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Complexes of Ni(II) and Zn(II) as models for hydrolytic enzymes

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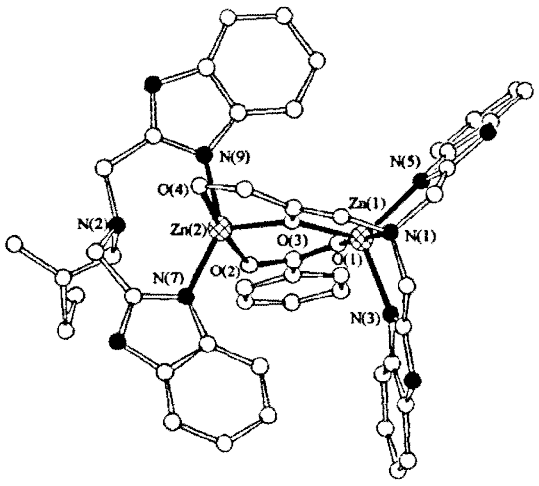

Hydrolytic enzymes play an important role in nature. In order to mimic the active sites of that type of enzymes we synthesized complexes of Zn(II) and Ni(II) with the new ligand 1-[N,N-bis(benzimidazolylmethyl)]amino-2,3-dihydroxypropane (bdapoh). The complexes were characterized by X-ray crystallography and tested for their hydrolytic activity towards 4-nitrophenylacetate (npa).

Crystals of $[Zn_2(bdapo)_2\ C_6H_5CO_2](NO_3)_2 \cdot 2CH_3OH$ **(1)** were obtained from $Zn(NO_3)_2 \cdot 6H_2O$, $Na(C_6H_5CO_2)$ and bdapoh in methanol. $[Ni_3(bdapo)_2(CH_3COO)_2(ClO_4)_2] \cdot C_4H_{10}O \cdot 6CH_3OH$ **(2)** was obtained as dark green crystals from $Ni(ClO_4)_2 \cdot 6H_2O$, $Ni(CH_3COO)_2 \cdot 4H_2O$ and bdapoh in methanolic solution.

Kinetic measurements were carried out in buffered ethanol-water mixtures 1:1 at constant pH. We used the biological buffers mops (pH<7) and hepes (pH>7). The hydrolysis rate of npa was measured by monitoring the increase of the absorption at 400 nm of the released 4-nitrophenolate. The activity of the complex decreases from Zn^{2+} ($k = 1.69\ 10^{-3}\ mol^{-1}\ s^{-1}$) to Ni^{2+} ($k = 0.66\ 10^{-3}\ mol^{-1}\ s^{-1}$). At higher pH the hydrolytic activity of the complexes increases. Using low temperature ^{1}H-NMR we determined an equilibrium of mono- and dinuclear species in solution for **(1)**. The free enthalpy of activation for the dinuclear complex is -91.2 kJ/mol.