Regioselective Catalytic C-H Oxidation of Hydrocarbons in Aqueous Solution

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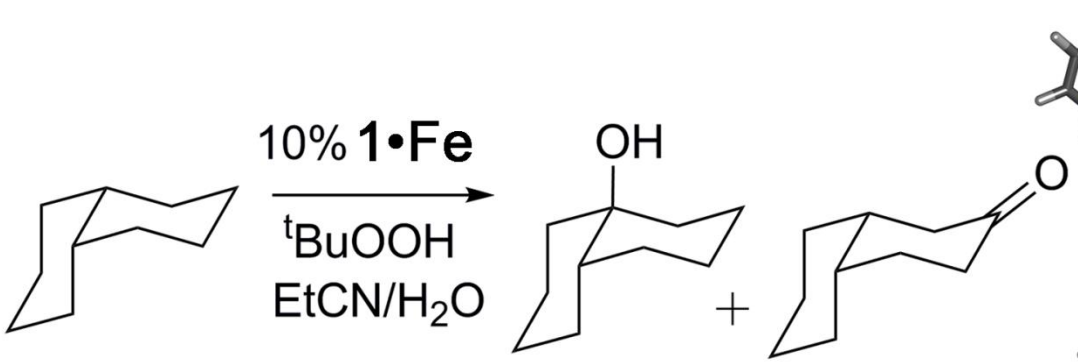
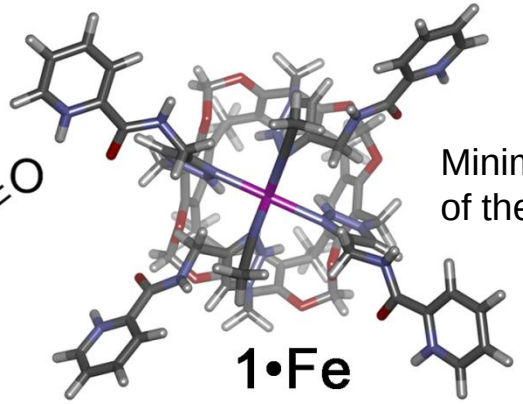
We aim to prepare new biomimetic catalysts that can *both* selectively bind substrate and activate it for reaction. This behavior is the hallmark of enzymatic catalysis: we seek to apply this to non-natural reactions such as hydrocarbon oxidation.

To achieve this, we have synthesized a series of water-soluble receptor molecules (cavitands) that can coordinate high oxidation state metal ions in aqueous solution while still retaining a defined cavity for molecular recognition. These cavitands that are water-soluble, able to *self-fold* upon coordination with suitable metals and can perform catalytic C-H oxidation reactions of unfunctionalized alkanes with little to no degradation in aqueous solvents. The catalysts are tolerant to the oxidation conditions and are capable of challenging oxidation reactions under mild conditions. The next challenge is to apply these successes to a host that displays a larger cavity for guest recognition and does not suffer from cavity blockage by the bound metal ions.





Minimized representation of the **1**:Fe(II) complex