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The covalent radii derived from the first-principle data

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The concept of atomic covalent radius forms the basis for one of the simplest parameterizations for prediction of the covalent bond length and recovering molecular graphs from the set of interatomic distances. In the present contribution we adopt the recently proposed dataset [1] of covalent bond lengths resulting from the first-principle calculations to derive the covalent radii for H, B, C, N, O, F, Si, P, S, Cl, Ge, As, Se and Br elements within the additive covalent bond length model. The obtained first-principle covalent radii are shown to be in good agreements ones based on empirical data [2]. Availability of the large-size dataset of covalent bond lengths enabled the further analysis of errors in approximating the covalent bond length with the sum of the covalent radii. In particular, the effects of electronic conjugation and the chemical elements electronegativity difference were investigated [3].

[1] Nikolaienko, T. Y., Chuiko, V. S., & Bulavin, L. A. (2019). The dataset of covalent bond lengths resulting from the first-principle calculations. Computational and Theoretical Chemistry, 112508.
[2] Pyykkö, P. (2015). Additive covalent radii for single-, double-, and triple-bonded molecules and tetrahedrally bonded crystals: a summary. The Journal of Physical Chemistry A, 119(11), 2326-2337.
[3] Nikolaienko, T. Y., Chuiko, V. S., & Bulavin, L. A. (2019). The covalent radii derived from the first-principle data. arXiv preprint arXiv:1906.11724

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