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

Shpatakovskaya G. V.

KIAM RAS, Moscow, Russia
shpagalya@yandex.ru

Experimental [1], [2] and theoretical [3] data on electronic binding energies $|E_{nlj}^{(Z)}|$ in N shells (n = 4) in the main state of transitional metals of the palladium group are considered. Special coordinates [4] are used to provide a compact view of the data:

$$\sigma_n = \pi n Z^{-1/3}; \tag{1}$$

$$e_n = E_{n0}^{(Z)} Z^{-4/3}, \quad l = 0; \tag{2}$$

$$d_{nlj} = \left(E_{nlj}^{(Z)} - E_{n0}^{(Z)} \right) Z^{-2/3} (l + 1/2)^{-2}, \quad l > 0. \tag{3}$$

Here $E_{nlj}^{(Z)}$ are energy levels of electrons taking into account spin-orbital interaction, Z is an atomic number, $n, l, j = l \mp 1/2$ are quantum numbers.

There is a spread in measurements of 4p- binding energies in different sources and almost complete absence of experimental data on 4d-energies in these elements. The divergence of measurements and calculations by the local density functionality [3] is also discussed. To estimate and correct the measurements of electronic binding energies, it is proposed to use the empirical law of similarity on the atomic number [5].

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