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Estimation of the chemical shifts in Mössbauer spectra on the basis of quantum-chemical calculations by Density Functional Theory

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Abstract

The calculated electron density at the nucleus of iron atom was analyzed on the bases of density functional theory. The bond lengths and electron density at the nucleus of iron atom correspond to the known structural and Mössbauer data. For ferrates the chemical shift depends on the population of 4s-orbitals of iron. The calculations performed allowed us to estimate the chemical shifts of tetraoxoferrate(VII), $KFeO_4$, and iron oxide(VIII), FeO_4.