

P007 Ligand Field Molecular Mechanics Calculations on Copper Type 3 Enzymes

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The description of transition metal complexes with conventional force field methods poses a significant problem if electronic effects like the Jahn-Teller distortion are relevant for the electron configuration of interest. The Ligand Field Molecular Mechanics (LFMM) method, developed in our group, deals with these effects by adding a “ligand field stabilisation energy” term to the otherwise conventional force field. This approach has been proven to be very successful for single metal systems.

The importance of multi metal metalloproteins prompted us to test LFMM also for systems with more than one transition metal centre. The performance of the model was critically analysed for a set of small compounds which model the $[\text{Cu}_2\text{O}_2]^{2+}$ centre in copper type 3 (T3) enzymes. On the basis of the very encouraging results for these molecules we carried out geometry optimisations and molecular dynamics simulations on the T3 enzymes Hemocyanin and Tyrosinase for which crystallographic data are available. We present first results of these simulations which emphasise the importance of a proper treatment of the d-electronic effects for a reasonable description particularly of the dynamic behaviour of these systems.