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Title: Synthesis and characterization of bio-inspired copper complexes as models for lytic polysaccharide monooxygenases

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Abstract:

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This work is inspired by the naturally occurring enzyme named lytic polysaccharide monooxygenases. Lytic polysaccharide monooxygenases (LPMOs) are enzymes that use an oxidative mode of action to cleave the glycosidic bonds of polysaccharides. The exact identity and mechanistic aspects of catalytically active species of LPMOs are still unknown. Here, we aim to develop a copper hydroperoxo species with an N3 coordination site mimicking the active site of

LPMOs and study whether the intermediate performs the oxidative cleavage of glycosidic bonds. In this context, six mononuclear copper(II) complexes were synthesized by changing the secondary coordination sphere to explore the effect of flexibility vs. rigidity of complexes on copper hydroperoxo intermediate. Then the reactivity of copper(II) complexes with hydrogen peroxide were checked. Complex 5 was found suitable to generate copper hydroperoxo intermediate. Therefore, structural rigidity plays a vital role in stabilizing hydroperoxo moiety. This study can be extended further to investigate the oxidative cleavage of

glycosidic bonds.

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