New Functional and Structural Copper Model Systems for the Active Site of Catechol Oxidase

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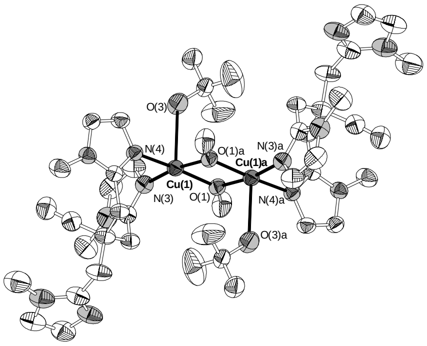
The coordination chemistry of dinuclear Cu(II) complexes has been the subject of extensive investigations with the goal of synthesizing model compounds that mimic the active sites of the type 3 copper proteins/enzymes such as hemocyanin, tyrosinase and catechol oxidase. The oxidation of a wide range of *o*-diphenols to *o*-quinones is catalyzed by the catechol oxidases. Recent reports of the crystal structure of the *met*-form of catechol oxidase from sweet potatoes (*Ipomoea batatas*) depicts a mono-hydroxo-bridged Cu(II)-Cu(II) active site with a distorted $(His)_3Cu(\mu\text{-}OH)Cu(His)_3$ coordination.[1,2]

New biomimetic model complexes were synthesized with tridentate ligands consisting solely of imidazole nitrogen atoms. The ligands 3-(1-methylimidazol-2-yl)-2,2-bis((1-methylimidazol-2-yl)methyl)propanenitrile and 1,1,2-tris(1-methylimidazol-2-yl)ethanol exhibit N_3-donorsets with the addition of an alcohol group to the second ligand. Dinuclear copper(II) complexes were synthesized, in which the ligands lead to similar coordination of the two copper sites.



The structures of the complexes were characterized by X-ray crystallography. Both compounds show substantial catalytic activity with respect to the aerial oxidation of 3,5-di-*tert*-butylcatechol.

[1] T. Klabunde, C. Eicken, J. C. Sacchettini, B. Krebs, *Nature Struct. Biol.* **1998**, *5*, 1084.
[2] C. Eicken, F. Zippel, K. Büldt-Karentzopoulos, B. Krebs, *FEBS Lett.* **1998**, *436*, 293.