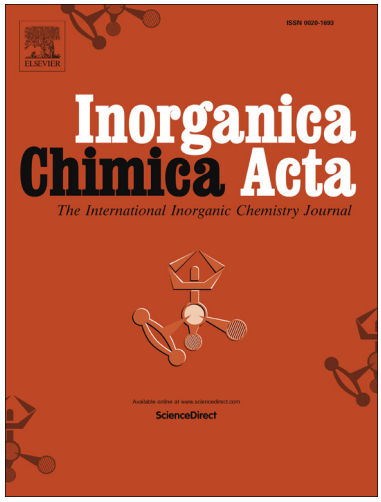

Research paper

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Effects of Denticity and Ligand Rigidity on Reactivity of Copper Complexes with Cumyl Hydroperoxide

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KEYWORDS: Copper coordination chemistry, oxidation reactions, complex characterization, O-O bond cleavage mechanism, cumyl hydroperoxide

ABSTRACT

Cu(II) complexes bearing N2/Py2 tetradentate ligands consisting of two pyridyl arms and a flexible ethyldiamine backbone, [(BPMEN)Cu(ClO_4)$_2$] (**1**), with rigid cyclohexyl backbone [(BPMCN)Cu(ClO_4)$_2$] (**2**), and substituted with bispyrrolidyl [(PDP)Cu(ClO_4)$_2$] (**3**), and Cu(II) complex bearing N2/Py3 pentadentate ligand, [(TPMEN)Cu(ClO_4)$_2$] (**4**), were synthesized and structurally characterized. Reactivity of **1-4** with cumyl hydroperoxide was investigated to study the effects of ligand rigidity and denticity on the mechanism of O-O bond cleavage. Results presented herein illustrate that **1-3** favors homolysis, however **4** showed little to almost no impact on O-O bond cleavage.