Refinement of the relationship between effective radii and ionization energies of alkali metal atoms

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Abstract

One of the key explanations for the peculiarities of the change in the first ionization energies (IE E_{i1}) of the elements of the periodic table is based on the postulation of an unambiguous relationship between E_{i1} and atomic radii (rat). Due to the certain conventionality of the rat parameters, they do not belong to the category of attributive atomic characteristics. Usually they are found either by implementing various kinds of theoretical or semi-empirical calculation schemes, or by using experimental data on E_{i1} for the corresponding approximations. As follows from the literature data, the known values of rat, even in the case of "quasi-hydrogen-like" alkali metals (AM), relatively simple manyelectron systems - are characterized, as a rule, by a significant scatter. In addition, the canonical analytical formulas describing r_{at} within the framework of a hydrogen-like model with two effective interaction parameters (according to Slater) do not ultimately lead to adequate results in this set of elements.

In this work, to correct the relationship $r_{at} = f(E_{i1})$ related to the properties of the aggregate of alkaline elements, the publication of the effective Slater radii (r_{eff}) and Weber-Cromer orbital radii (r_{orb}), and some results of later data are used. The effective principal quantum numbers n_* for each of the AM (except for Li, for which it is assumed that $n_*=n=2$) are estimated on the basis of the values of E_{i1} . A further step, by introducing n_* , made it possible to use the criterion for optimizing the value of the effective radius r_* and to correct the formula that determines its relationship with E_{i1} in the form of a simple power function. At the same time, the radii Li, Na, and Fr have been refined towards some underestimation, compared with r_{orb} . Arguments are presented in favor of the reliability of the proposed approach.

It is shown that the obtained estimates of r_* correlate better with the amplitudes of the solution of the wave equation covering all AMs than the known corresponding values of $r_{\rm orb}$ and $r_{\rm eff}$.

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