Kinetics and DFT Studies on the Reaction of Copper(II) Complexes Supported by *N,N*-Bis(2-quinolylmethyl)amine Tridentate Ligands toward H_2O_2

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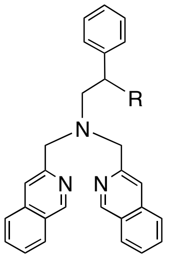
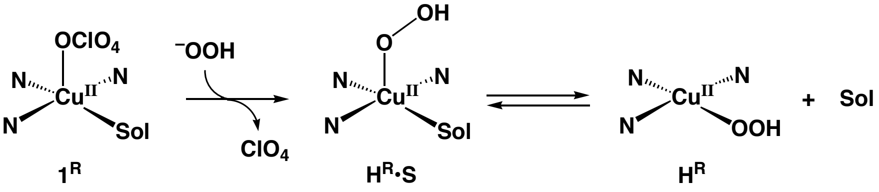
Kinetics and DFT studies on the reaction of copper(II) complexes supported by bulky tridentate ligands L1^R (*N,N*-bis(2-quinolylmethyl)amine tridentate ligands) toward H_2O_2 have been investigated in detail.



L1^R
R = H and Ph

The copper(II) complexes exhibit a square pyramidal structure containing a coordinated solvent molecule at an equatorial position and a weakly coordinated counter anion (or water) at an axial position. They reacted readily with H_2O_2 at a low temperature to give mononuclear hydroperoxo copper(II) complexes. Stopped-flow kinetics and DFT studies have suggested that, in the initial stage of the reaction, deprotonated hydrogen peroxide attacks the cupric ion, presumably from the axial position, to give a hydroperoxo copper(II) complex retaining the coordinated solvent molecule (**H^R**•S). **H^R**•S then loses the solvent to give a tetragonal copper(II)-hydroperoxo complex (**H^R**), in which the –OOH group may occupy an equatorial position (Scheme 1). The copper(II)-hydroperoxo complex **H^R** exhibits a relatively high O–O bond stretching vibration at 900 cm^{-1} compared to other previously reported examples.

***Scheme 1*.**



Sol = Solvent Molecule