Mimicking the CuD Site of pMMO via a Copper Cage-Complex

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Abstract:

Understanding of particulate methane monooxygenase (pMMO) is of great interest due to its ability to oxidize methane selective to methanol. Currently, different proposals for its active site and its mechanism of action exist. Among them is the recently found Cu_D site which offers two imdazoles and one amide coordinating to copper.[1] Our group has the interest to model (potential) enzymatic active sites via endohedral functionalized cages. As such, we recently reported a mimicking of the Cu_C site of pMMO.[2] Here we extend this approach towards a structural mimicking of the Cu_D site (Figure 1). The resulting Cu(I) cage complex can catalyze aerobic oxidative transformations such as the selective oxidation of benzylic alcohols to aldehydes. Further, its Cu(II) cage complex was obtained and characterized.

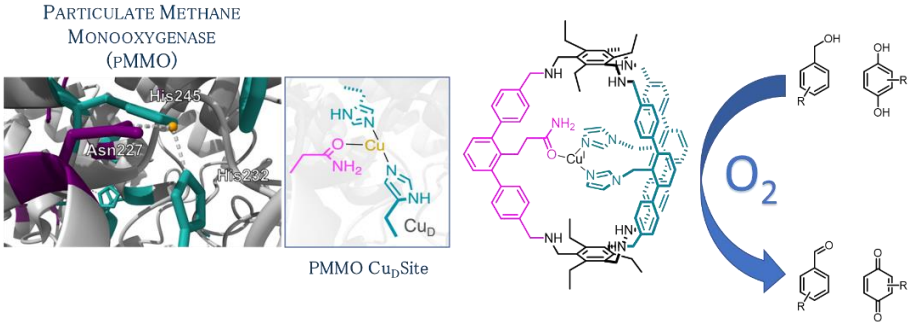

Figure 1: Cu_D site in pMMO, synthesized copper(I) cage complex, and aerobic oxidations of benzyl alcohol and hydroquinone.

[1] C. W. Koo *et al.,* Science, 2022, **375**, 1287-129.
[2] S. C. Bete *et al.,* Angew. Chem. Int. Ed., 2022, **61**, e202206120.