

# Mimicking Copper Active Sites with Cage Ligands

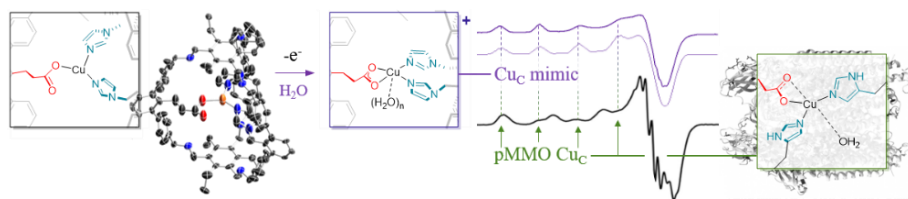
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Imidazole units are a reoccurring motive in the active sites of copper enzymes e.g. tyrosinase (Tyr) or the Cu<sub>B</sub> site of particulate methane monooxygenase (pMMO). Heteroleptic coordination environments are known, where copper is additionally coordinated by other ligands such as carboxylates, like in the Cu<sub>C</sub> site of pMMO. *Endo*-Functionalized cage compounds have been shown to act as ligands towards transition metals, leading to catalysts with interesting properties for example unusual selectivity, increased turnover number or a switchable behavior.<sup>[1]</sup>

Here, *endo*-functionalized organic cages are presented, that mimic the ligand spheres found in enzymes. For instance, they offer three imidazole units, coordinating to copper in a mode, which is reminiscent to the ones occurring at enzymatic active sites.<sup>[2]</sup> These can be used as catalysts for the aerobic oxidation of organic substrates. We could expand this strategy of cages to coordinate to metal centers in a bio-inspired fashion towards a heteroleptic ligation.<sup>[3]</sup> Such cages can be used to mimic the coordination in the Cu<sub>C</sub> site of pMMO (Figure 1).<sup>[4]</sup>



**Figure 1:** Mimicking the Cu<sub>C</sub> site of pMMO via an endohedral-functionalized cage.

[1] M. Otte, Eur. J. Org. Chem. 2023, e202300012.

[2] S.C. Bete, M. Otte, Chem. Commun. 2019, 55, 4427-4430.

[3] S.C. Bete, M. Otte, Angew. Chem. Int. Ed. 2021, 60, 18582-18586.

[4] S.C. Bete, L.K. May, P. Woite, M. Roemelt, M. Otte, Angew. Chem. Int. Ed. 2022, 61, e202206120.