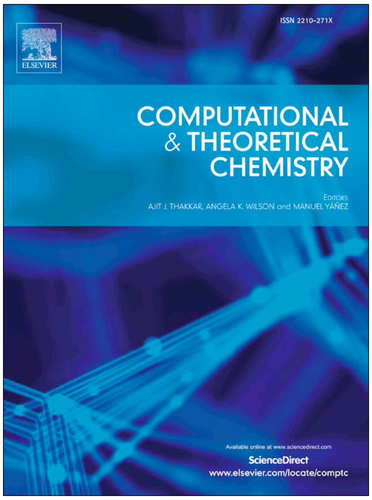

Ligand field splitting in homoleptic tetrahedral d^{10} transition metal complexes. Spectrochemical series

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Ligand field splitting in homoleptic tetrahedral d^{10} transition metal complexes. Spectrochemical series

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A B S T R A C T

The ligand field splitting Δ_t in a number of homoleptic tetrahedral complexes of Cu(I) and Ni(0) are determined from electronic structure calculations by DFT at the BP86/6-31+G(d,p) and BP86/LanL2DZ levels. Some ligands are monodentate (e.g. CO, NH_3, Cl^- etc.) and some are bidentate (e.g. ethylenediamine, 2,2′-bipyridine etc.). The Δ_t values obtained with the two basis sets for a given metal ion are comparable except for the phosphines. They correlate linearly with Shimura’s d_{Co} parameters which are considered to be most effective for constructing a spectrochemical series. Earlier it was believed that the d_{Co} parameters are applicable only to the octahedral complexes of cobalt(III). It is further shown that the d_{Co} parameters bear a linear relationship with Chatt’s ligand constants P_L. Implications are discussed.

Keywords: copper(I); Nickel(0); DFT; spectrochemical series; d_{Co} parameters.

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