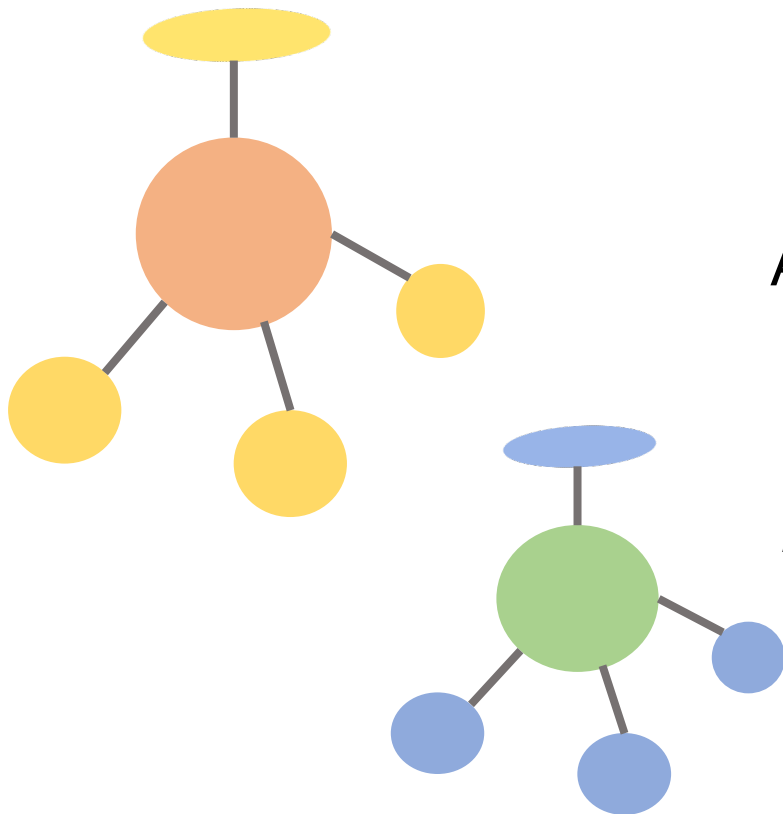


Design and Analysis of Organometallic Catalysts for the Synthesis of Better Fuels



Anna Eblen, Chemistry B.S. Major
Alexander Miller, PhD.
Chemistry Department

Additional Support: Allison Smith, PhD candidate

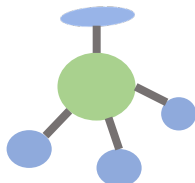


THE UNIVERSITY
of NORTH CAROLINA
at CHAPEL HILL



What catalyst designs improve the conversion of ethanol to n-butanol at lower temperatures and aqueous conditions?

catalyst (noun) -



A catalyst is a molecule or complex that lowers the activation energy required for a reaction to occur, thereby promoting the reactions occurrence.

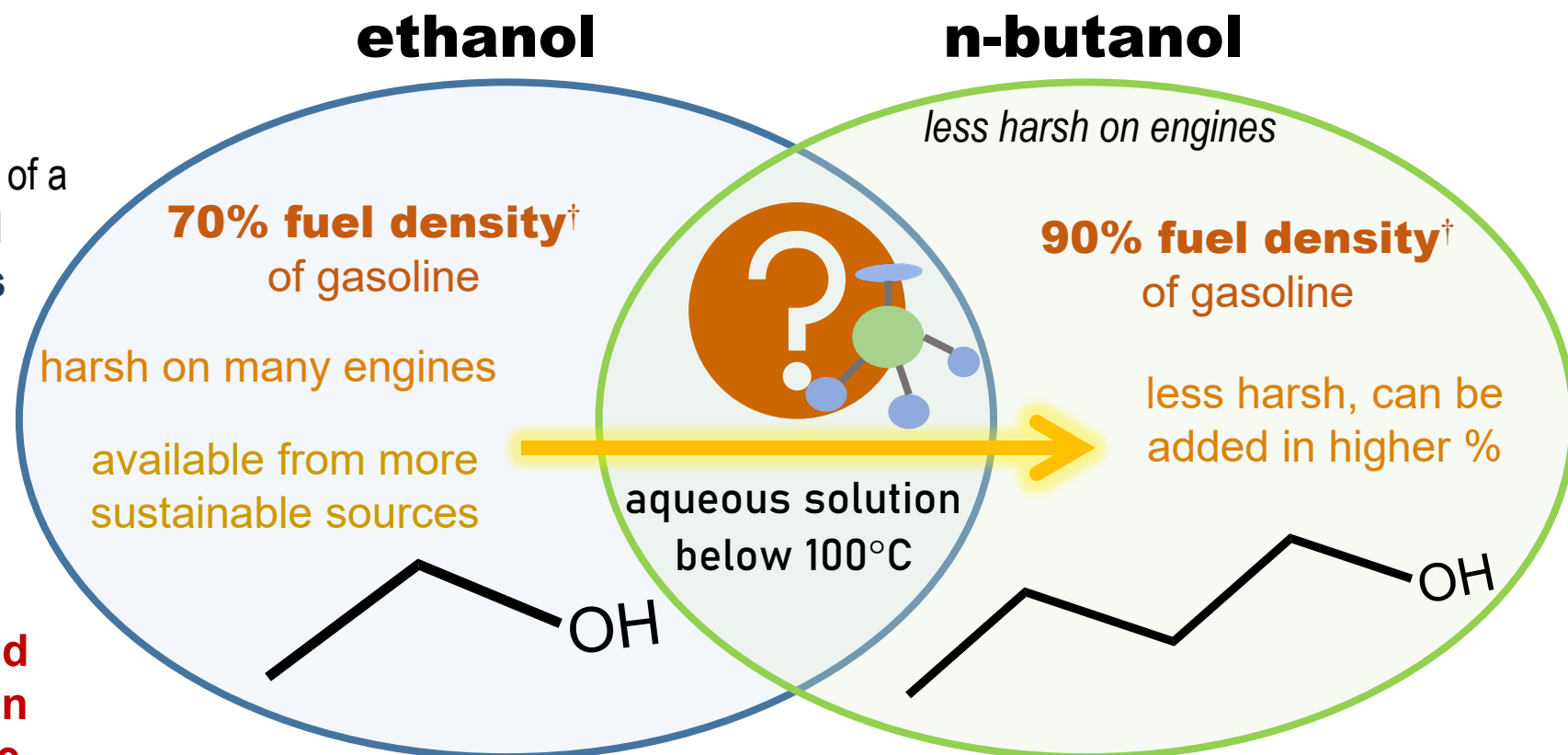
Inorganic catalysts usually consist of a **center metal** atom and connected atoms or molecules called **ligands**

By changing these components we can change how well the catalyst works for our reaction and under what conditions.

Fuel additives that work better and can be used in a higher proportion decrease our reliance on gasoline

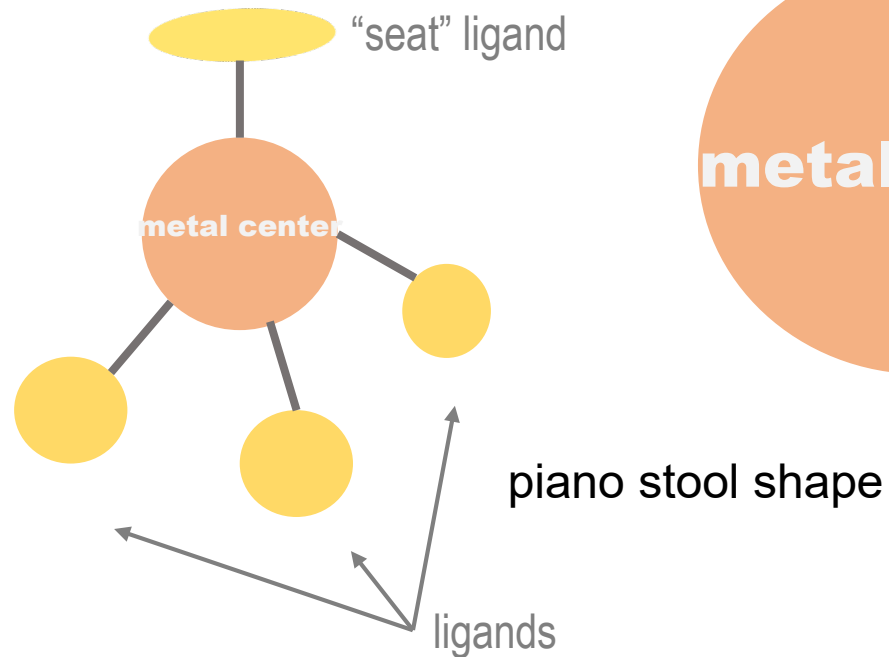


Ethanol is commonly used as a fuel additive in gasoline.



[†] Chakraborty, S.; Piszal, P. E.; Hayes, C. E.; Baker, R. T.; Jones, W. D. Highly Selective Formation of n -Butanol from Ethanol through the Guerbet Process: A Tandem Catalytic Approach. *J. Am. Chem. Soc.* **2015**, 137 (45), 14264-14267 DOI: 10.1021/jacs.5b10257

"Piano Stool" Configuration



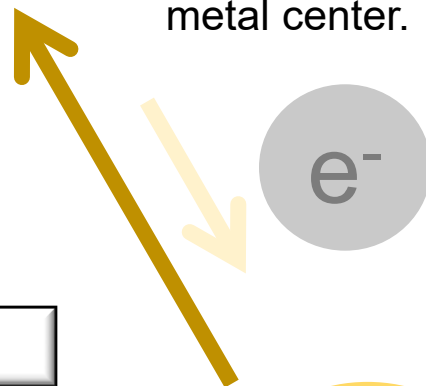
MAJOR DESIGN PRINCIPLES

For all of us...

Being one step closer towards the ability to convert ethanol to butanol means one step away from reliance on gasoline and one step towards more sustainable fuel sources.

Electron Donating Ligands

Ligands can move electron density towards or away from the metal center which affects the reactivity. Electron donating ligands move electron density towards the metal center.



Metal Center

Iridium

or

Ruthenium

Cobalt centers were also tested, but not as successful.

For chemists and collaborators...

Knowing and understanding the trends in design that improve the conversion to butanol will not only allow fine-tuning of this conversion, but can be used to explore other similar processes.

Whether a ligand donates or withdraws electron density depends on its identity and modifier groups called substituents.