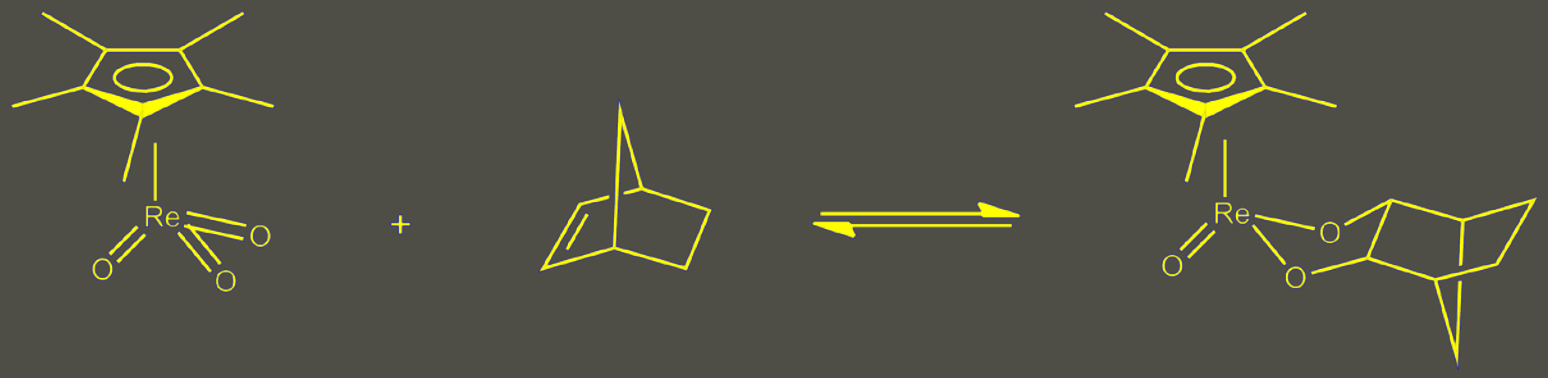
Ligands for Selective Metal Binding

Kevin P. Gable

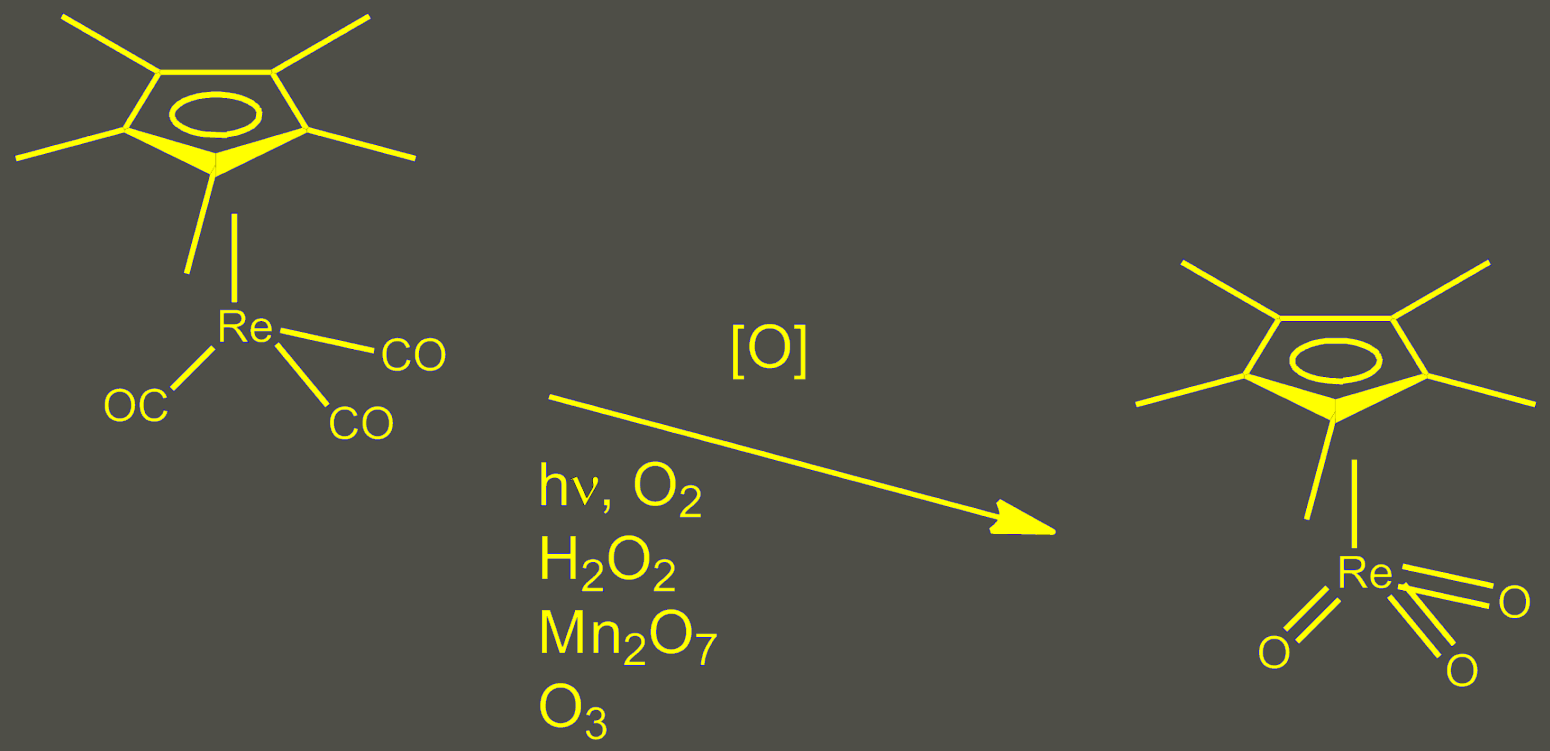
Department of Chemistry

Oregon State University

Ligand-based Metal Chemistry



Synthesis



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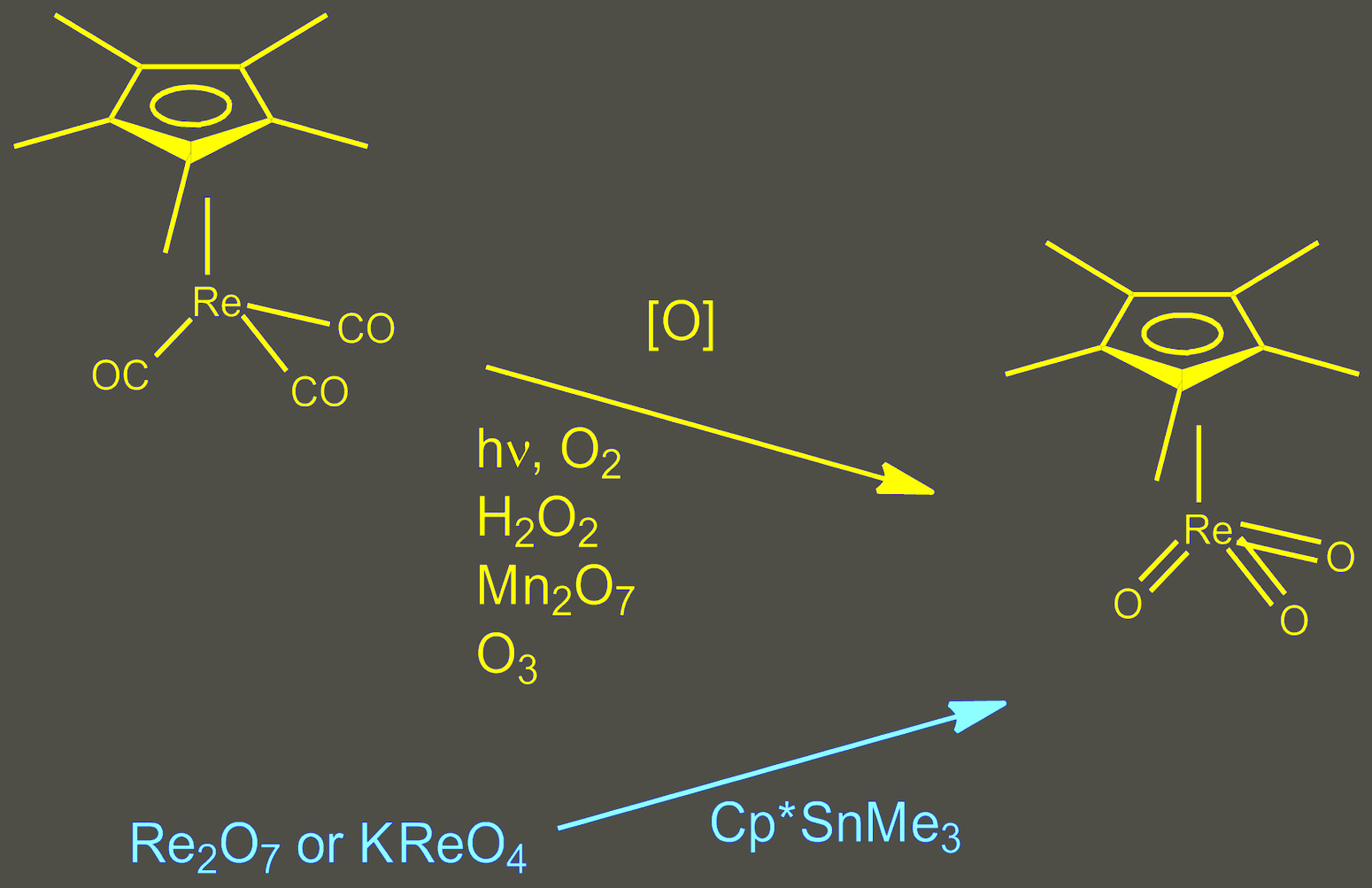
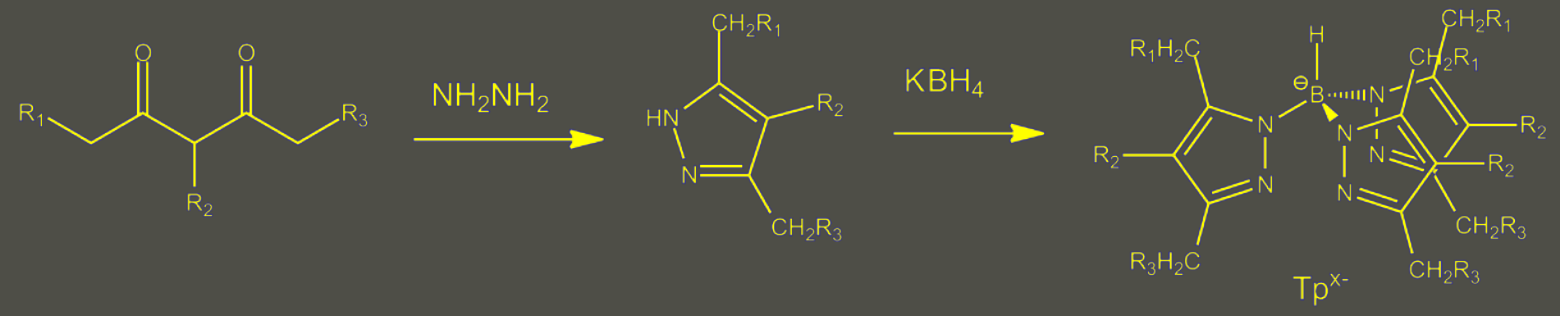
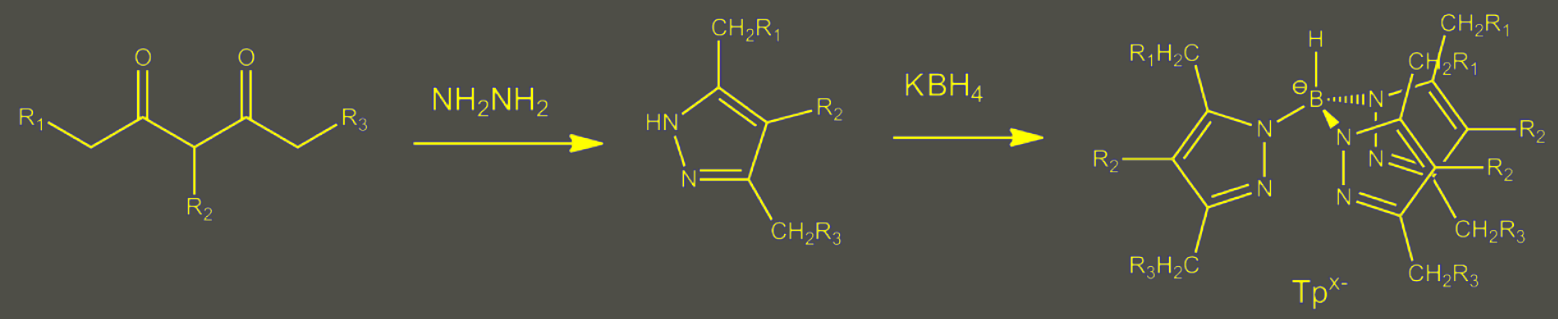
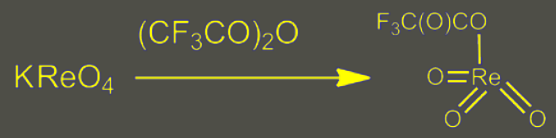


Ligand Variation

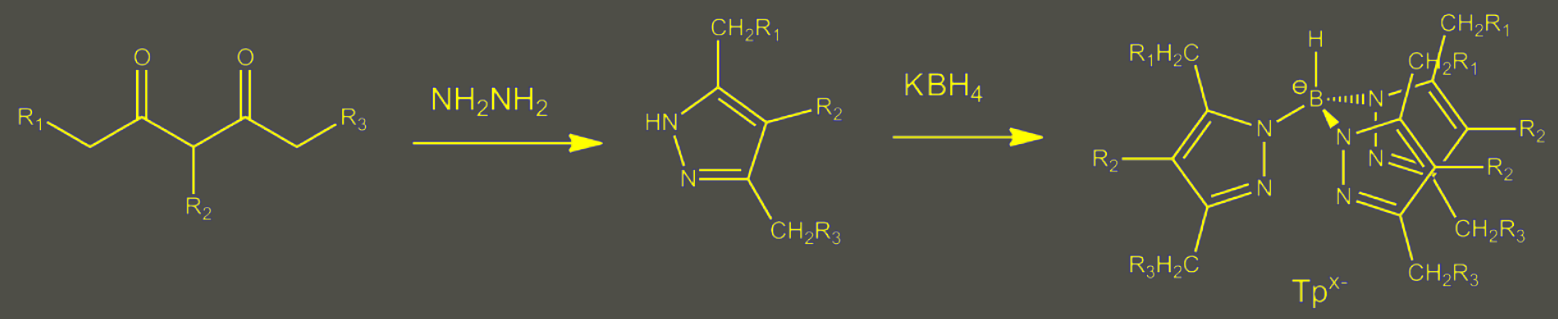


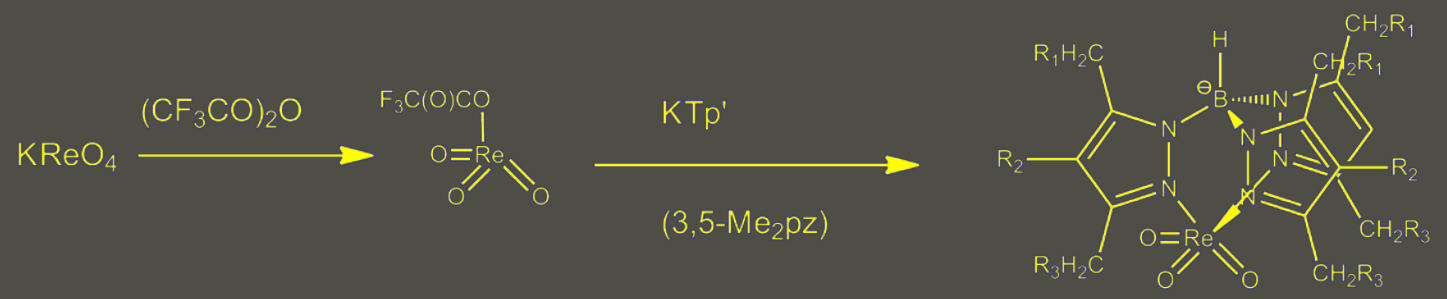
Ligand Variation



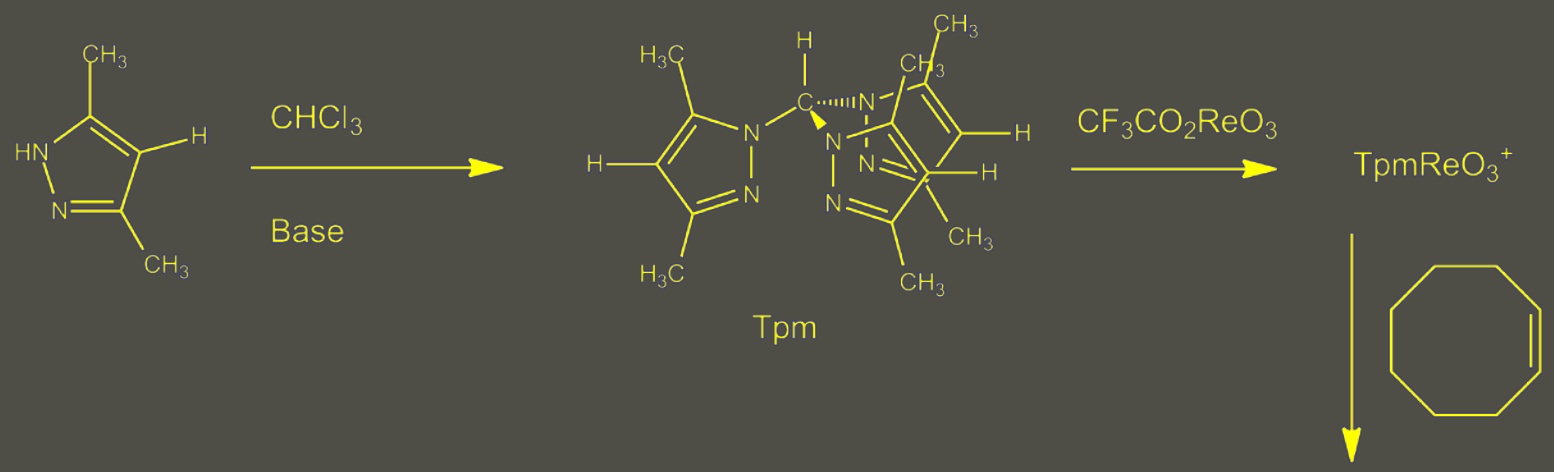


Ligand Variation



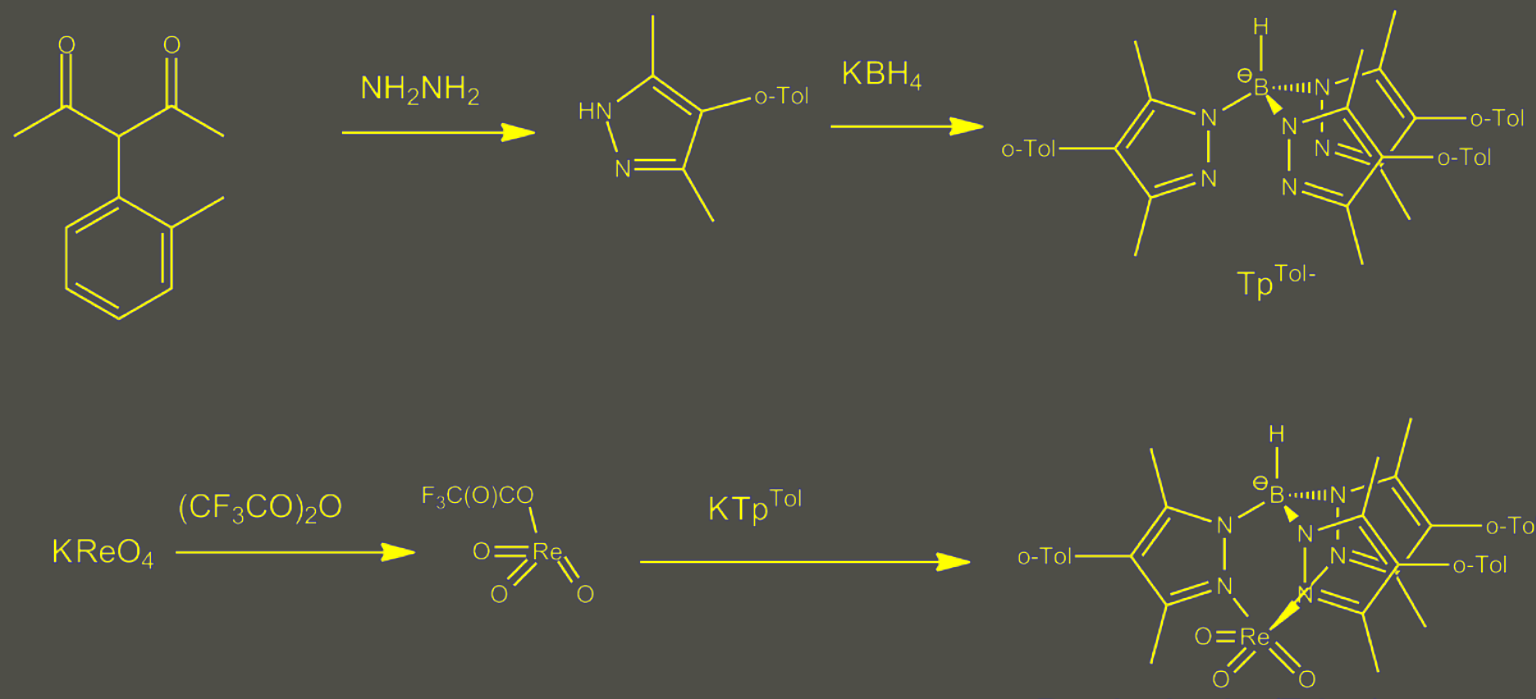


Ligand Control of Chemistry



Thermodynamics agree with computational modeling (B3LYP/LACVP*)

Ligand Control of Chemistry



Rotation barrier (Tol-pz)
= 10 kcal/mol

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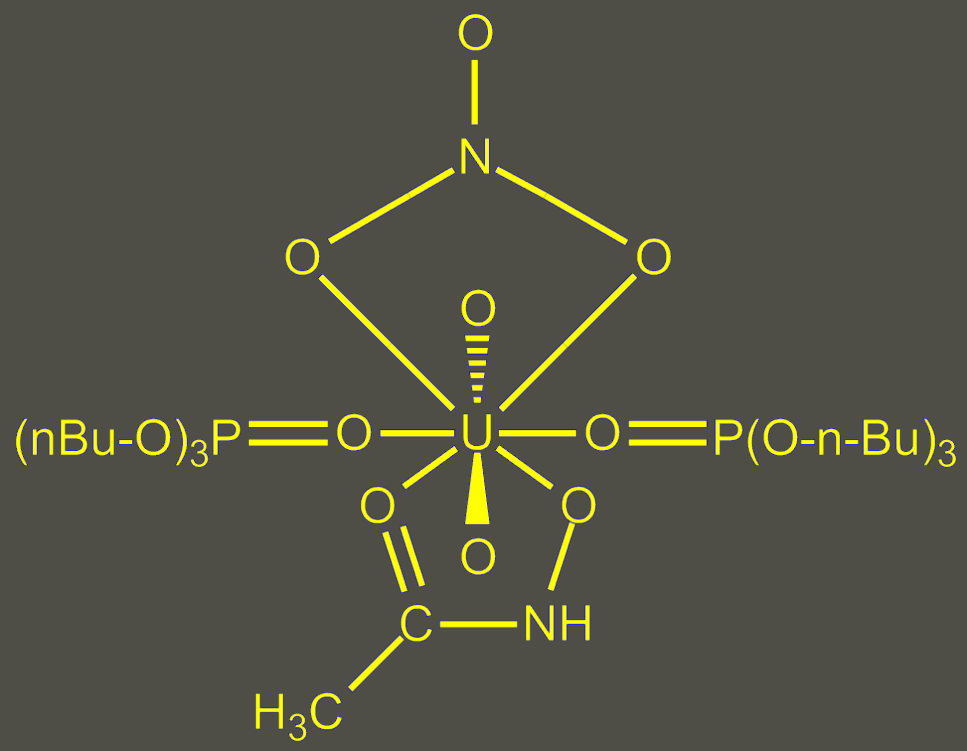
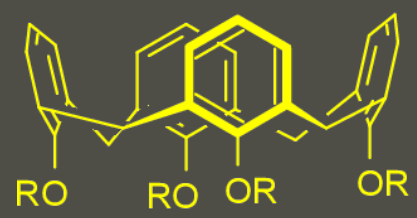
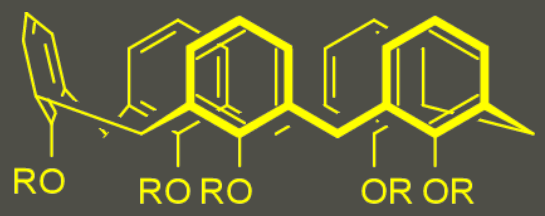
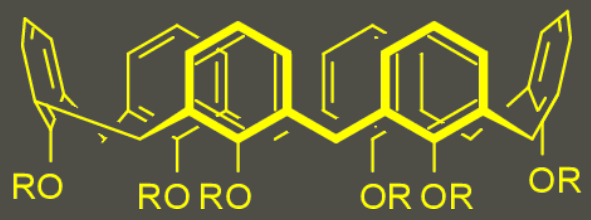


Tkac, P.; Paulenova, A.; Gable, K. P. *Appl. Spectr.*, **2007**, *61*, 772-776

Ligands for Selective Binding







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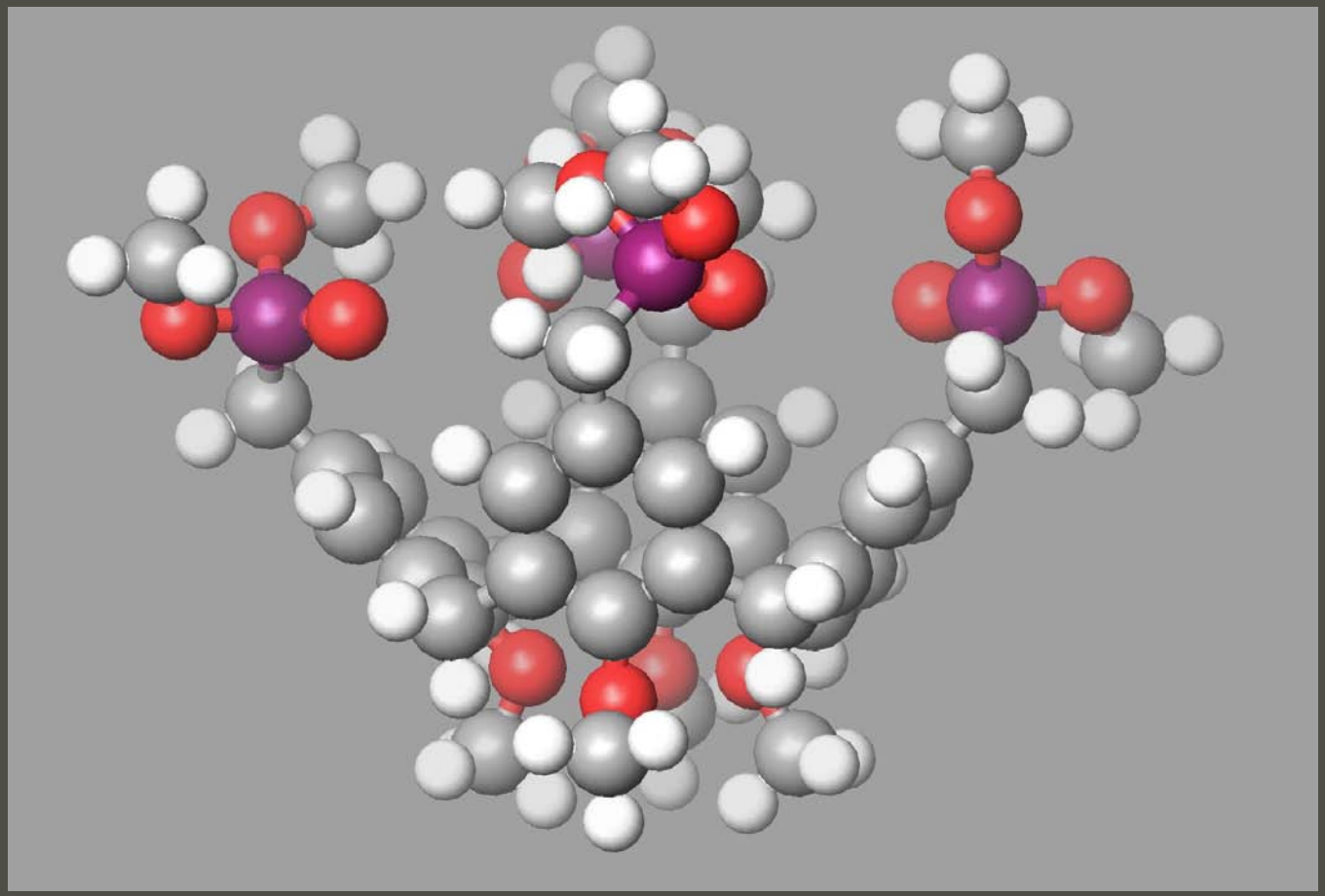
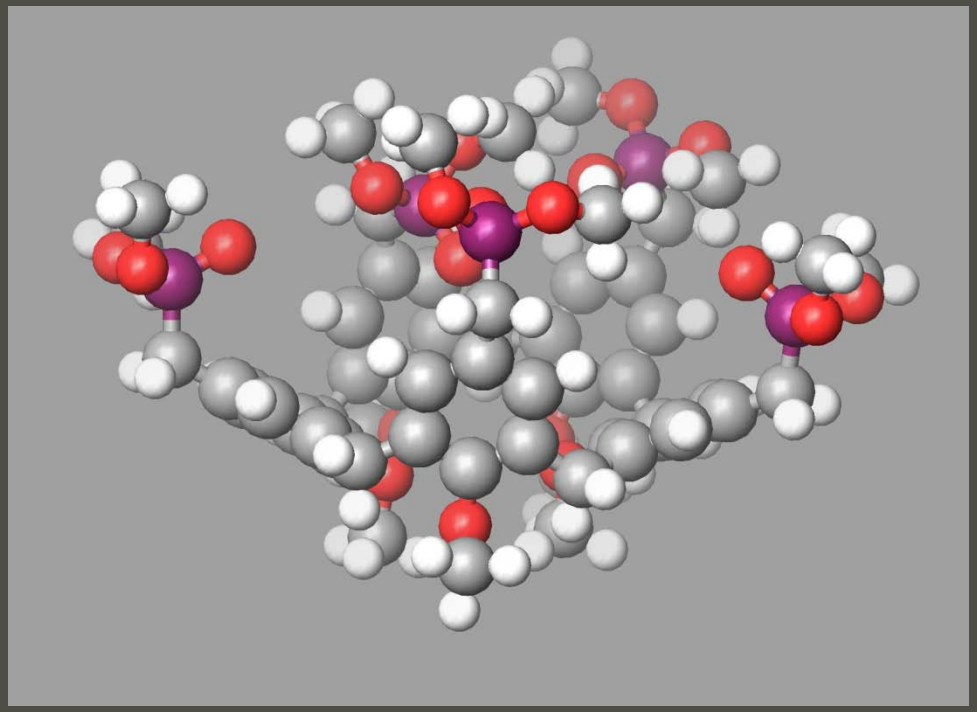


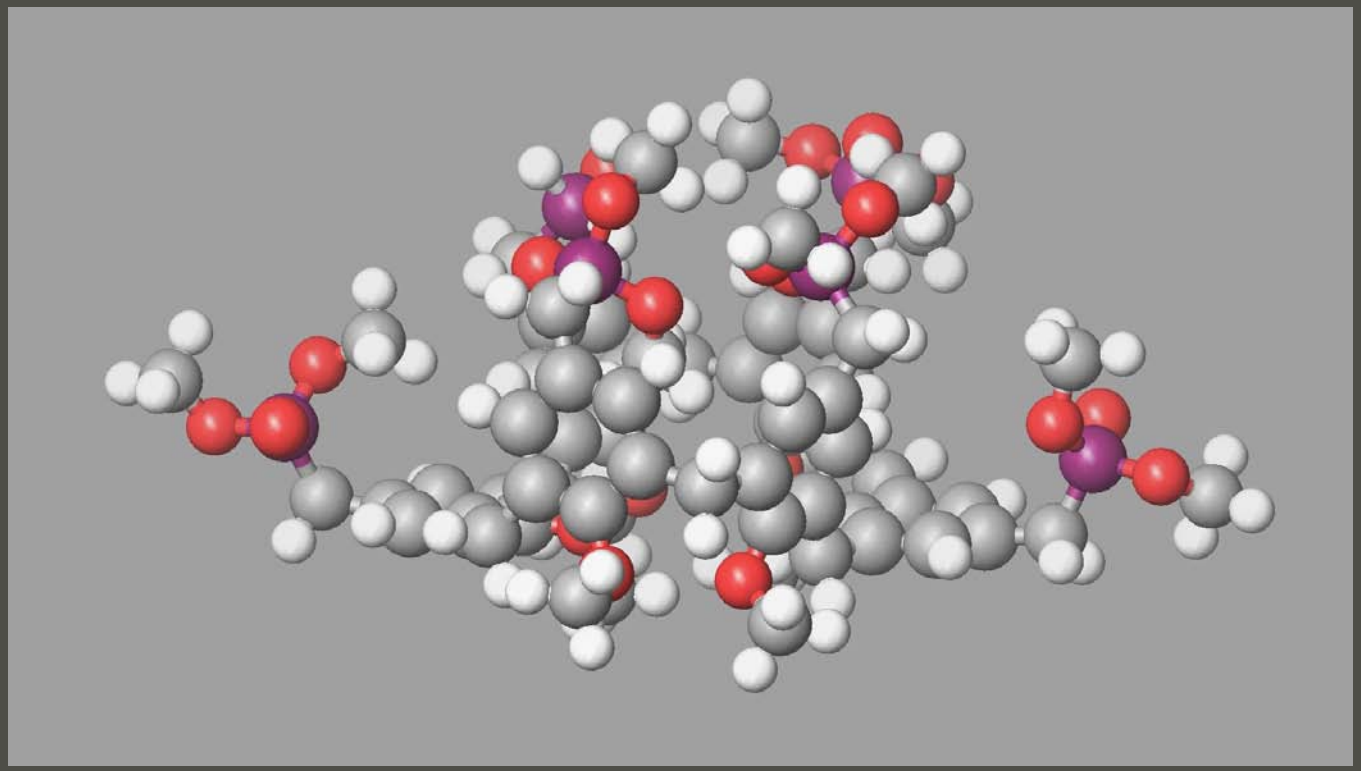
Calix-4-arene (B3LYP/6-31G*): Cavity = 6.55 Å

Ligands for Selective Binding



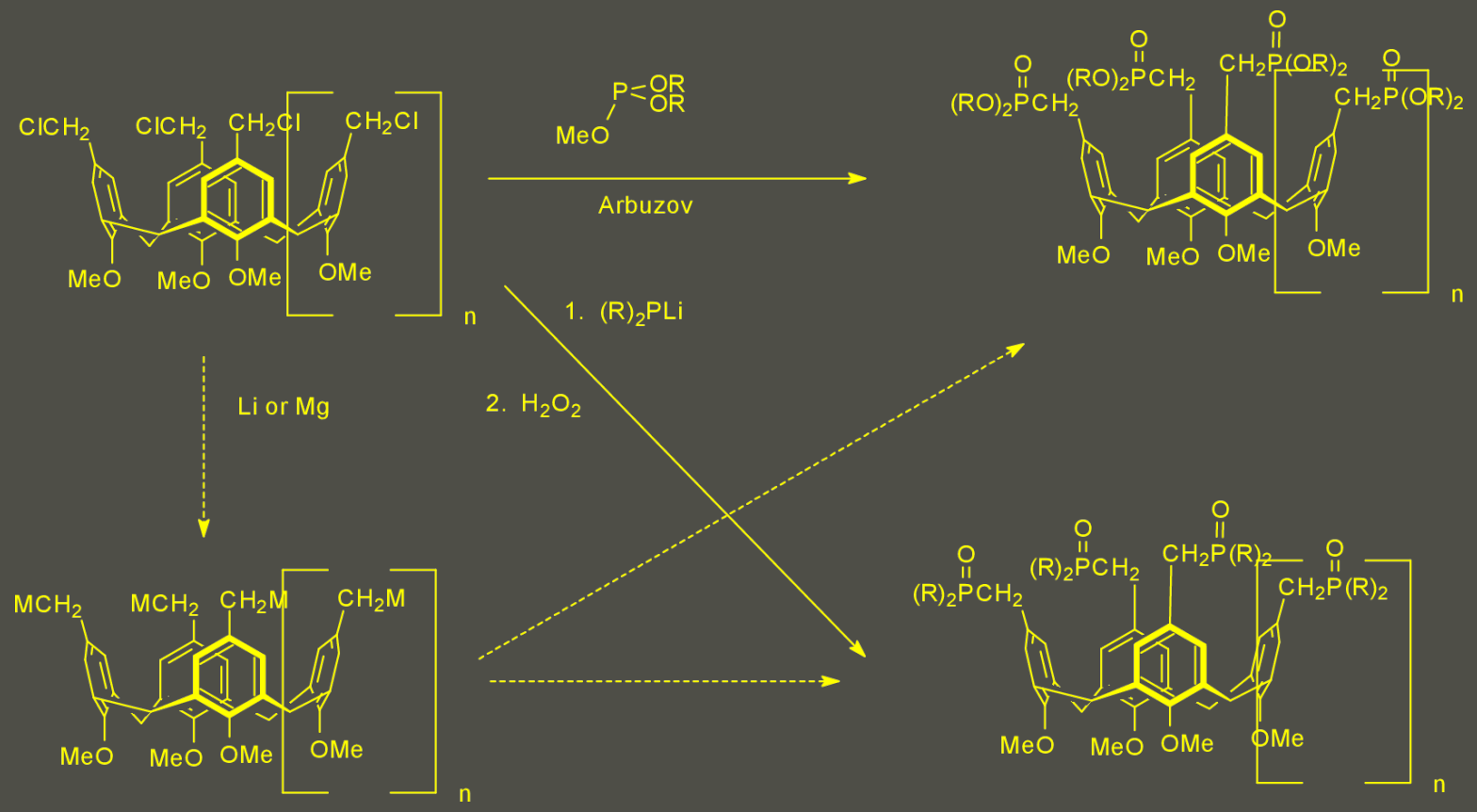
Calix-5-arene (B3LYP/6-31G*)
Cavity = 6.97 Å

Ligands for Selective Binding



Calix-6-arene (B3LYP/6-31G*)
Cavity = 7.82 Å

Ligands for Selective Binding



Conclusion

- Our program at OSU has the capacity to synthesize a variety of ligands for metal binding
- We can model binding affinity
- We can predict consequences of structural variation