Regularities in filling procedure of electron shells   
in transition metals[[1]](#footnote-1)\*)

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Experimental [1], [2] and theoretical [3] data on electronic energies  in the ground state of atoms in three groups of transition metals, iron (n = 3), palladium (n = 4), platinum (n = 5), are considered in special reduced coordinates [4]:

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where Z is the atomic number of the element, n, l, j = l ± ½ are quantum numbers..

There is a scatter of measurements of the binding energies in different sources and the lack of experimental data on the energies of d-states in these groups. The discrepancy between the results of measurements and calculations by the density functional method is discussed (Figs. 1a, 1b). To estimate the measurements of electronic binding energies, it is proposed to use the empirical law of similarity in atomic number [5] and polynomial approximation of functions .

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| --- | --- |
| Pd_Expt | Pd_RLDA |
| Fig.1a Experimental dependence according to data from databases [1], [2] | Fig.1b Calculation by the relativistic model of the local density functional RLDA [3] |

References

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1. \*) [abstracts of this report in Russian](http://www.fpl.gpi.ru/Zvenigorod/XLVIII/Lt/ru/EB-Shpatakovskaya.docx) [↑](#footnote-ref-1)