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Spectrochemical series

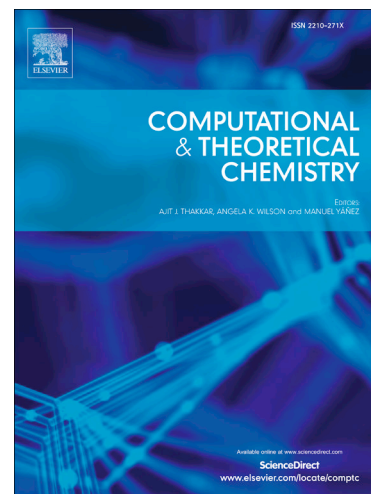
Shati G. Patra, Dipankar Datta

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

Shati G. Patra and Dipankar Datta\*

*Department of Inorganic Chemistry, Indian Association for the Cultivation of Science, Calcutta 700 032, India*

## ABSTRACT

The ligand field splitting  $\Delta_t$  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<sub>3</sub>, Cl<sup>-</sup> etc.) and some are bidentate (e.g. ethylenediamine, 2,2'-bipyridine etc.). The  $\Delta_t$  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.

\* Corresponding author. Tel: +91 33 2473 5374; fax: +91 33 2473 2805.

*E-mail address:* icdd@iacs.res.in (D. Datta)

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