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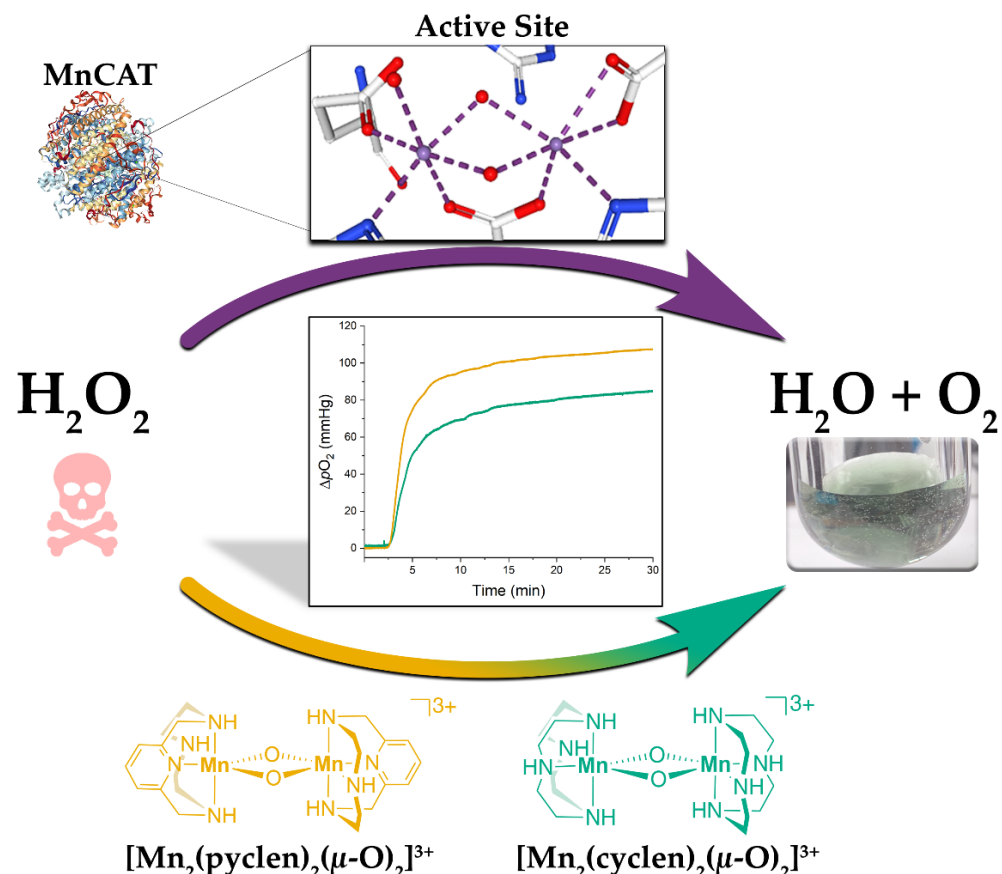


Hydrogen Peroxide Disproportionation with Manganese Macrocyclic Complexes of Cyclen and Pyclen

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Mn Pyridinophanes as Catalysts for H_2O_2 Disproportionation



- **ROS is a threat to multiple types of tissues and cells**
 - Contributes to the development of neurodegenerative, pulmonary, and cardiovascular diseases as well as promote a number of inflammation pathways
- **Catalase family of enzymes**
 - Mitigate the risk from ROS
 - Most catalase enzymes contain an iron-protoporphyrin IX prosthetic group (FeCAT)
 - Some bacteria use manganese-based catalases (MnCAT)

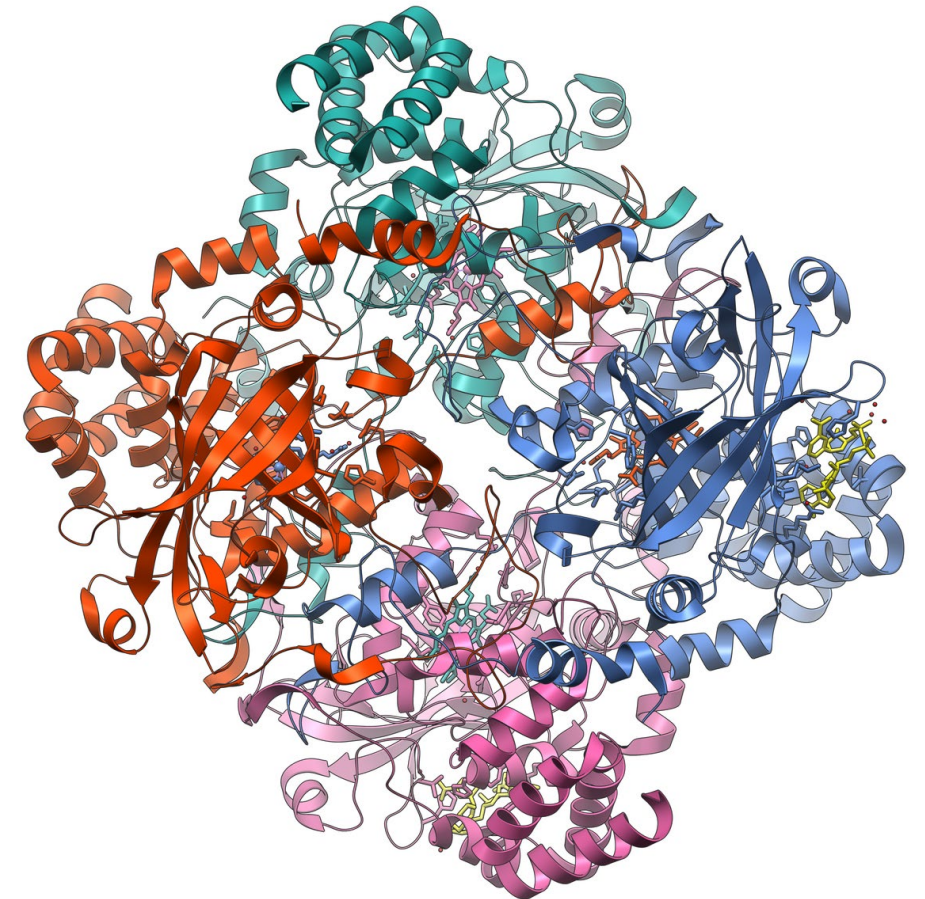
Catalase

The Enzyme that Balances ROS

- Found in living organisms exposed to oxygen
- It catalyzes the decomposition of hydrogen peroxide to water and oxygen.

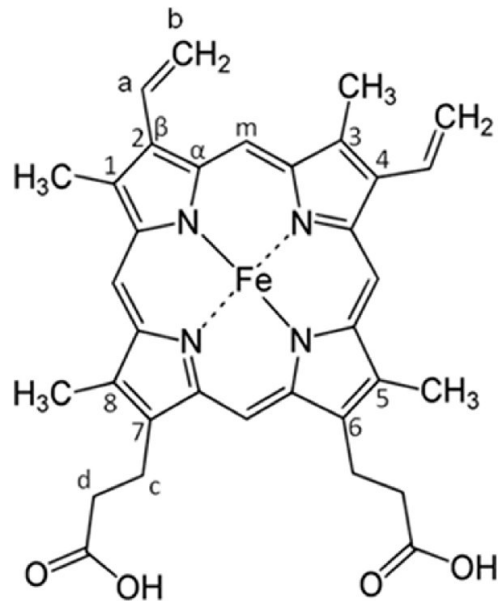


- It protects the cell from oxidative damage by reactive oxygen species (ROS).
- One catalase molecule can convert millions of hydrogen peroxide molecules to water and oxygen each second



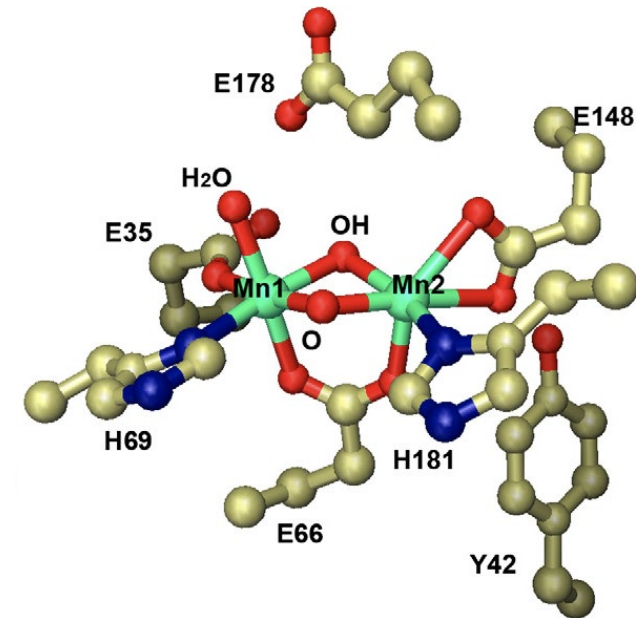
Metal Centers Found in Catalases

Fe-Based Catalases



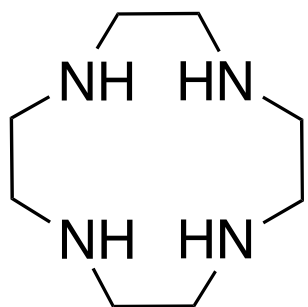
Fe(III) Protoporphyrin IX Prosthetic Group
(Heme)

Mn-Based Catalases

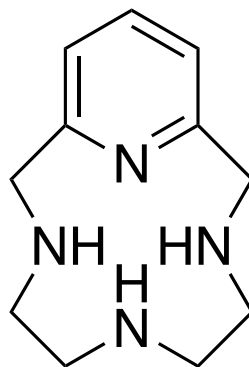


Binuclear Manganese Active Center

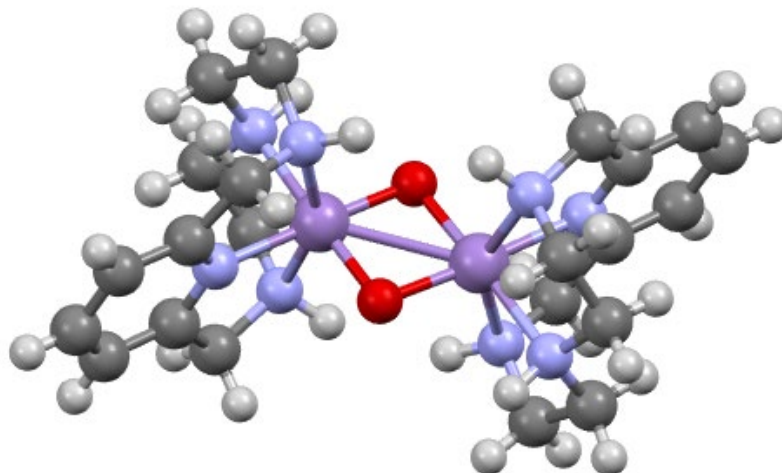
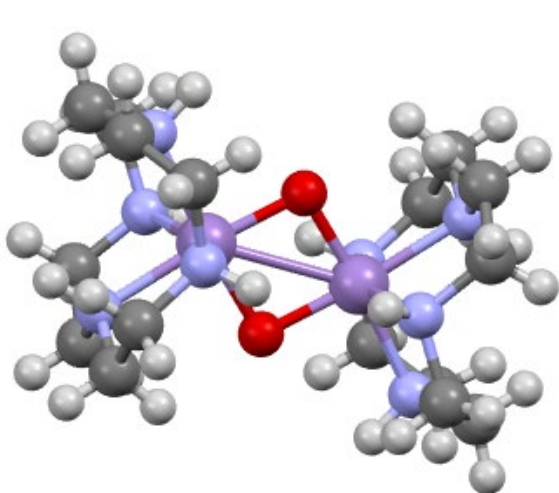
Mn Complexes Synthesized within the Green Group



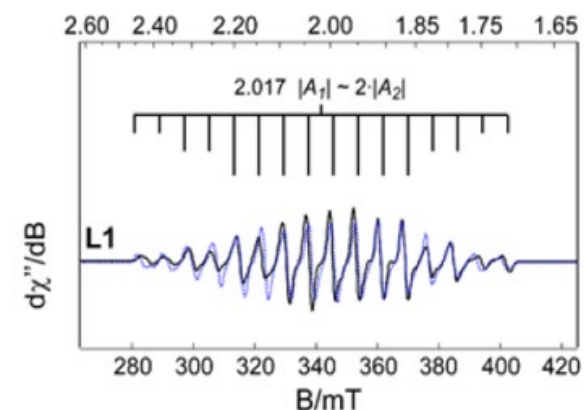
Cyclen



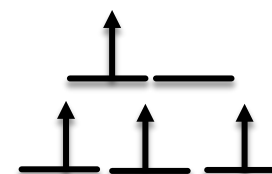
Pyclen



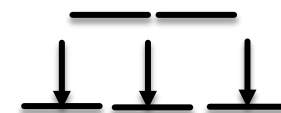
Electron Paramagnetic Resonance (EPR)



16-Line EPR Spectra MnCAT
Centered at ~2.00 Ghz

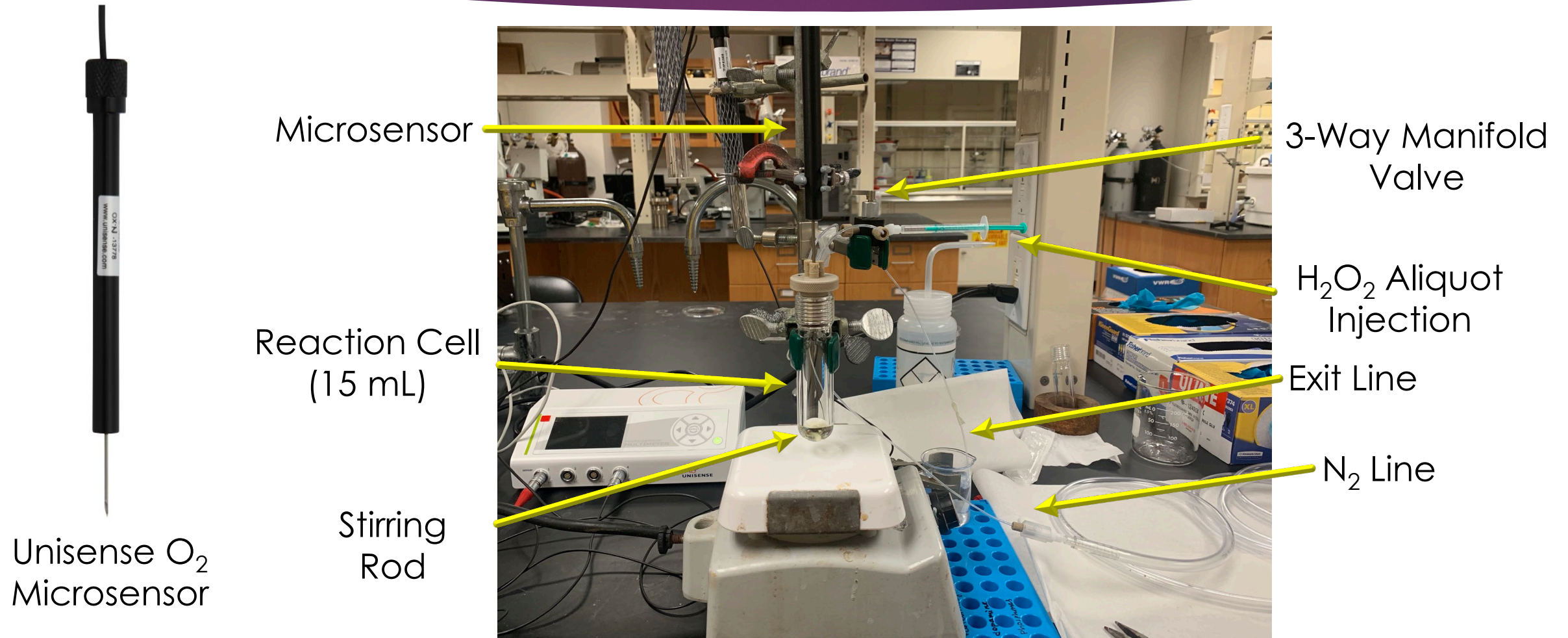


Mn(III) d^4



Mn(IV) d^3

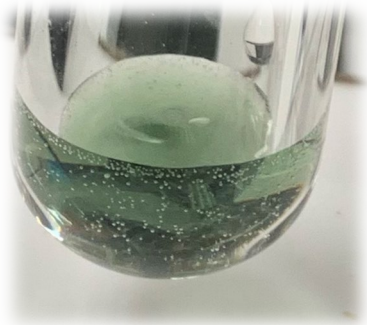
How did we measure O_2 production?



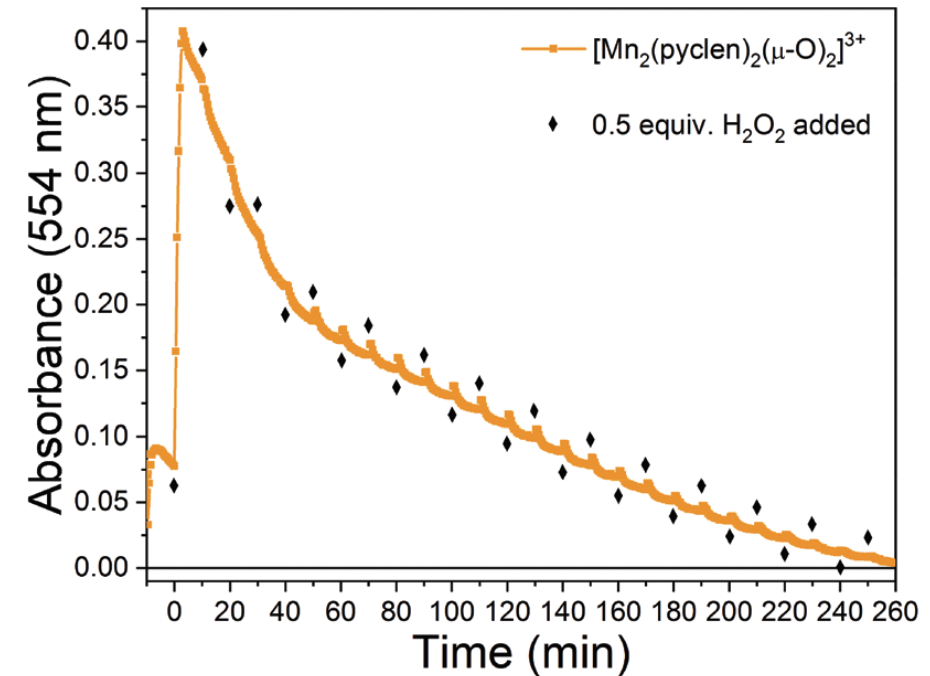
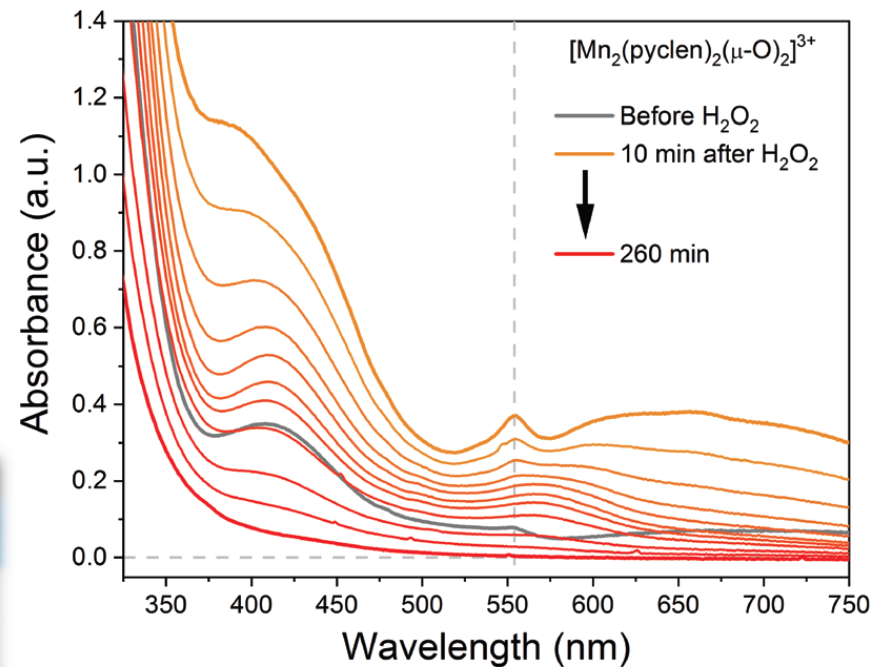
O₂ Production and Color of the Solutions

UV-Visible Spectroscopy

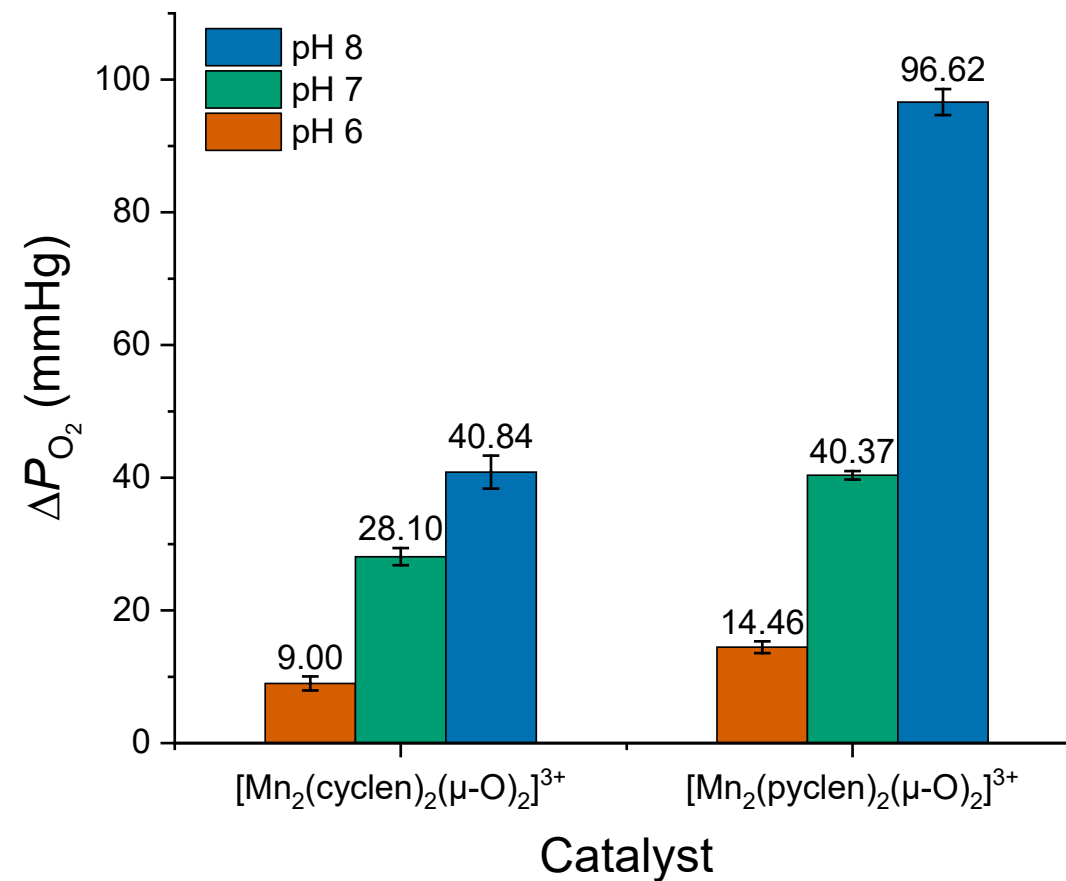
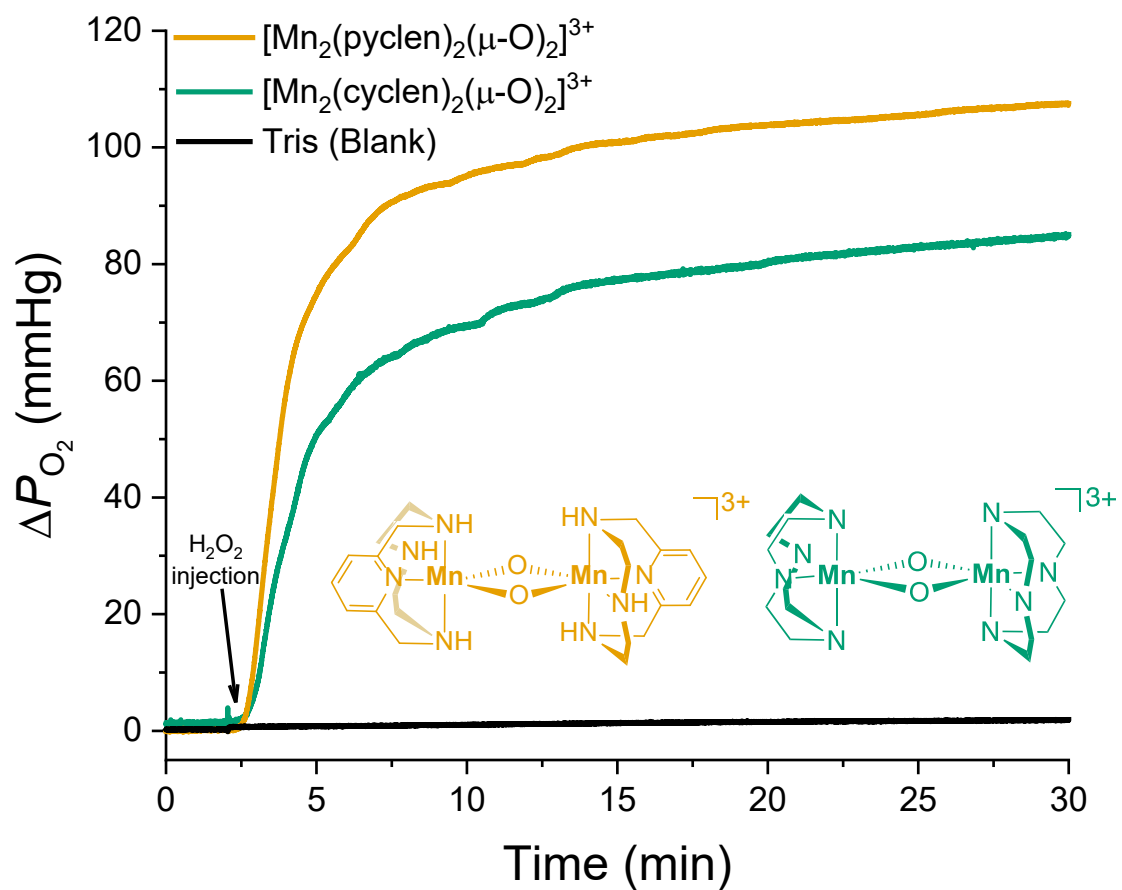
Immediately
after injection
of H₂O₂



~30 seconds
after injection
of H₂O₂

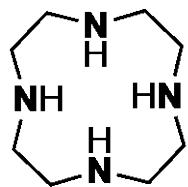


Structure of the Ligand and Reactivity

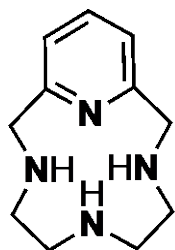


Future Directions

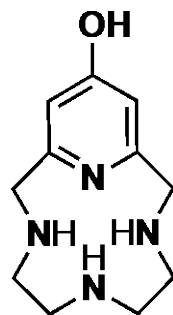
Kinetics and computational methods involving a bigger library of ligands



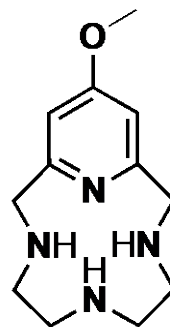
Cyclen (N_4)



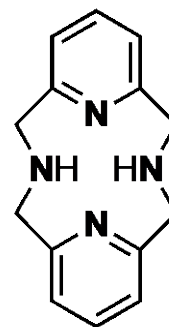
Pyclen (PyN_3)



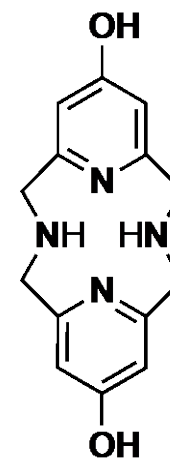
$OH-PyN_3$



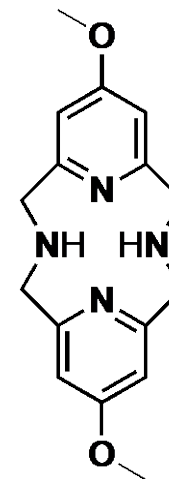
$OMe-PyN_3$



Py_2N_2



$OH,OH-Py_2N_2$



$OMe,OMe-Py_2N_2$

Acknowledgements

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Thank you for your attention!

