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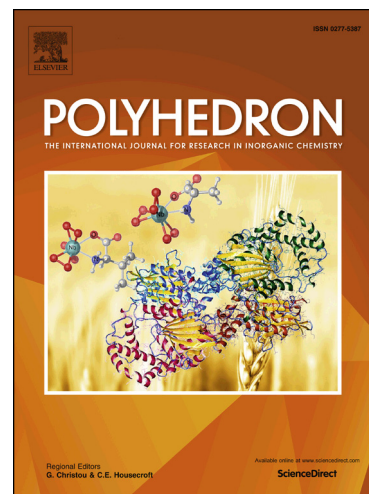
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On the nature of the coordination bonding of metal–organics for ions with the d^{10} electronic configuration – experimental and theoretical analyses

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Abstract

The fundamental goal of this work in applying high resolution crystallographic X-ray measurements of single crystals as well as *ab initio* and density functional computational methods is to provide a correlation between the experimental electron densities and valence states of atoms with the theoretically predicted ones by methodological approaches of quantum chemistry. In order to test the reliability of the data, we chose to examine statistically the crystallographic datasets of nine metal-organics with Zn^{2+} , Ag^+ and Cu^{2+} ions. There are several premises to the argument for this choice: (i) the different nature of M–L interactions, (ii) various geometries of the chromophores and (iii) distinguishable chemical behavior of the dentate atoms in the inner coordination sphere (L = O, N, Cl). New insights about the nature of the M–L interactions are gained for the following bonding fashions: (a) bonded $Ag^I-X(Y)$ fragments (X, Y = O and/or N) in tetrahedral (T_d) and square planar AgX_2Y_2 symmetries, (b) bonded $Zn^{II}-X(Y)$ cores (X, Y = O and/or N; or Cl) in T_d $Zn^{II}X_2Y_2$ or $Zn^{II}X_2$ chromophores, (c) $Zn^{II}-OH_2$ interactions in the discrete octahedral $\{[Zn^{II}(H_2O)]^{2+}\}$ charged complex and (d) bonded $Cu^{II}-X(Y)$ systems (X, Y = O and/or N) in square planar AgX_2Y_2 chromophores as comparative examples of complexes with the d^9 configurations of the metal ion. The methods of ‘atoms in molecules’ (AIM), ‘natural bond orbital analyses’ (NBO) and electrostatic potentials were employed. The analyses include employment of the bond valence (BV) methodology and non-covalent interaction (NCI) analysis. Quantum chemical prediction of multi-pole moments, orbital population and charge transfer effects (CT), bond covalence, iconicity, different bond order methodologies (BOs); electron density distribution and Laplacian of the total electron density

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