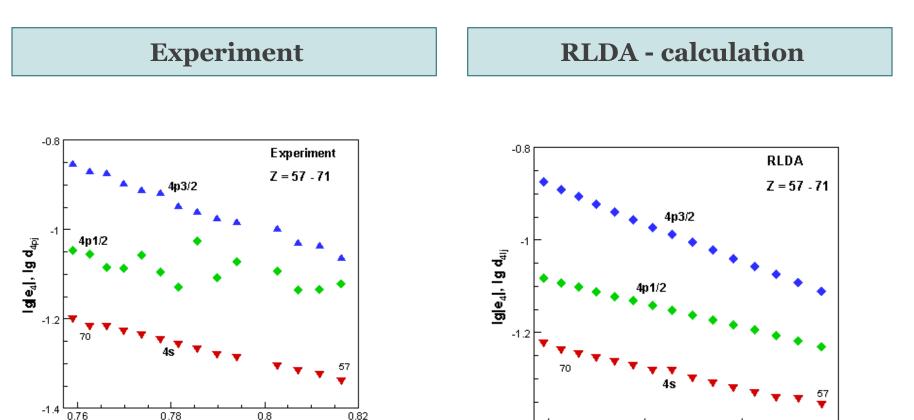
0.78

σ

0.8

0.82

2.2 Subshells 4s, 4p1/2, 4p3/2 in rare-earth elements through functions $e(\sigma)$ and $d(\sigma)$. $\sigma = \pi Z^{-1/3}$. JETP 131 385 (2020)



-1.4

0.76

0.78

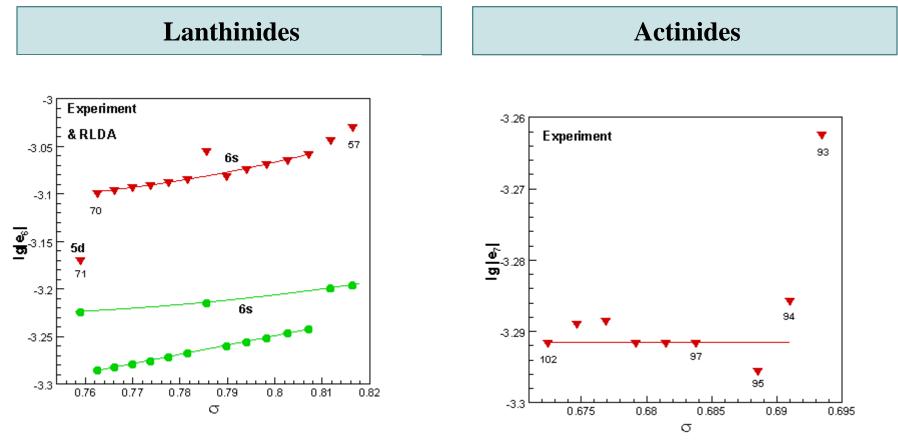
σ

0.8

0.82



2.3 Measured first potentials of **lanthinides and actinides** through functions $e(\sigma)$ and $d(\sigma)$. $\sigma = \pi z^{-1/3}$. *JETP Lett.* **111** 463 (2020)





1

0.5

-0.5

-1

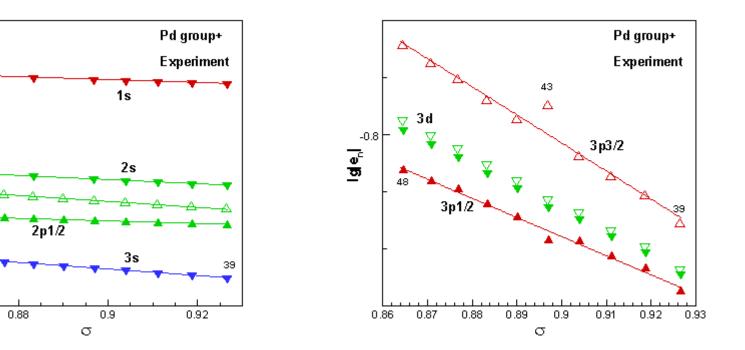
0.86

lge_

3.1 *K*, *L*, *M* shells in **Pd atomic group** through functions $e(\sigma)$ and $d(\sigma)$. $\sigma = \pi Z^{-1/3}$.



Experiment: 3p, 3d

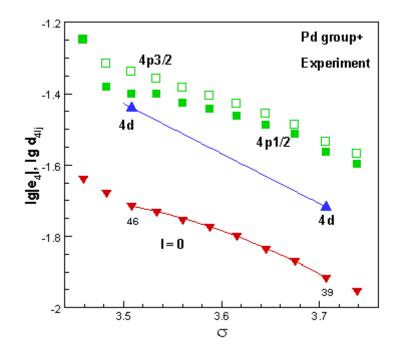


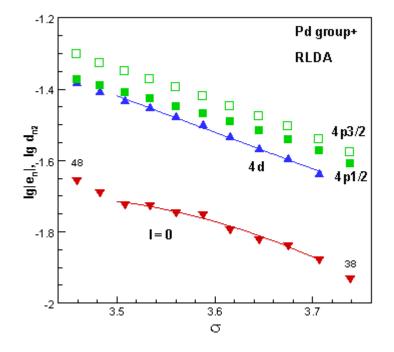


3.2 *N* shell in **Pd atomic group** through functions $e(\sigma)$ and $d(\sigma), \sigma = \pi Z^{-1/3}$.

Experiment

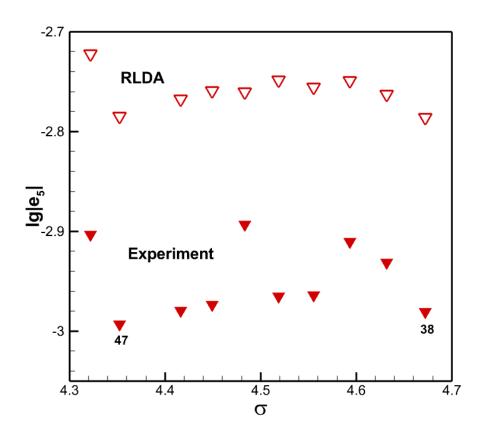
RLDA - calculation







3.3 Measured and RLDA first potentials of **Pd group atoms**





<u>4. Conclusion</u>

- 1. There are lack and scatter of some experimental data in internal shells of atoms.
- 2. However most points in the reduced coordinates form smooth dependence on atomic number, that is atomic number similarity law .
- 3. The deviation from the law raises doubts and needs additional experimental verification.
- 4. The found atomic number similarity law provide a way to recover missing or erroneous data.
- 5. The available theoretical RLDA model does not satisfactorily describe the orbital binding energies, which indicates its incompleteness.