Synthesis and structural properties of copper complexes toward the active center model of galactose oxidase

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As part of our long-term project designed to investigate structural properties of active center model of copper containing enzymes and coordination chemistry of monocopper complexes, we synthesized a series of copper complexes by using tripodal ligands bearing pyridyl and phenolic or phenyl arms. In this paper we report the synthesis and crystal structures of two copper complexes containing [bis(2-pyridylethyl)aminoethyl]cresol(Crepy2) and [bis(2-pyridylethyl)aminoethyl]benzene(Phepy2) toward the active center model of galactose oxidase. The results of crystal analysis have showed that the crystal of $[\text{Cu}(\text{Crepy}2)\text{Cl}_2] \cdot \text{CH}_2\text{Cl}_2$ (I) belongs to monoclinic system, space group $P2_1/n$ with unit cell dimensions of $a=9.002(1)$, $b=2.871(4)$, $c=22.817(11)\text{\AA}$, $\beta=97.03(6)^\circ$; $V=2623.7(14)\text{\AA}^3$; $Z=4$; the final structure gave the R 0.051, R_w 0.046, and the crystal of $[\text{Cu}(\text{Phepy}2)(\text{ClO}_4)_2](\text{II})$ belongs to orthorhombic system, space group $Pna2_1$ with unit cell dimensions of $a=18.003(1)$, $b=15.376(1)$, $c=9.054(1)\text{\AA}$; $V=2506.3(6)\text{\AA}^3$; $Z=4$; the final structure gave the R 0.055, R_w 0.049. The copper atom exhibits trigonal bipyramidal coordination geometry in $[\text{Cu}(\text{Crepy}2)\text{Cl}_2] \cdot \text{CH}_2\text{Cl}_2$ but distorted square pyramidal coordination geometry in $[\text{Cu}(\text{Phepy}2)(\text{ClO}_4)_2]$. Their structural properties compared with those of active centers of galactose oxidase and other copper-containing enzymes were described.

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