Day 13: Catalytic Carbonylation

TODAY'S TOPICS

-Monsanto acetic acid process
-Cativa process
-Hydroformylation with cat. Co
-Hydroformylation with cat. Rh
-Hydroaminomethylation
-Related reactions

CHEMIST OF THE DAY

name?
known for?

QUOTE OF THE DAY

"The cave you fear to enter holds the treasure you seek."

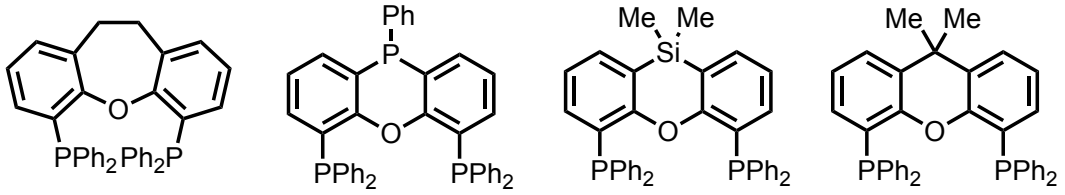
- Joseph Campbell

READING

Hartwig: Ch. 17
Crabtree: Ch. 9.4

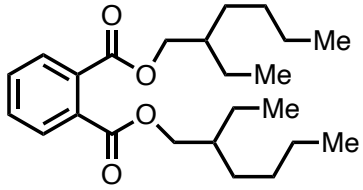
PROBLEMS OF THE DAY

#1 In Rh-catalyzed hydroformylation, the bite angle of the bisphosphine ligand (β_n) is known to influence the equitorial/equitorial:equitorial/axial (ee:ea) ratio in which the bisphosphine coordinates in the catalyst resting state and the linear:branched (l:b) ratio of the product. Within the ligand series below: based on your mechanistic understanding, **predict (A) whether wide or narrow bite angles favor the *linear* product, and (B) whether there is a relationship between ee:ea ratio and l:b ratio.**



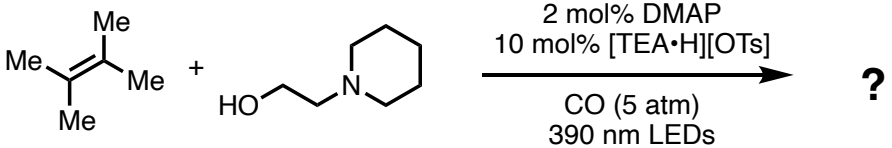
1. Homoxantphos (102.0°) **2**. Phosxantphos (107.9°) **3**. Sixantphos (108.5°) **4**. Xantphos (111.4°)

#2 Di(2-ethylhexyl)phthalate (DEHP or "dioctyl phthalate") is a plasticizer for polyvinyl chloride and is thus ubiquitous is modern society. **Propose a synthesis of DEHP from ≤ C3 and aromatic feedstocks.**



(DEHP)

#3 Consider the following reaction below. **Predict that major product and provide a plausible catalytic cycle that accounts for involvements of light, [TEA•H][OTs]. and DMAP.**



(1 equiv) (1 equiv)