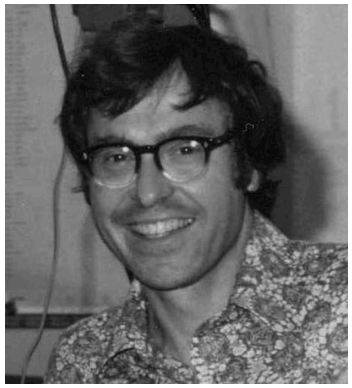
Day 9: Principles of Catalysis and Ancillary Ligand Design

TODAY'S TOPICS

- Principles of catalysis
- Phosphine
- NHCs

CHEMIST OF THE DAY



name?
known for?

QUOTE OF THE DAY

"Today is gone. Today was fun.
Tomorrow is another one.
Every day,
from here to there,
funny things are everywhere."

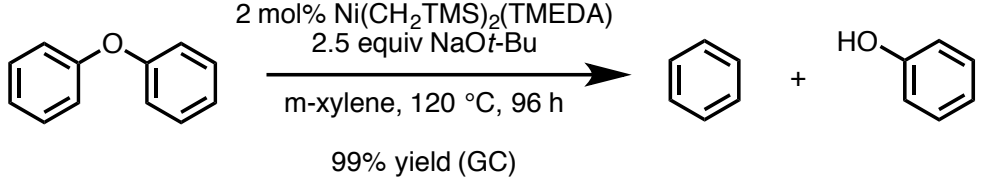
- Dr. Seuss

READING

Hartwig: Ch. 2.3, 14
Crabtree: Ch. 4.2, 4.3

PROBLEMS OF THE DAY

#1 Consider the following diaryl ether hydrogenation method reported by Hartwig (*JACS* **2012**, *134*, 20226). **Propose one or more experiment(s) to elucidate whether the reaction is homogenous or heterogeneous.**

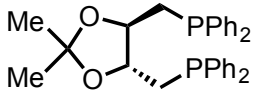


99% yield (GC)

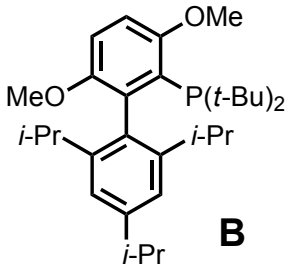
#2 **A.** Imagine a generic mono-phosphine complex of the form $(CO)_3Ni(PR_3)$. **Predict how the CO stretching frequency would compare to that of $Ni(CO)_4$.**

B. Now consider a series of $(CO)_3Ni(PR_3)$ complexes where R = aryl, alkyl, alkoxy. **Predict how the CO stretching frequency would vary across this series.**

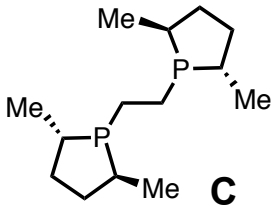
#3 For the following three phosphine ligands below, **propose a preparative route, provide the name, and the give the name of the inventor.**



A



B



C

#4 **A.** Consider the following two complexes below and **rationalize the observed ^{195}Pt NMR shifts.**

[(SIMes)Pt(dmso)(Cl)$_2$]	[(IMes)Pt(dmso)(Cl)$_2$]
991.8 ppm	1017.0 ppm

B. Based on your answer for part A, **design one or more additional experiment(s) to further test your working hypothesis.**