Topical Seminar
Bioderived Jet Fuels

Carli Kovel
6-14-2022

From Fuels to Batteries: Distinctions Between Powering Automobiles and Aircrafts

Automobiles

Gasoline

12 gallons, $5.72/gallon NJ = $68.64

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Jet Fuel

High energy content per volume

Challenges: fossil-fuel derived and emissions

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Next Steps: Sustainable Fuels as Drop-In Replacement for Jet Fuel

Current Production of Jet Fuel

1

Desalting
removes H_2O and salts from crude oil

https://www.bp.com/en/global/air-bp/aviation-fuel/jet-fuel.html

Current Production of Jet Fuel

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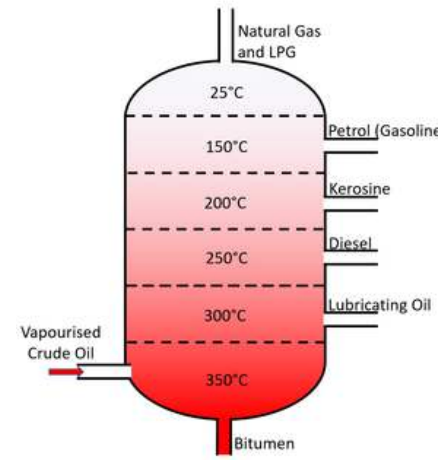

Distillation
Kerosene 175-270 °C

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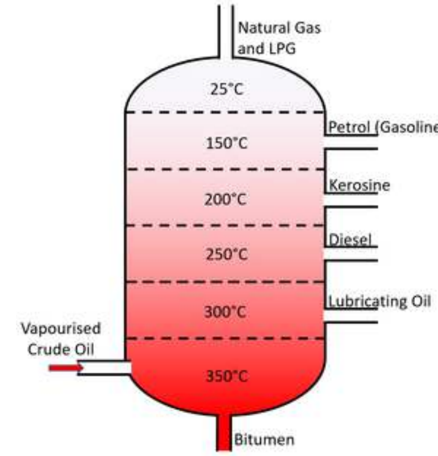

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Processing
Removal of acids, sulphurs, and metals

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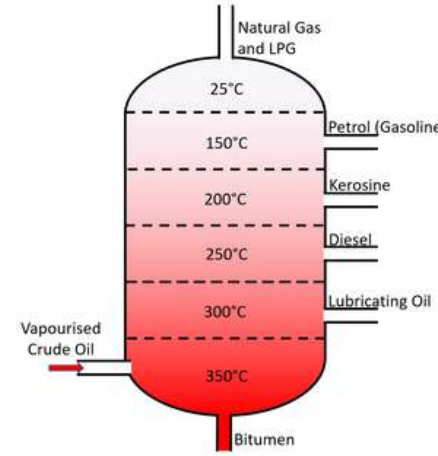

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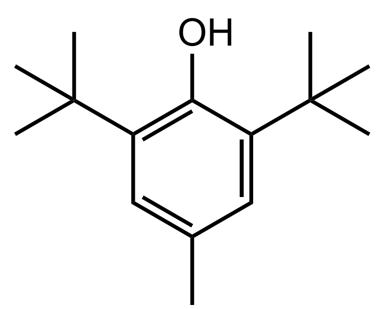

Additives
Improve fuel performance and stability

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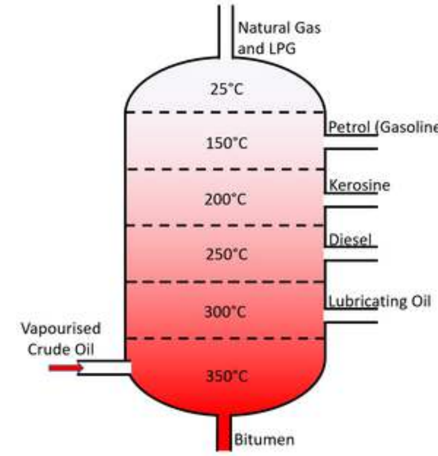

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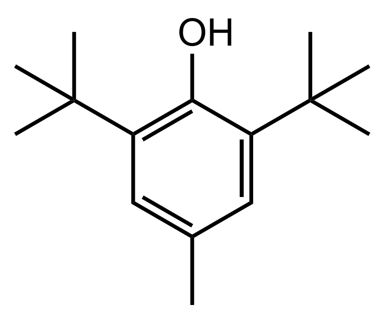

Additives
Improve fuel performance and stability

5

Fuel Delivered to Airplane

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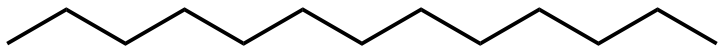
Petroleum-Derived Jet Fuels

Alkanes



- Short Ignition Delays

Muldoon, J. A.; Harvey, B. G., *ChemSusChem* **2020,** *13*, 5777-5807.

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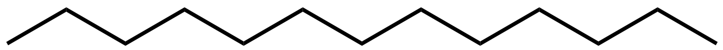

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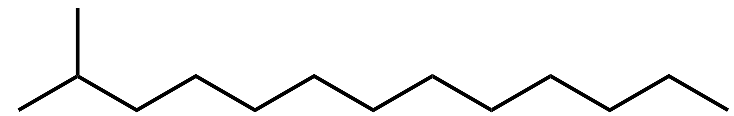

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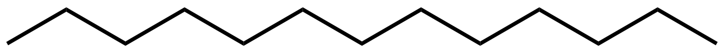

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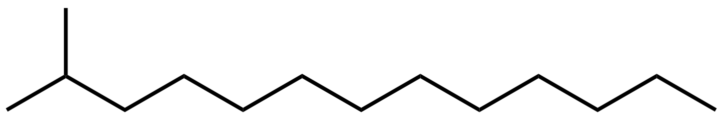

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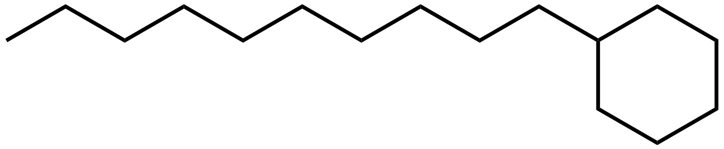
Cycloalkanes



- Increased fuel density compared to acyclic alkanes

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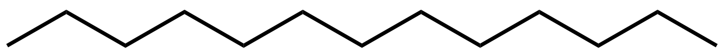

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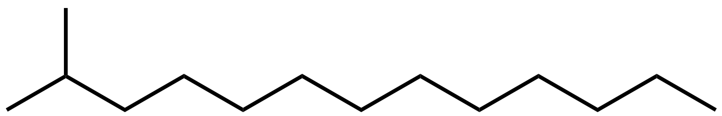

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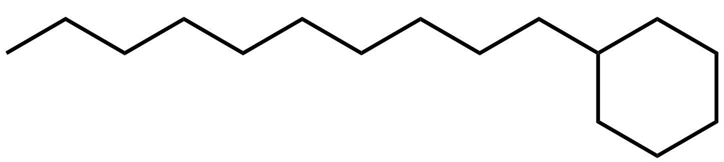

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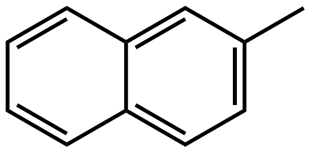
Aromatic Compounds



- Increased fuel density
- Promote O-ring swelling
- Poor combustion properties - result in particulates

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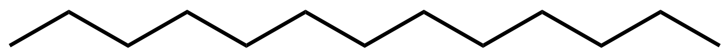

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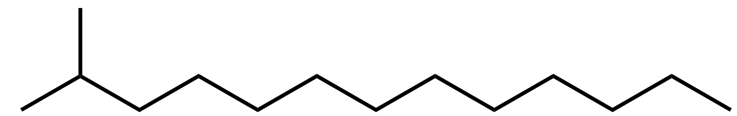

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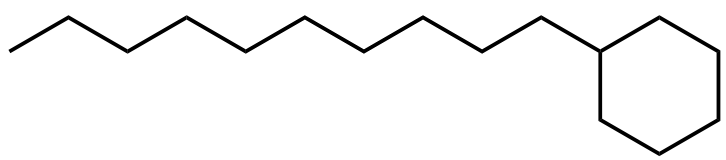

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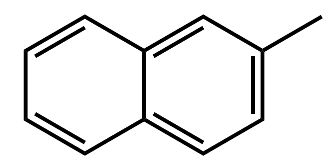

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4 Classes of Carbon Atoms: C_9-C_{16}

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Current State of Aviation Fuel: Kerosene Jet Fuel

Jet A - Civil Aviation Fuel

Toxilogical profile: https://www.atsdr.cdc.gov/ToxProfiles/tp121-c4.pdf Civil Aviation Fuel: https://www.shell.com/business-customers/aviation/aviation-fuel/civil-jet-fuel-grades.html

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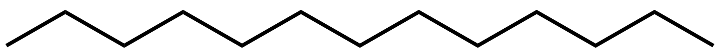
n-parraffins

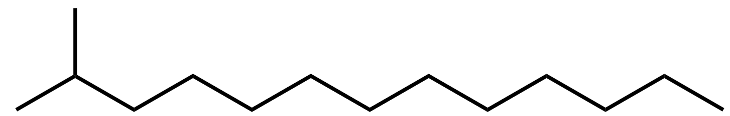
26.8 mass %



C9-C16

iso-parraffins

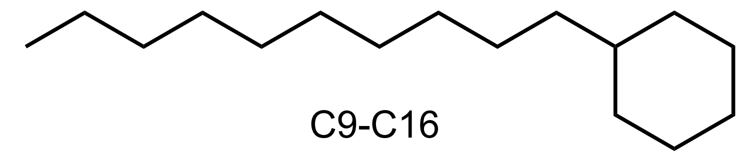
39.7 mass %



C9-C16

cycloparraffins

20.1 mass %



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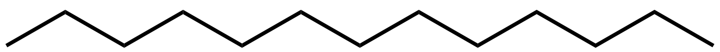

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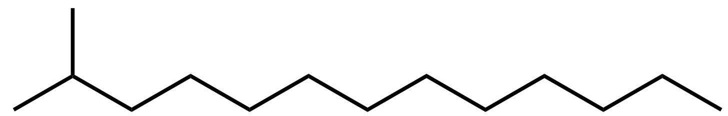

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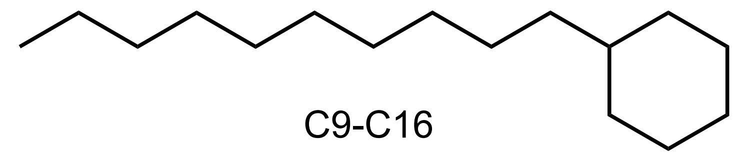
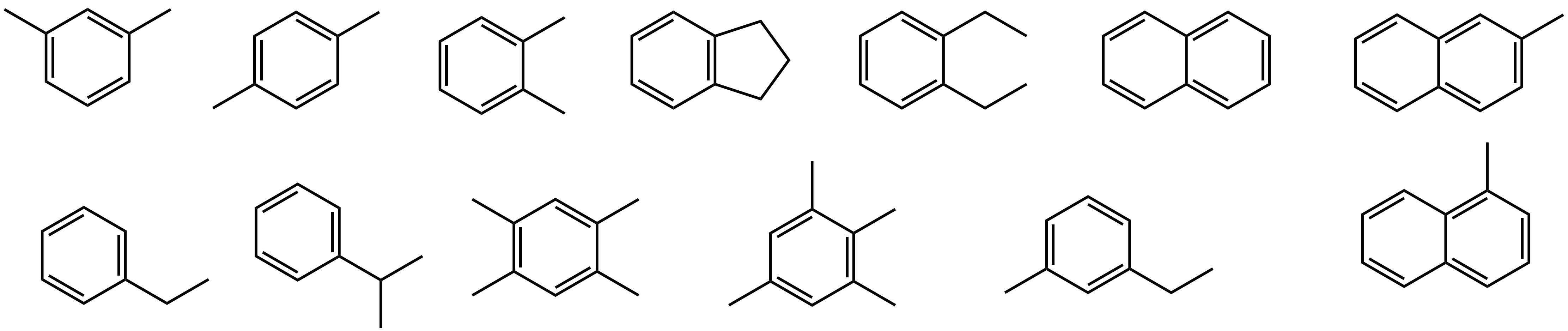


C9-C16

aromatics

13.4 mass %



+ more aromatics

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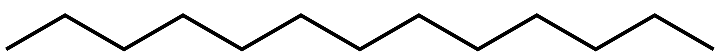

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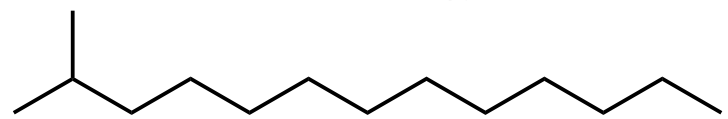

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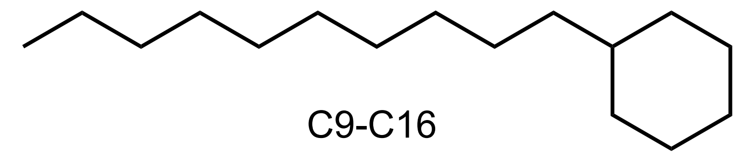

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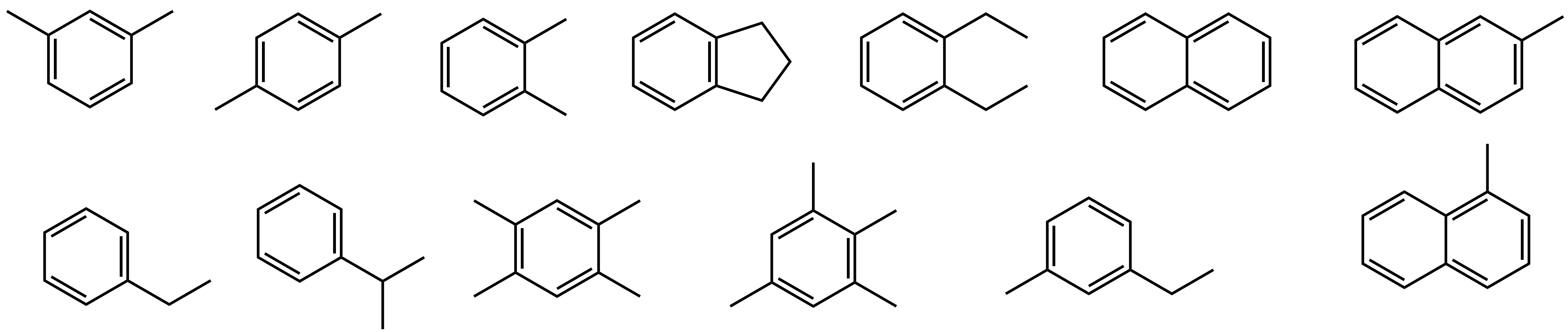

+ more aromatics

Jet A Requirements

Density: ≥ 0.775 (15 °C)

NHOC: ≥ 42.8 MJ/kg

Kinematic Viscocity: ≤ 8.0 (-20 °C) mm^2/s

Freezing Point: ≤ -40 °C

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Jet Fuel Requirements

Density

- Jet fuels are filled by volume
- Important for determining aircraft load

Density: acyclic alkanes > isoalkanes > cyclic alkanes > aromatics

A.; Park, A. C.; Zhang, W. T. J.; Trice, R. W.; Kenttämaa, H. I.; Kilaz, G. *Fuel* **2019,** *235*, 1052-1060.

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Measure of fluid's internal resistance to flow under gravitational forces

$$v = \mu/\rho$$

μ: *dynamic viscosity* ***ρ***: *density of fluid*

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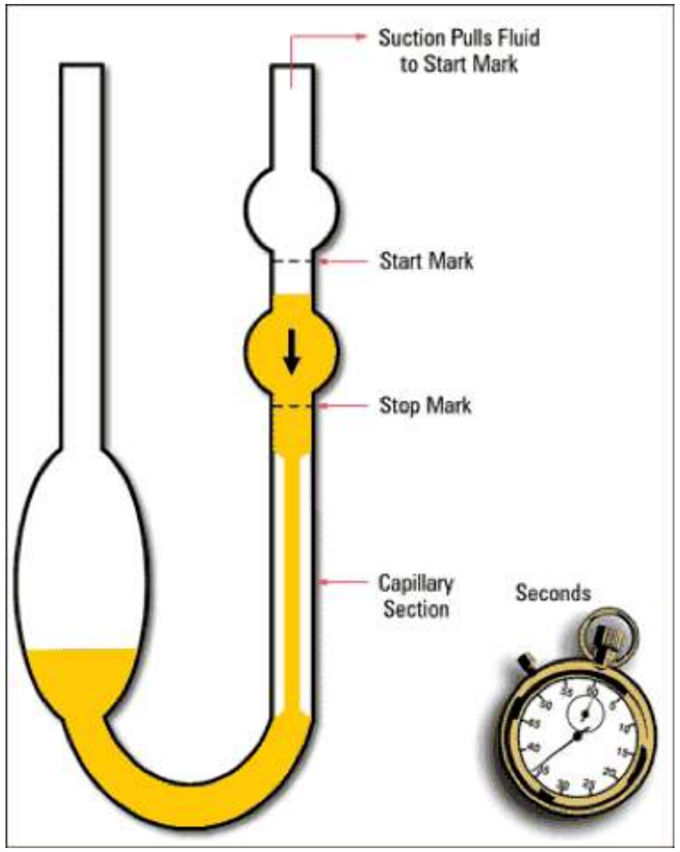

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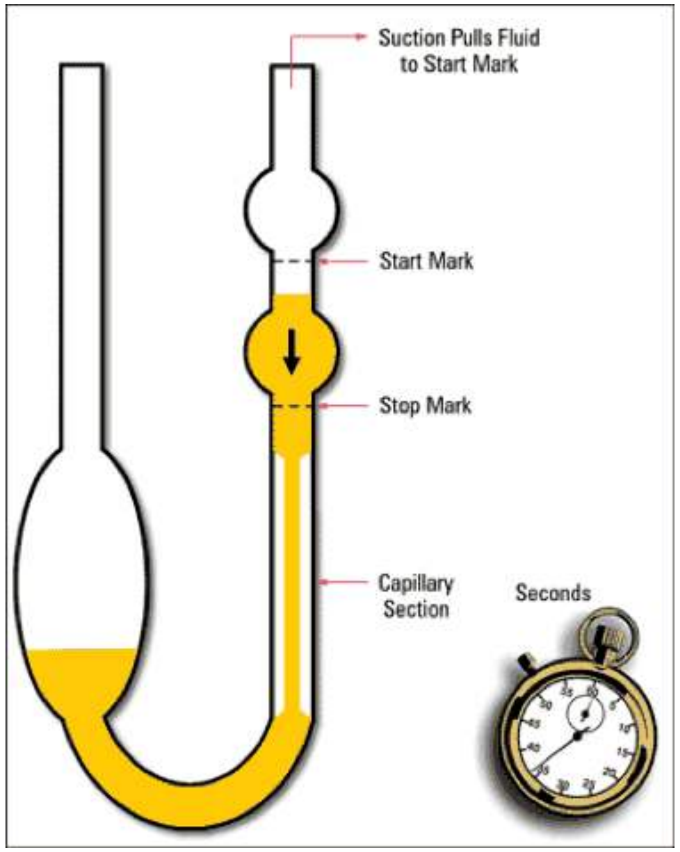

Net Heat of Combustion (NHOC)

- Maximize the energy per unit volume

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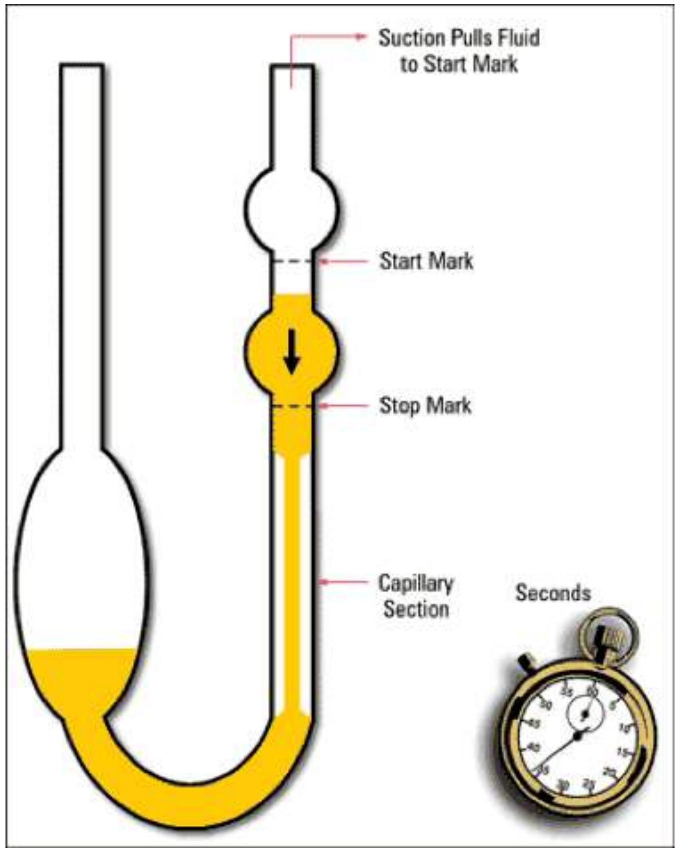

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Freezing Point

- As planes reach higher altitudes temperatures decrease

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Synthetic Parraffinic Kerosenes (SPKs)

Renewable substrates ⟶ *Acyclic SPKs*

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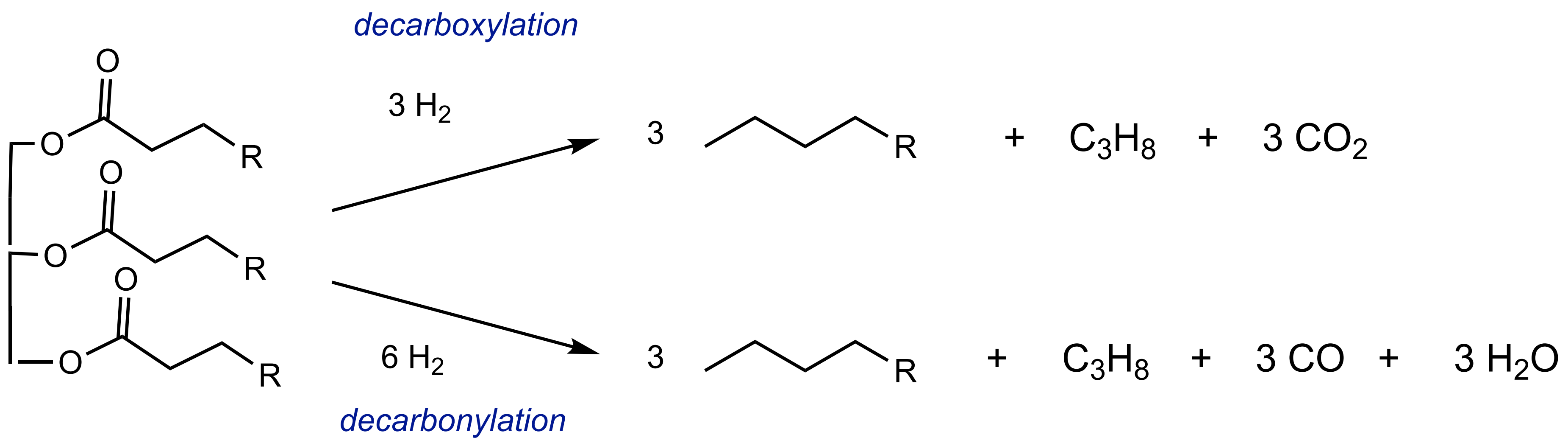
Renewable substrates → *Acyclic SPKs*

"Oil to Jet" Approach: Hydrotreatment of Esters and Fatty Acids (HEFA)



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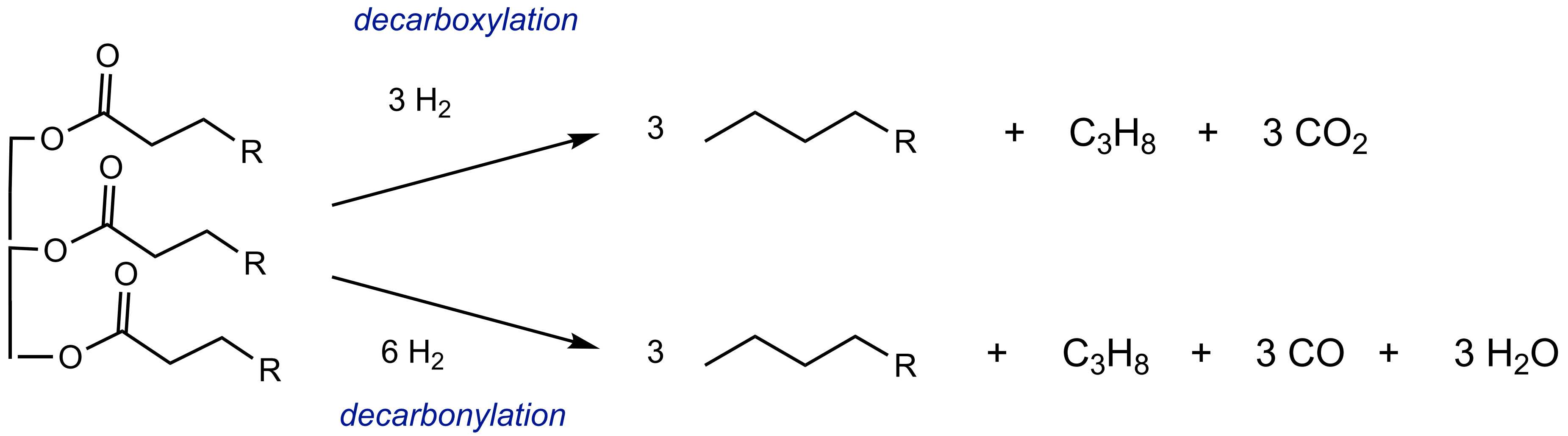

"Gas to Jet" Approach

Biomass → $CO + H_2$ —*Fischer-Tropsch*→ "tail gas" —ZSM-5, *oligomerization*→ C_9 - C_{15} alkenes —*Hydrogenation*→ C_9 - C_{15} alkanes

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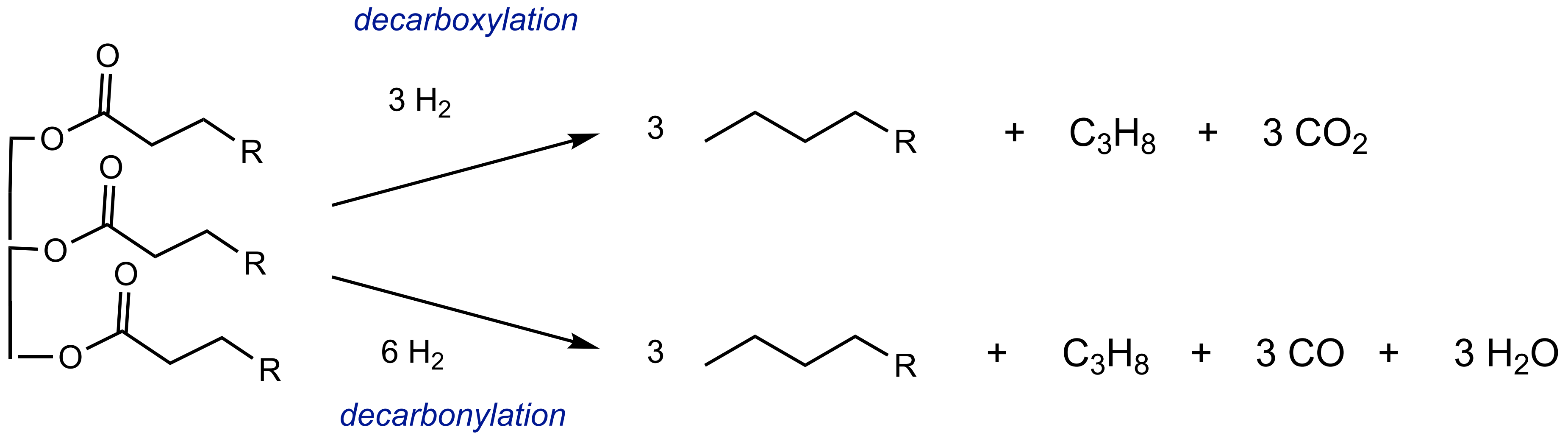

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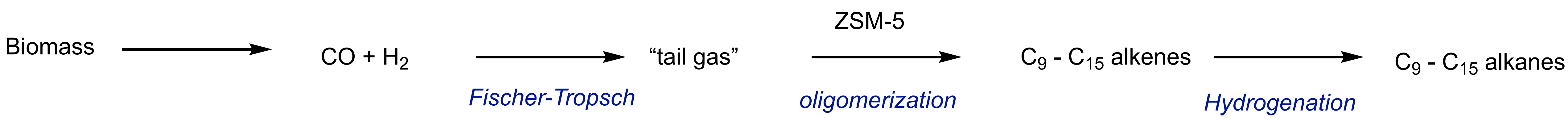
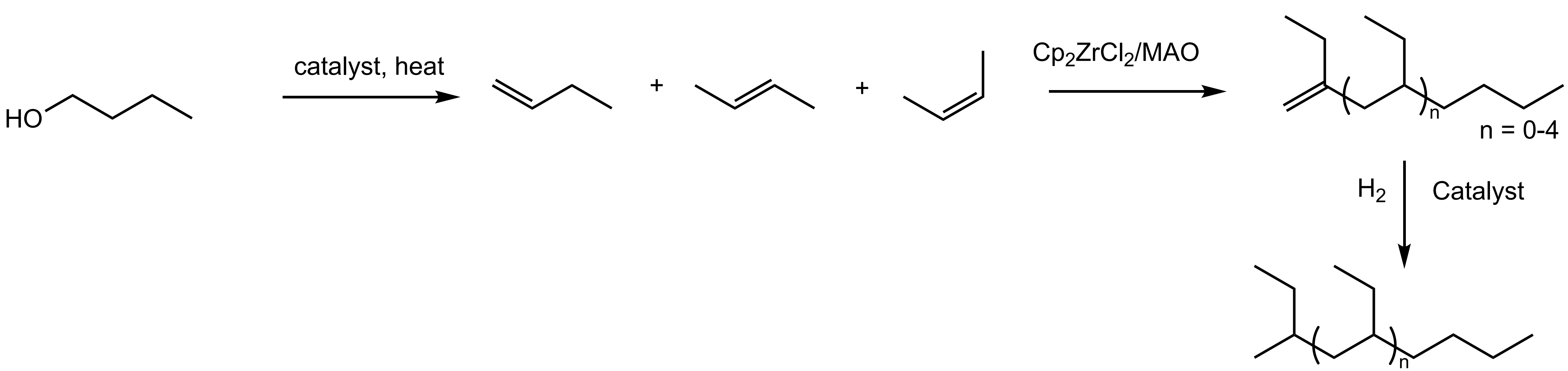


"Alcohol to Jet" Approach: Conversion of Bio-based alcohols to alkenes



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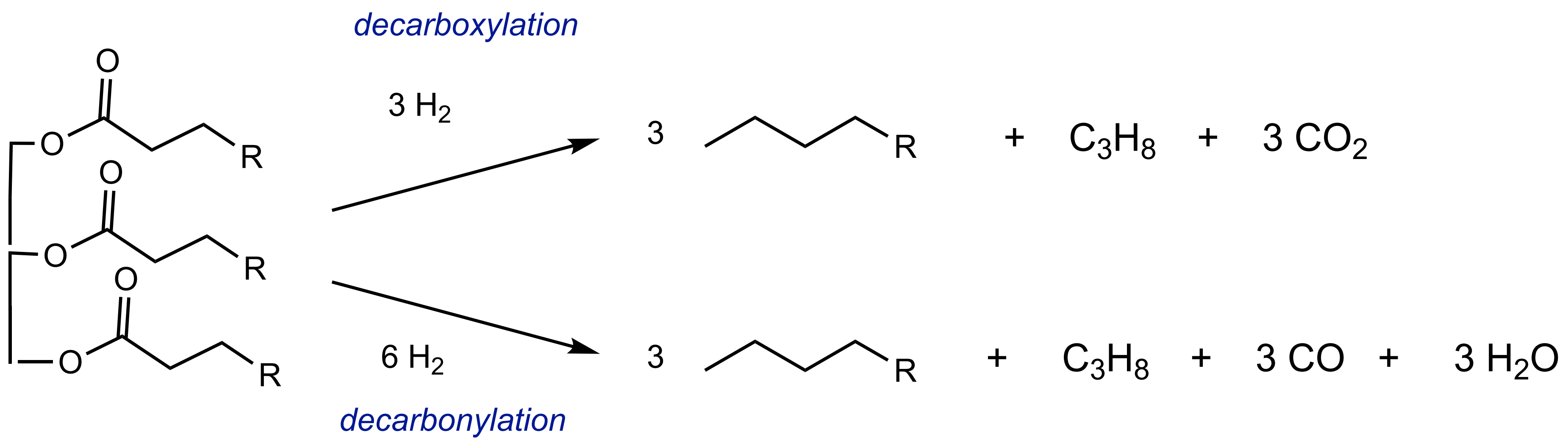
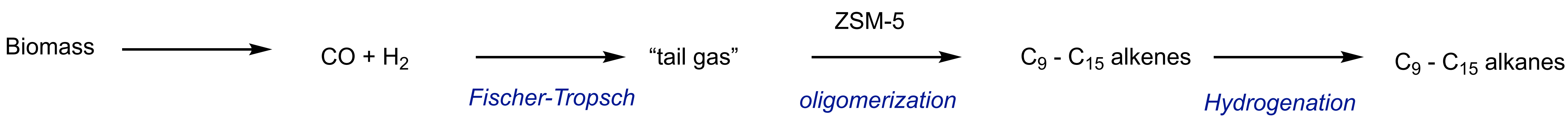
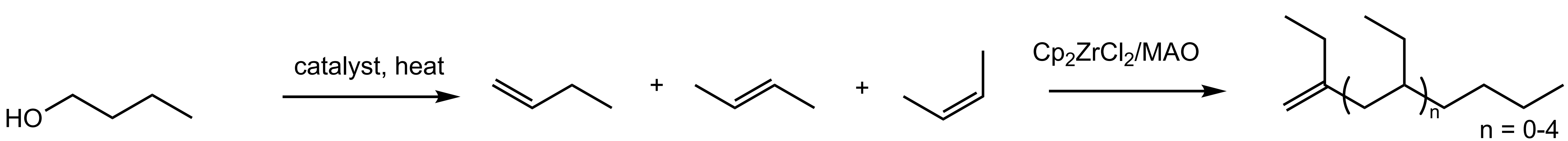
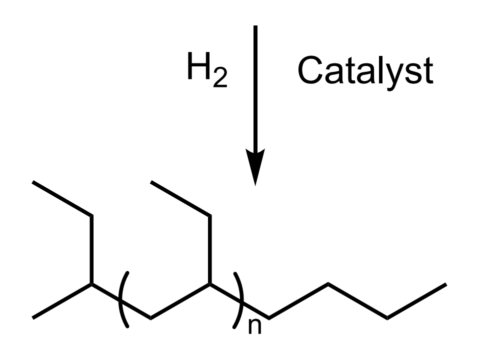


"Gas to Jet" Approach



"Alcohol to Jet" Approach: Conversion of Bio-based alcohols to alkenes





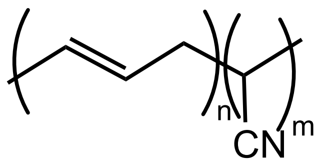
Acyclic jet fuels have low densities and heats of combustions and poor o-ring swelling

Halmenschlager, C. M.; Brar, M.; Apan, I. T.; de Klerk, A., **2016,** *55*, 13020-13031. Ng, K. S.; Farooq, D.; Yang, A., *Renewable and Sustainable Energy Reviews* **2021,** *150*, 111502. Monteiro, R. R.; dos Santos, I. A.; Arcanjo, M. R.; Cavalcante Jr, C. L.; de Luna, F. M.; Fernandez-Lafuente, R.; Vieira, R. S., P*Catalysts* **2022,** *12*, 237. Doliente, S. S.; Narayan, A.; Tapia, J. F. D.; Samsatli, N. J.; Zhao, Y.; Samsatli, S., *Frontiers in Energy Research* **2020,** *8*.

Current Focus of Bioderived Fuel Synthesis: Synthesis of Cycloalkanes

O-Ring Swelling

Aromatics



O-ring material:
butadiene-nitrile rubber

- *Swelling of nitrile rubber increases with polarity and H-bonding character of aromatics*
- *Disrupt interactions between cyano-groups by promoting cyano-aromatic interactions*

R. C.; Myers, K. J.; Minus, D. K.; Harrison, W. E., *Energy & fuels* **2006,** *20*, 759-765. Landera, A.; Bambha, R. P.; Hao, N.; Desai, S. P.; Moore, C. M.; Sutton, A. D.; George, A., *Frontiers in Energy Research* **2022,** *9*.

Current Focus of Bioderived Fuel Synthesis: Synthesis of Cycloalkanes

O-Ring Swelling

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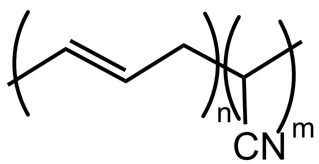

O-ring material:
butadiene-nitrile rubber

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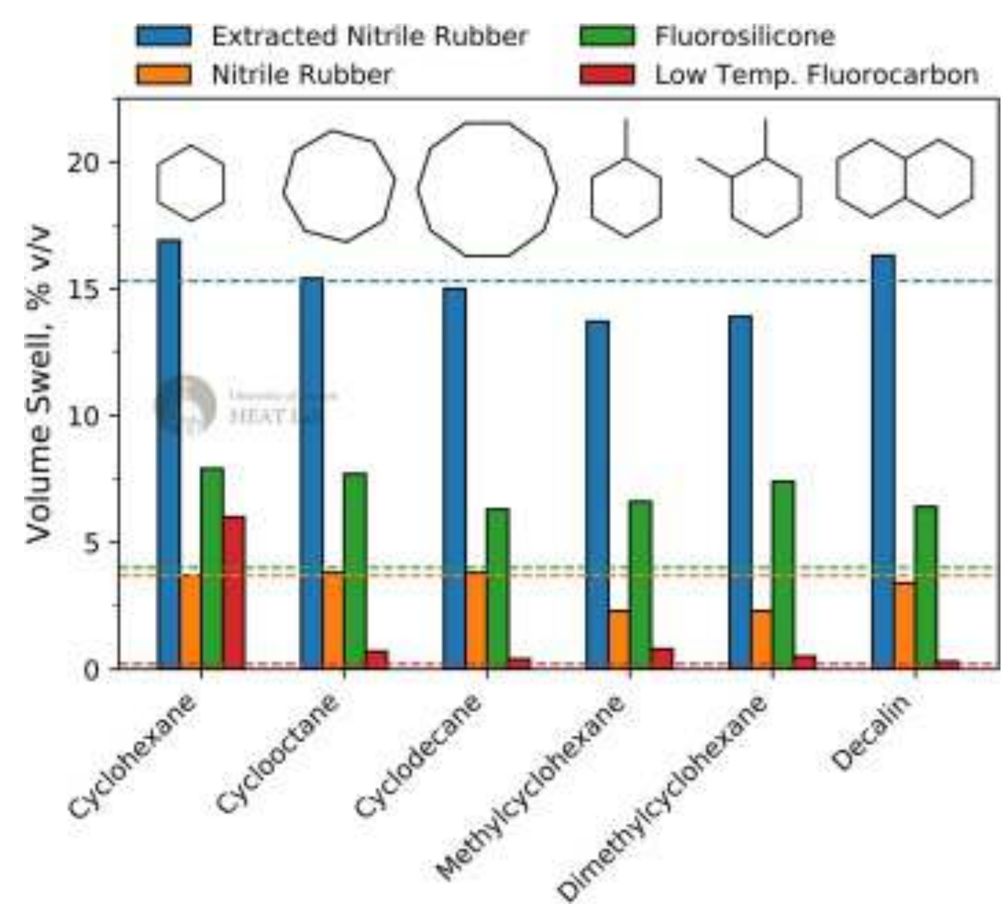
- *Disrupt interactions between cyano-groups by promoting cyano-aromatic interactions*

Cycloalkanes

- *Experimental and computational studies indicate cycloalkanes promote O-ring swelling more than isoalkanes and acyclic alkanes*



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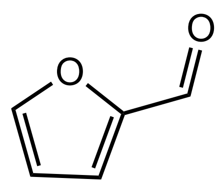
“Bioderived Toolbox”

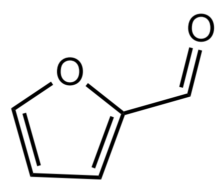


furfural

from hemicellulose and polysaccharides

Muldoon, J. A.; Harvey, B. G., *ChemSusChem* **2020,** *13*, 5777-5807.

“Bioderived Toolbox”



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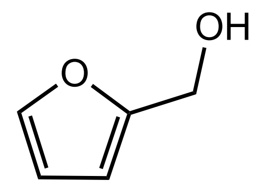
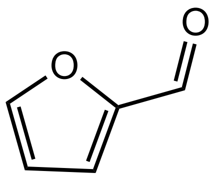


furfural alcohol

from hydrogenation of furfural

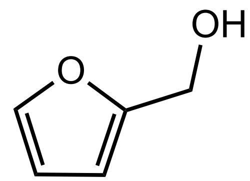
Muldoon, J. A.; Harvey, B. G., *ChemSusChem* **2020,** *13*, 5777-5807.

“Bioderived Toolbox”



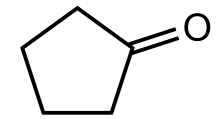
furfural

from hemicellulose and polysaccharides

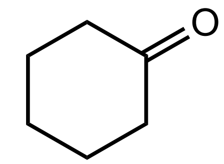


furfural alcohol

from hydrogenation of furfural



cyclopentanone

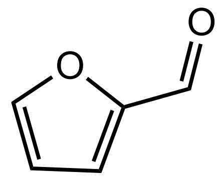


cyclohexanone

from lignocellulose

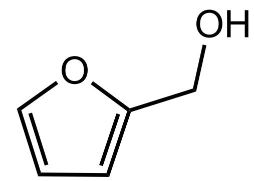
Muldoon, J. A.; Harvey, B. G., *ChemSusChem* **2020,** *13*, 5777-5807.

“Bioderived Toolbox”



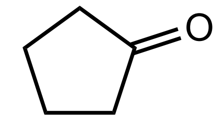
furfural

from hemicellulose and polysaccharides

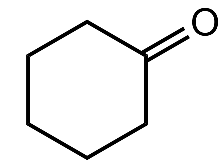


furfural alcohol

from hydrogenation of furfural

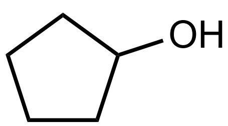


cyclopentanone

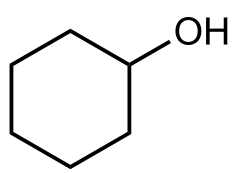


cyclohexanone

from lignocellulose



cyclopentanol

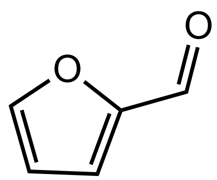


cyclohexanol

from hydrogenation of furfurals

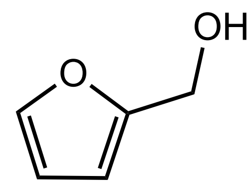
Muldoon, J. A.; Harvey, B. G., *ChemSusChem* **2020,** *13*, 5777-5807.

“Bioderived Toolbox”



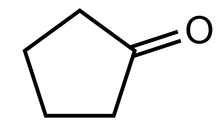
furfural

from hemicellulose and polysaccharides

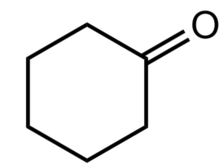


furfural alcohol

from hydrogenation of furfural

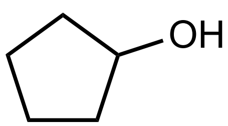


cyclopentanone

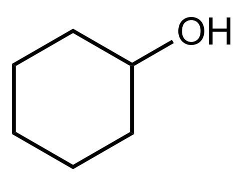


cyclohexanone

from lignocellulose

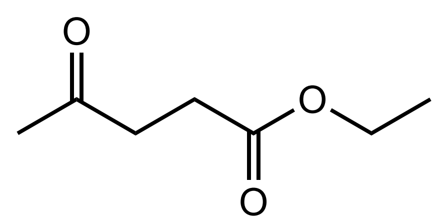


cyclopentanol



cyclohexanol

from hydrogenation of furfurals

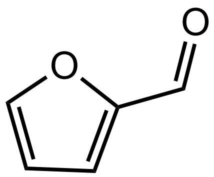


ethyl levulinate

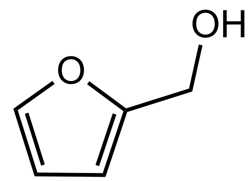
from levulinic acid

Muldoon, J. A.; Harvey, B. G., *ChemSusChem* **2020,** *13*, 5777-5807.

“Bioderived Toolbox”



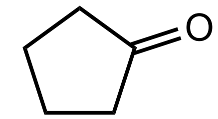
furfural



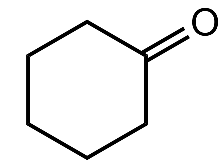
furfural alcohol

from hemicellulose and polysaccharides

from hydrogenation of furfural

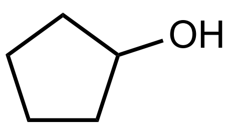


cyclopentanone

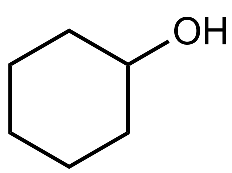


cyclohexanone

from lignocellulose

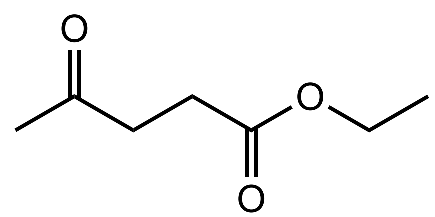


cyclopentanol



cyclohexanol

from hydrogenation of furfurals



ethyl levulinate

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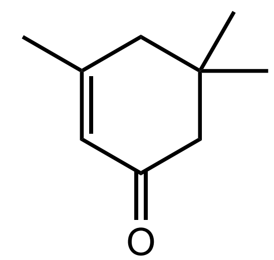
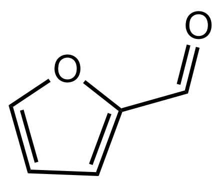


isophorone

condensation of bioderived acetone

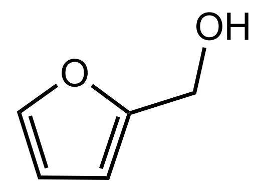
Muldoon, J. A.; Harvey, B. G., *ChemSusChem* **2020,** *13*, 5777-5807.

“Bioderived Toolbox”



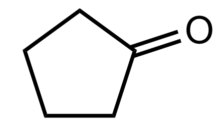
furfural

from hemicellulose and polysaccharides

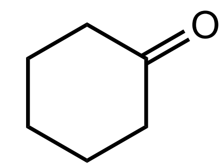


furfural alcohol

from hydrogenation of furfural

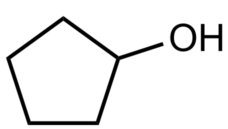


cyclopentanone

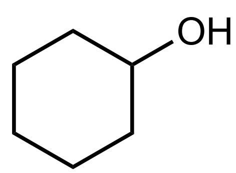


cyclohexanone

from lignocellulose

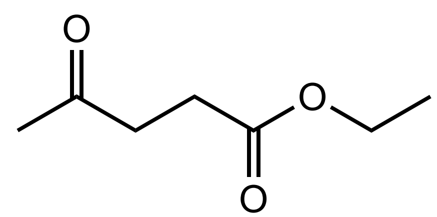


cyclopentanol



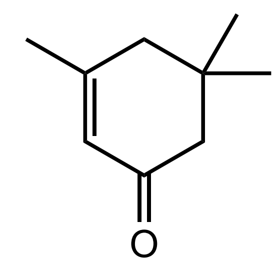
cyclohexanol

from hydrogenation of furfurals



ethyl levulinate

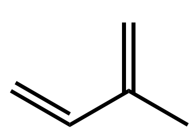
from levulinic acid



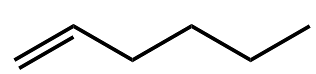
isophorone

condensation of bioderived acetone

Bio Based: Alkenes

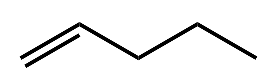


isoprene

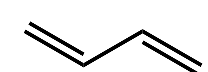


1-hexene

readily derived from biomass



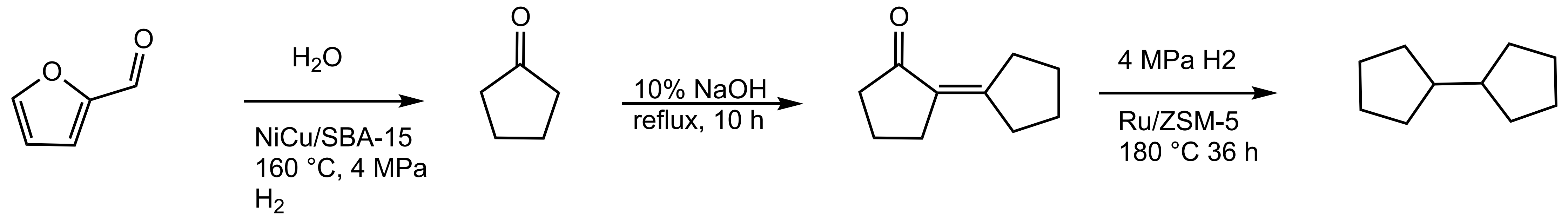
1-pentene



butadiene

Muldoon, J. A.; Harvey, B. G., *ChemSusChem* **2020,** *13*, 5777-5807.

Synthesis of Cycloalkane Fuels from Furfural



NHOC BCP: 42.53 MJ/kg
NHOC Requirment: ≥ 42.8 MJ/kg

Deng, Q.; Nie, G.; Pan, L.; Zou, J.-J.; Zhang, X.; Wang, L., *Green Chemistry* **2015,** *17* (8), 4473-4481. Yang, J.; Li, N.; Li, G.; Wang, W.; Wang, A.; Wang, X.; Cong, Y.; Zhang, T., *Chem. Comm.* **2014**, *50*, 2572-2574. Pino, N.; Hincapié, G.; López, D., *Energy & Fuels* **2018**, *32*, 561-573.

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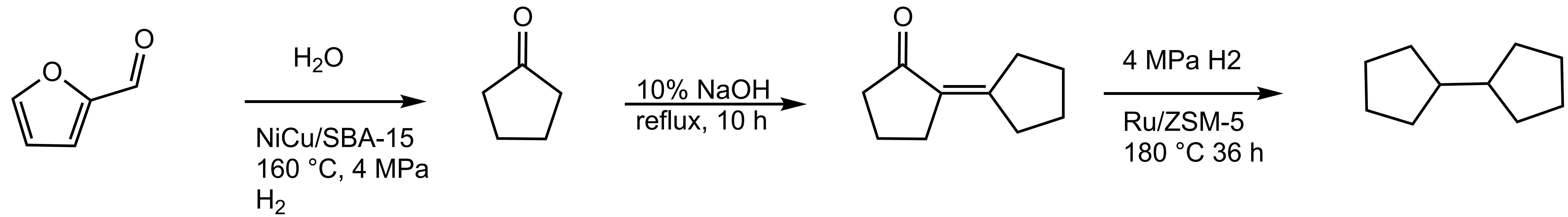

NHOC BCP: 42.53 MJ/kg
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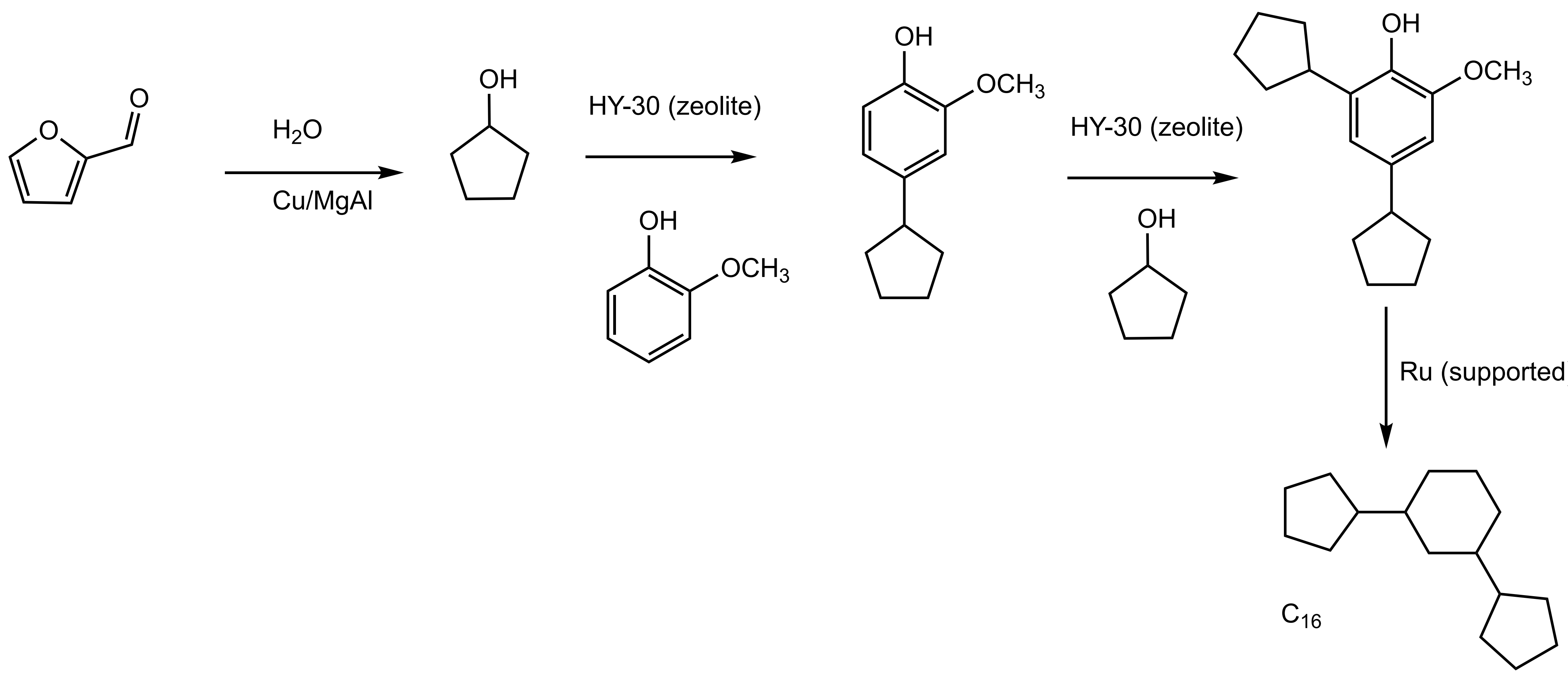
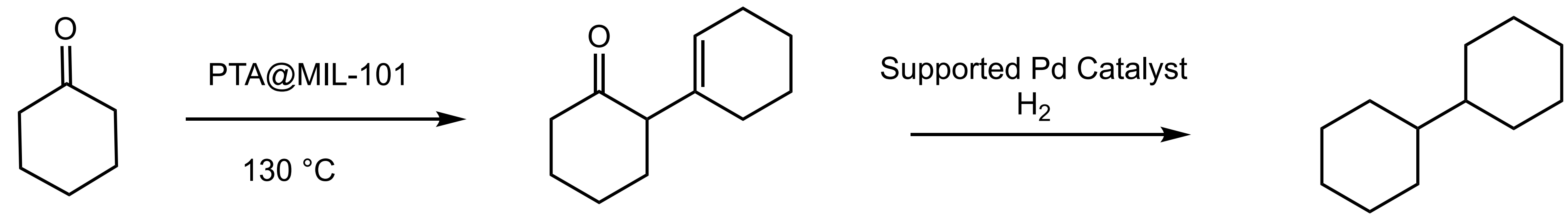


Met Jet A requirements

Yang, J.; Li, N.; Li, G.; Wang, W.; Wang, A.; Wang, X.; Cong, Y.; Zhang, T., *Chem. Comm.* **2014,** *50*, 2572-2574. Pino, N.; Hincapié, G.; López, D., *Energy & Fuels* **2018,** *32* , 561-573.

Synthesis of Fuels from Aldol-Self Condensation of Cyclic Ketones



Freezing point is 1.3 °C
Jet A: Freezing Point: ≤ -40 °C

Deng, Q.; Nie, G.; Pan, L.; Zou, J.-J.; Zhang, X.; Wang, L., *Green Chemistry* **2015,** *17* (8), 4473-4481.

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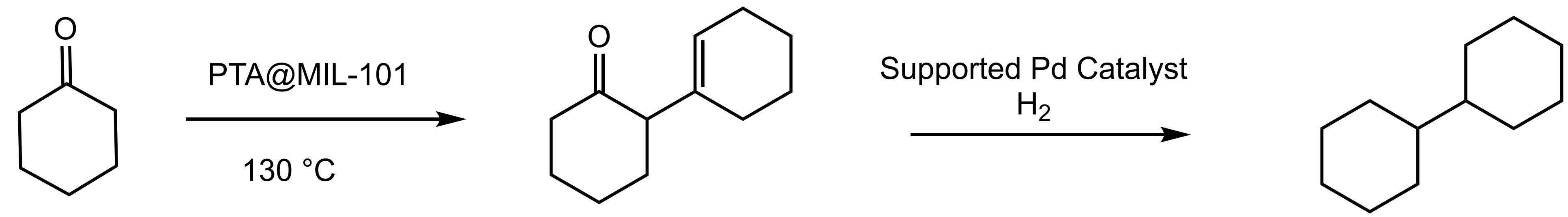

Freezing point is 1.3 °C
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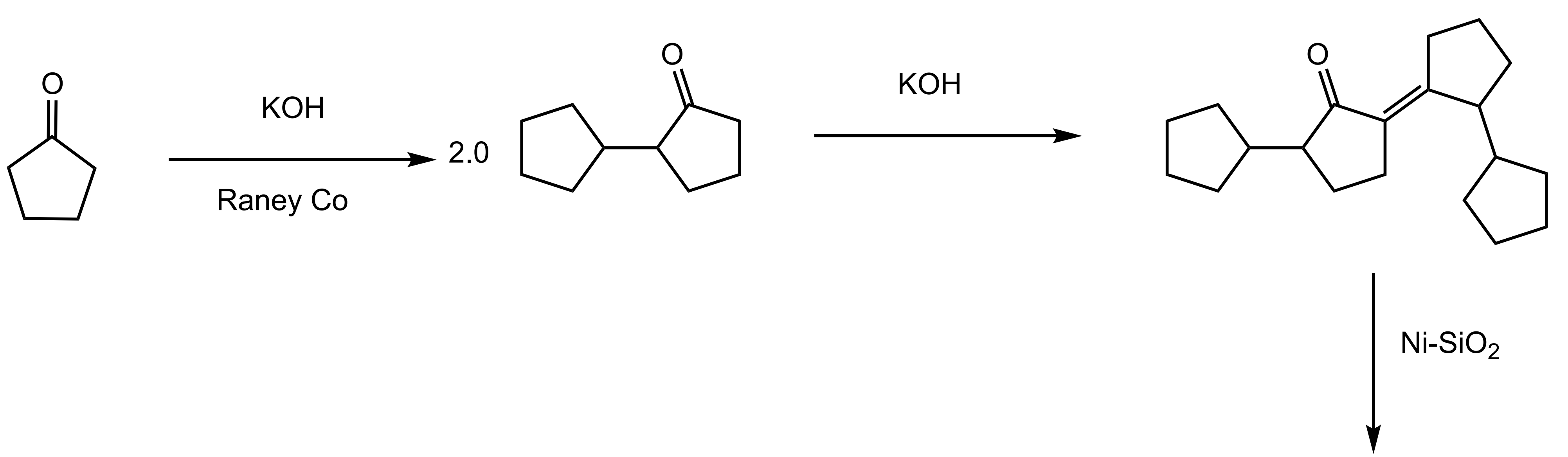
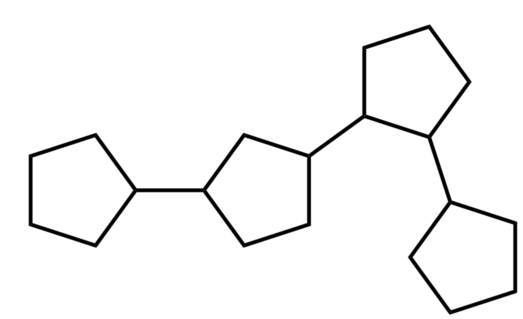
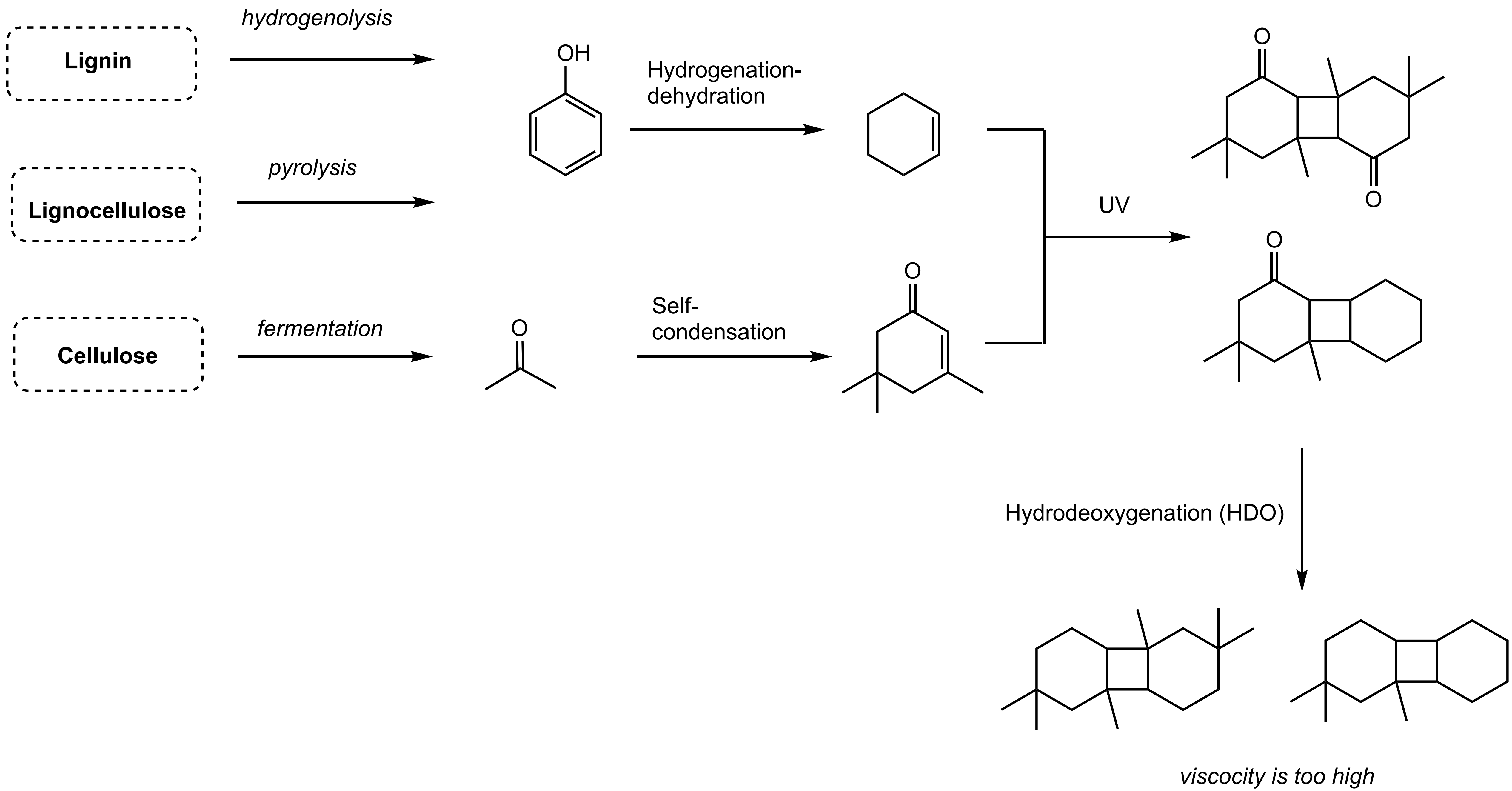


Freezing point is -39.3 °C
Jet A: Freezing Point: ≤ -40 °C



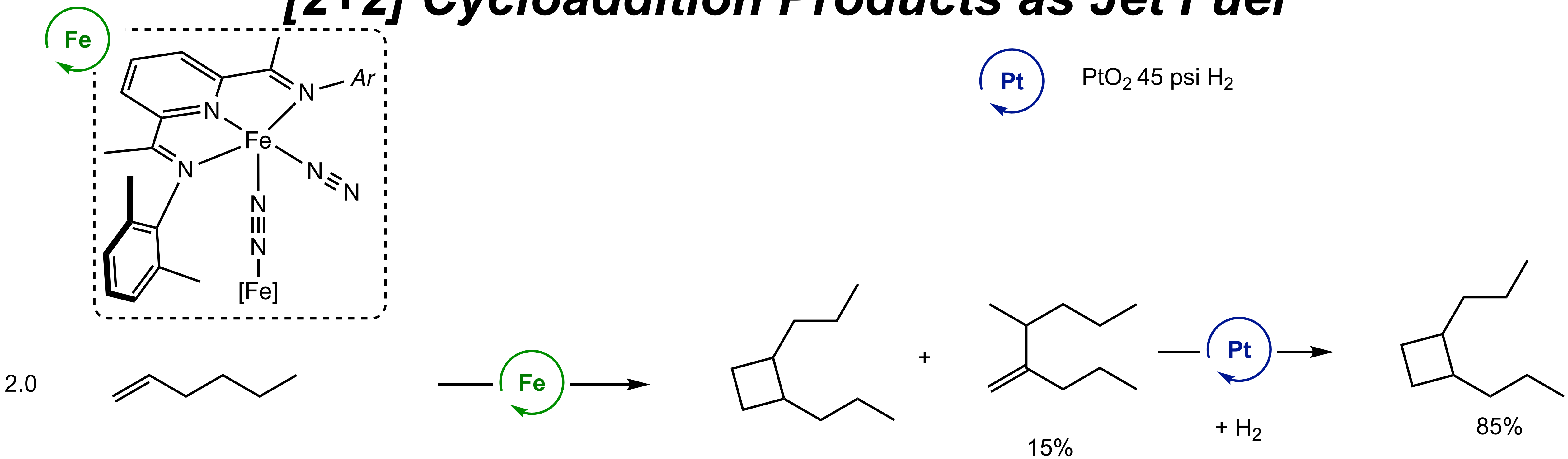
Deng, Q.; Nie, G.; Pan, L.; Zou, J.-J.; Zhang, X.; Wang, L., *Green Chemistry* **2015,** *17* (8), 4473-4481.

[2+2] Cycloaddition Products as Bioderived Fuels



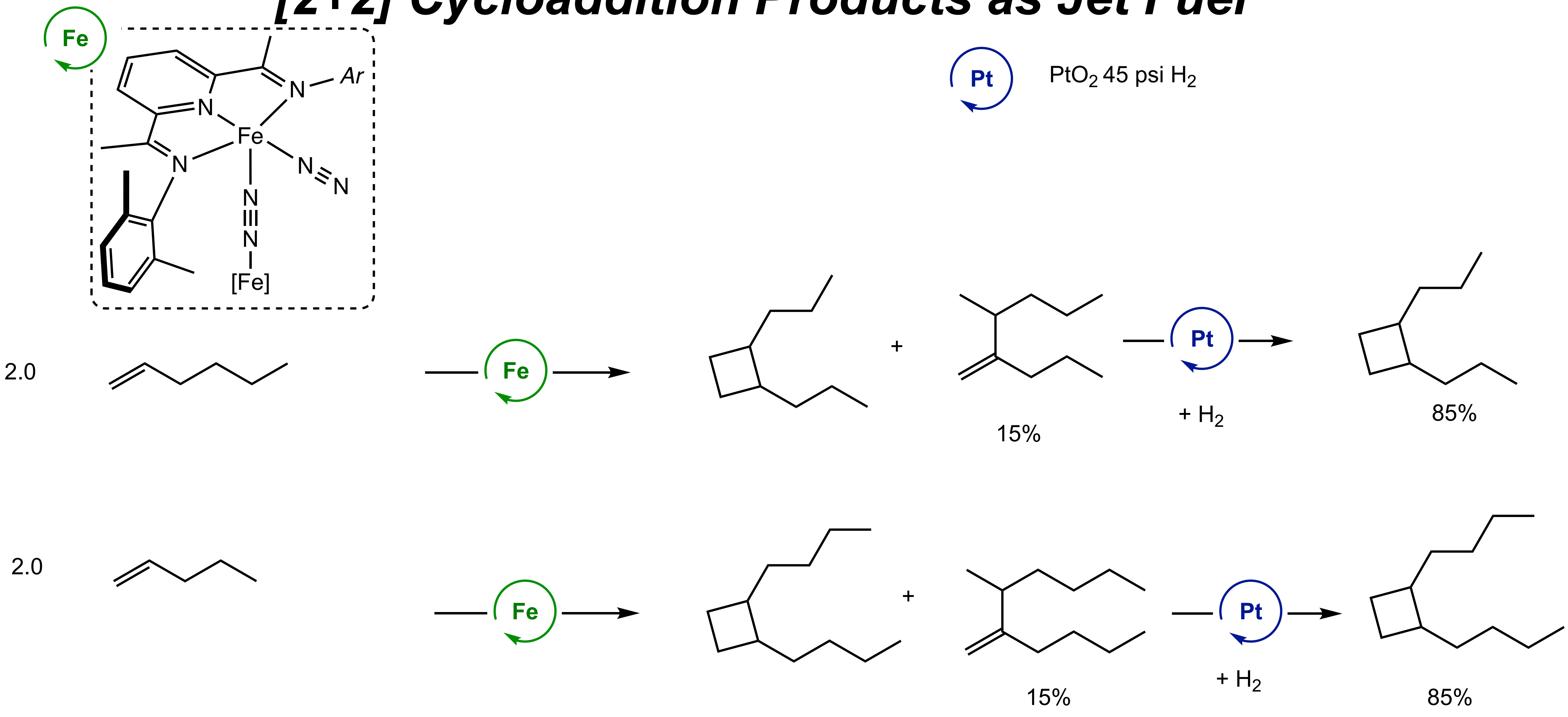
Xie, J.; Zhang, X.; Shi, C.; Pan, L.; Hou, F.; Nie, G.; Xie, J.; Liu, Q.; Zou, J.-J., *Sustainable Energy & Fuels* **2020,** *4*, 911-920.

[2+2] Cycloaddition Products as Jet Fuel



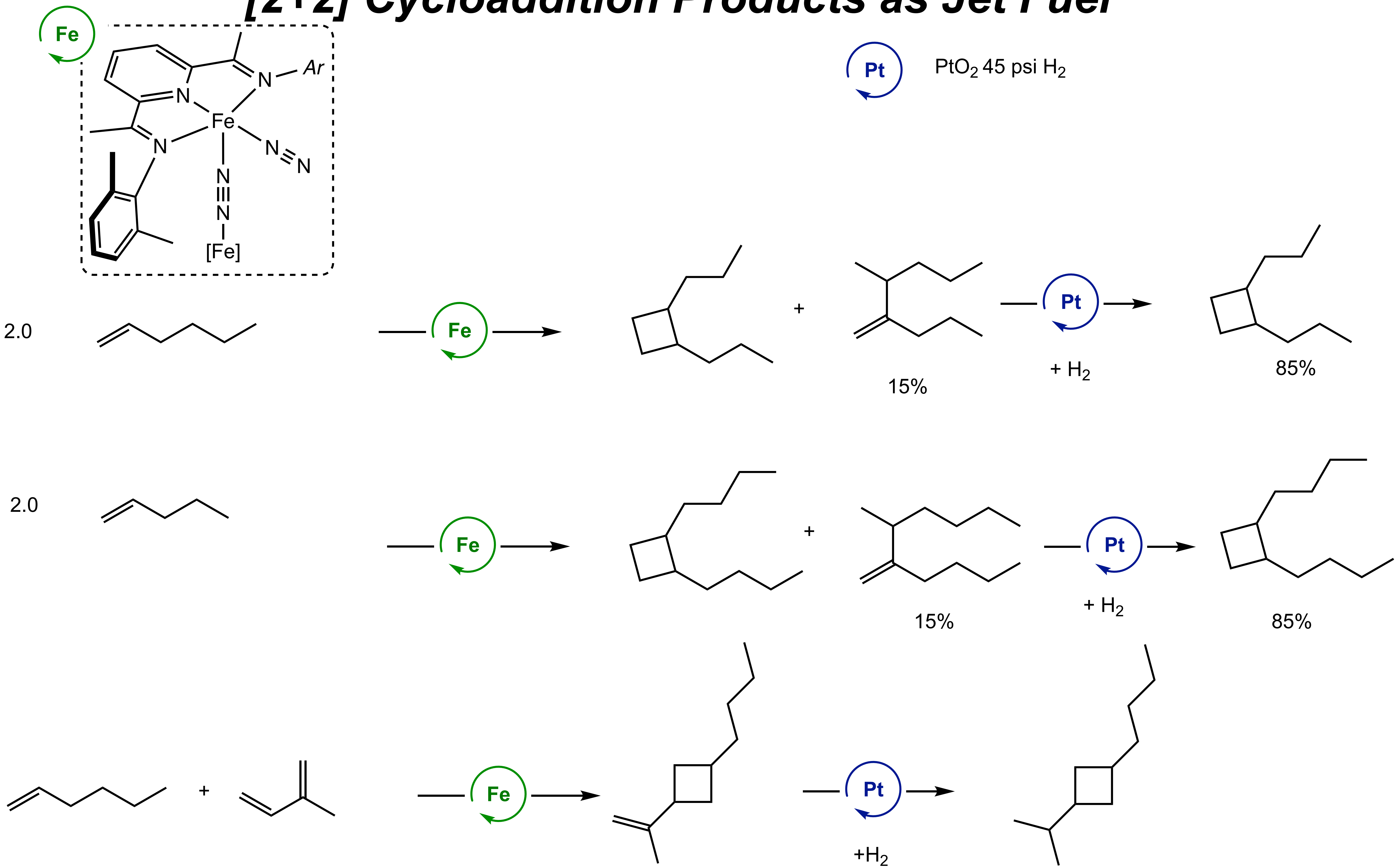
Morris, D. M.; Quintana, R. L.; Harvey, B. G.,. *ChemSusChem* **2019,** *12*, 1646-1652.

[2+2] Cycloaddition Products as Jet Fuel



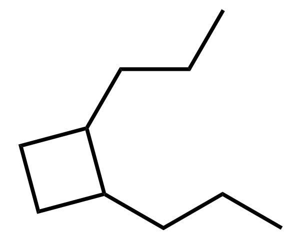
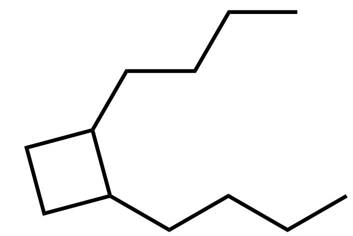
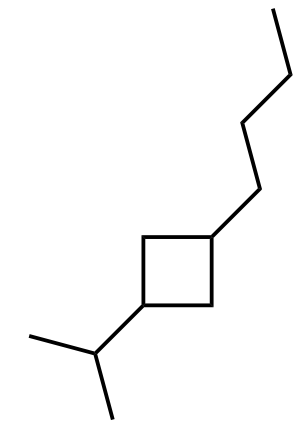
Morris, D. M.; Quintana, R. L.; Harvey, B. G.,. *ChemSusChem* **2019,** *12*, 1646-1652.

[2+2] Cycloaddition Products as Jet Fuel



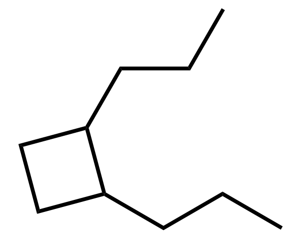
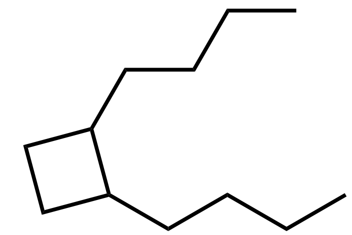
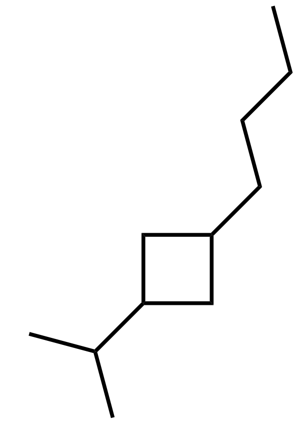
Morris, D. M.; Quintana, R. L.; Harvey, B. G.,. *ChemSusChem* **2019,** *12*, 1646-1652.

[2+2] Cycloaddition Products as Jet Fuel: Comparison of Properties

	Jet A			
density (g/mL)	>0.775	0.767	0.779	0.783

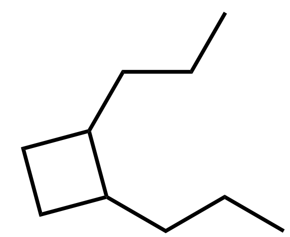
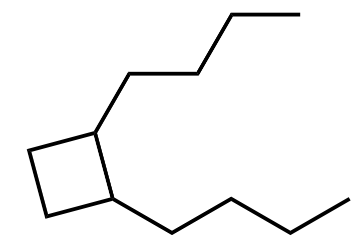
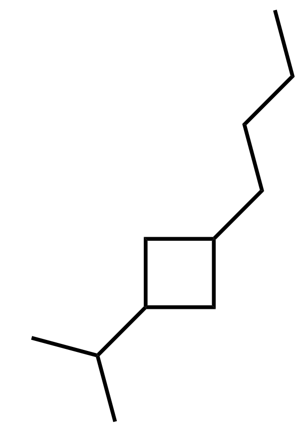
Morris, D. M.; Quintana, R. L.; Harvey, B. G.,. *ChemSusChem* **2019,** *12*, 1646-1652.

[2+2] Cycloaddition Products as Jet Fuel: Comparison of Properties

	Jet A			
density (g/mL)	>0.775	0.767	0.779	0.783
NHOC (MJ/kg)	>42.8	43.8	43.1	42.9

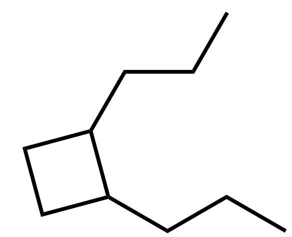
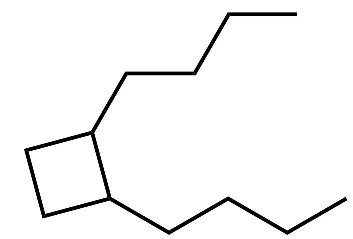
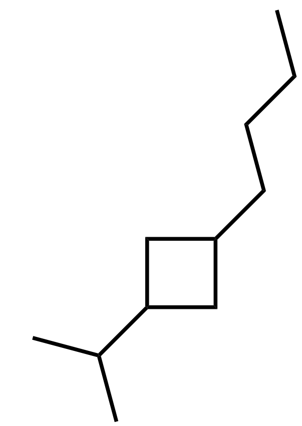
Morris, D. M.; Quintana, R. L.; Harvey, B. G.,. *ChemSusChem* **2019,** *12*, 1646-1652.

[2+2] Cycloaddition Products as Jet Fuel: Comparison of Properties

	Jet A			
density (g/mL)	>0.775	0.767	0.779	0.783
NHOC (MJ/kg)	>42.8	43.8	43.1	42.9
Kinematic Viscocity (mm^2/s)	<8	2.38	4.78	3.14

Morris, D. M.; Quintana, R. L.; Harvey, B. G.,. *ChemSusChem* **2019,** *12*, 1646-1652.

[2+2] Cycloaddition Products as Jet Fuel: Comparison of Properties

	Jet A			
density (g/mL)	>0.775	0.767	0.779	0.783
NHOC (MJ/kg)	>42.8	43.8	43.1	42.9
Kinematic Viscocity (mm^2/s)	<8	2.38	4.78	3.14

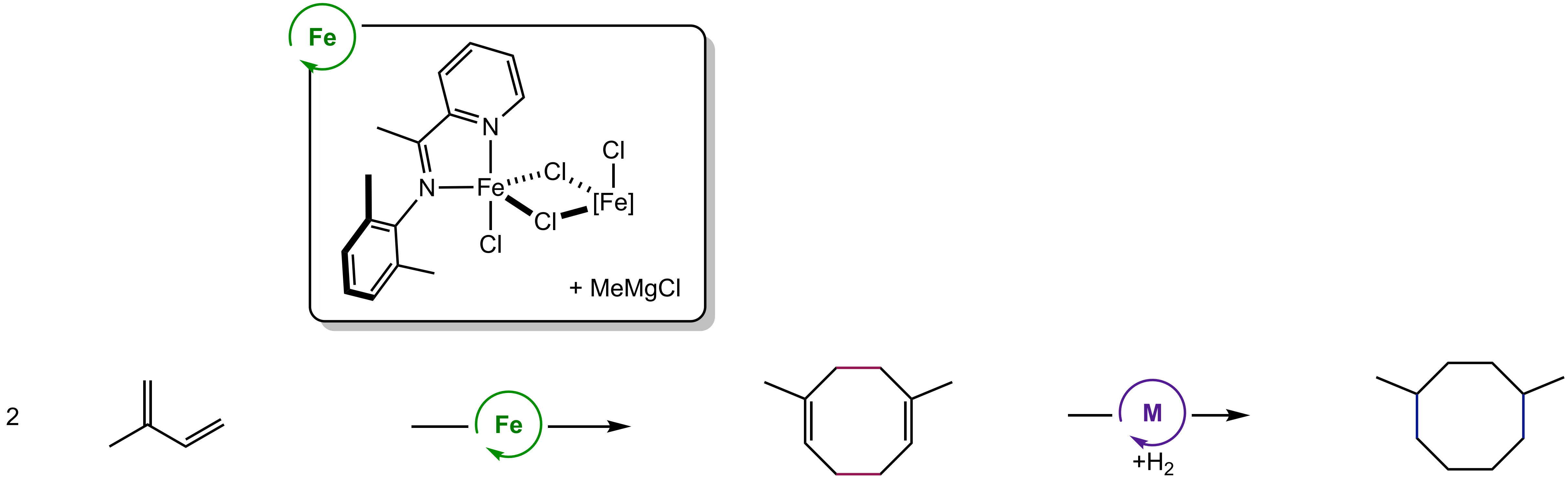
Freezing points below 80 °C

Fuels Meet Jet A Requirements

Challenges: *Need a more active 2+2 Catalyst [TON ~ 40]*

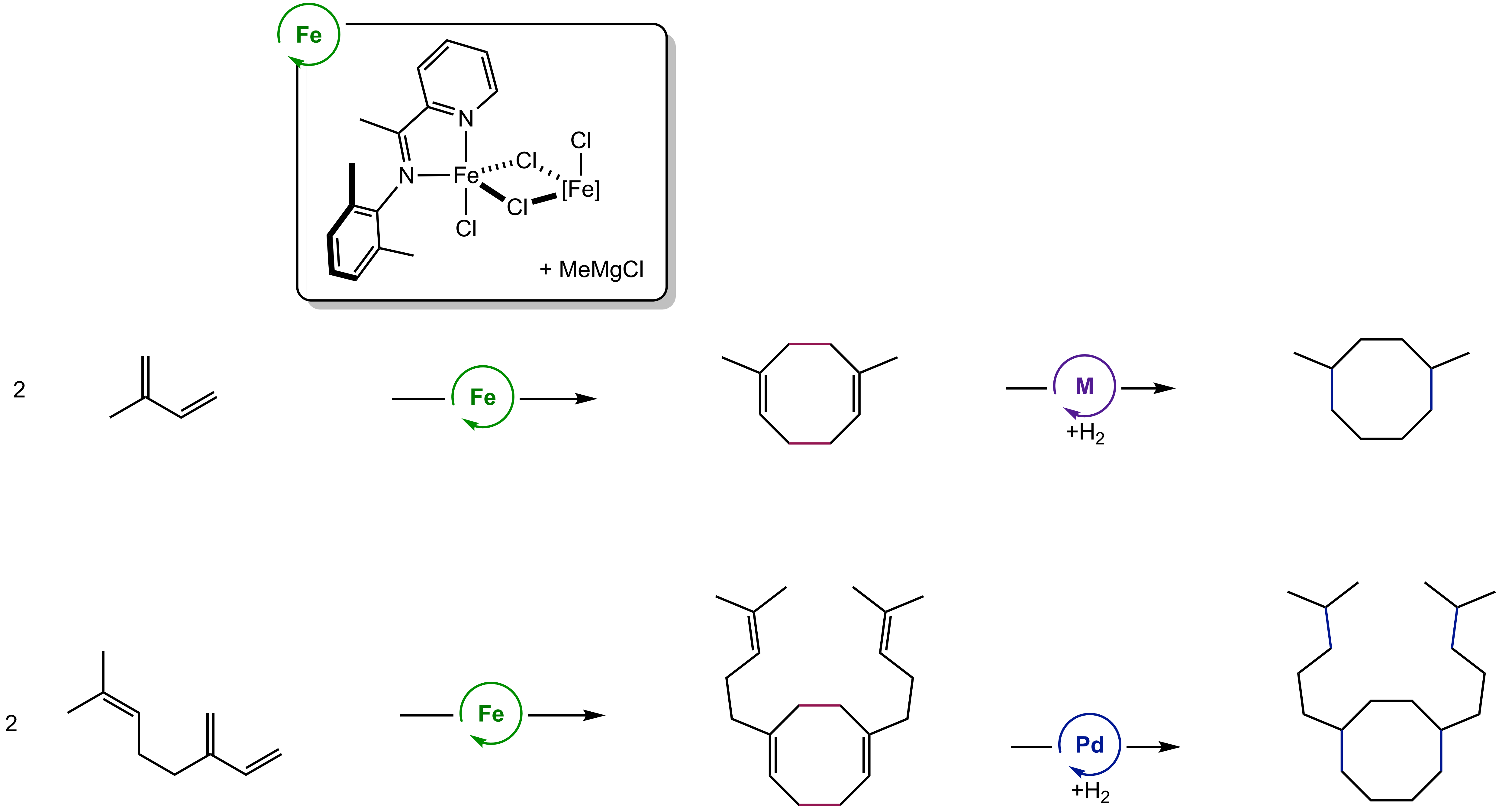
Morris, D. M.; Quintana, R. L.; Harvey, B. G.,. *ChemSusChem* **2019,** *12*, 1646-1652.

Bioderived Jet Fuels from [4+4] Cycloaddition Products



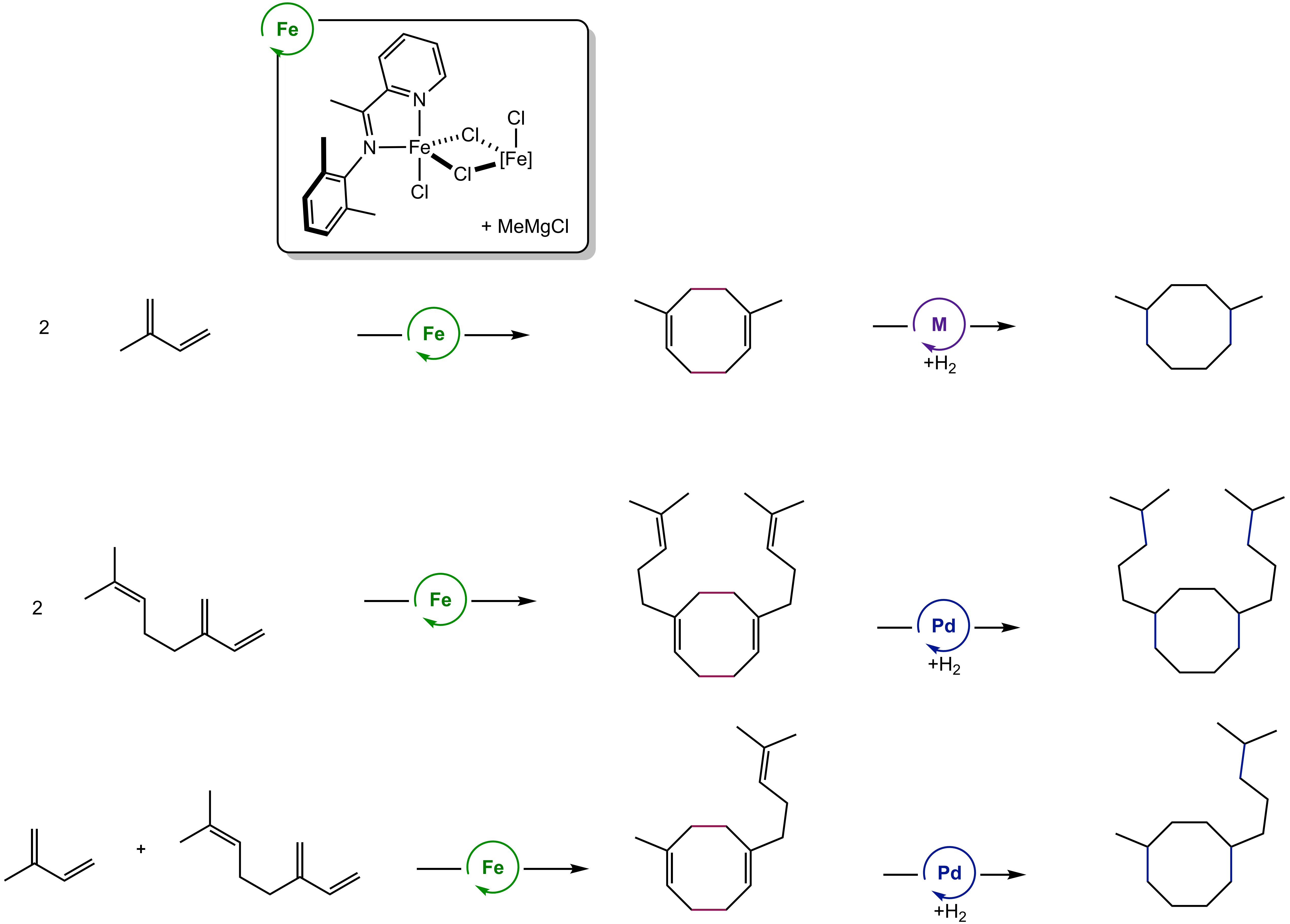
Rosenkoetter, K. E.; Kennedy, C. R.; Chirik, P. J.; Harvey, B. G.,*Green Chemistry* **2019,** *21*, 5616-5623. Woodroffe, J.-D.; Harvey, B. G. *Energy & Fuels* **2022,** *36*, 2630-2638.

Bioderived Jet Fuels from [4+4] Cycloaddition Products



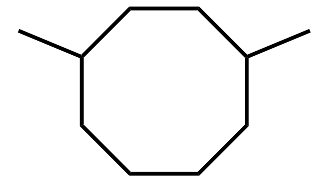
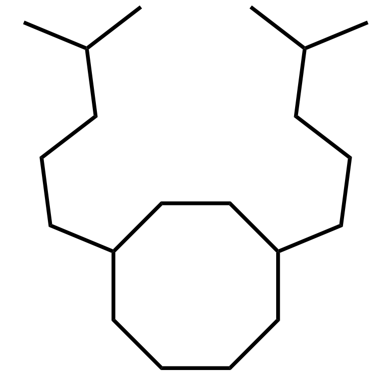
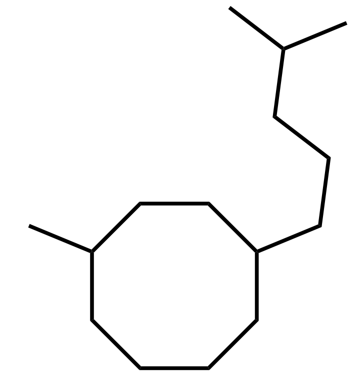
Rosenkoetter, K. E.; Kennedy, C. R.; Chirik, P. J.; Harvey, B. G., *Green Chemistry* **2019,** *21*, 5616-5623. Woodroffe, J.-D.; Harvey, B. G. *Energy & Fuels* **2022,** *36*, 2630-2638.

Bioderived Jet Fuels from [4+4] Cycloaddition Products



Rosenkoetter, K. E.; Kennedy, C. R.; Chirik, P. J.; Harvey, B. G., *Green Chemistry* **2019,** *21*, 5616-5623. Woodroffe, J.-D.; Harvey, B. G. *Energy & Fuels* **2022,** *36*, 2630-2638.

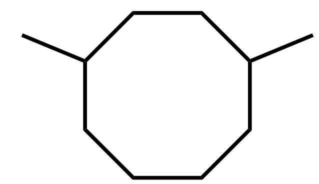
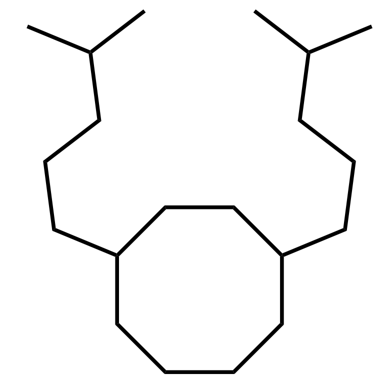
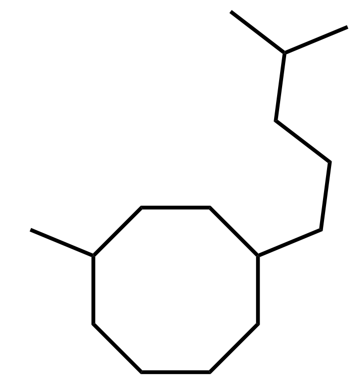
[4+4] Cycloaddition Products in Bioderived Fuels

	Jet A		 *	 *
density (g/mL)	>0.775	0.827	0.84	0.783

*** Main product in mixture**

Rosenkoetter, K. E.; Kennedy, C. R.; Chirik, P. J.; Harvey, B. G., *Green Chemistry* **2019,** *21*, 5616-5623. Woodroffe, J.-D.; Harvey, B. G. *Energy & Fuels* **2022,** *36*, 2630-2638.

[4+4] Cycloaddition Products in Bioderived Fuels

	Jet A		 *	 *
density (g/mL)	>0.775	0.827	0.84	0.783
NHOC (MJ/kg)	>42.8	43.82	43.63	43.68

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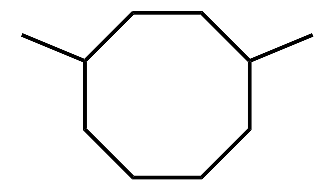
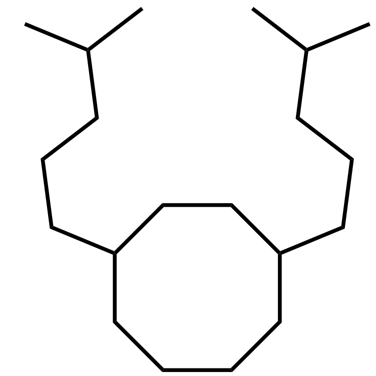
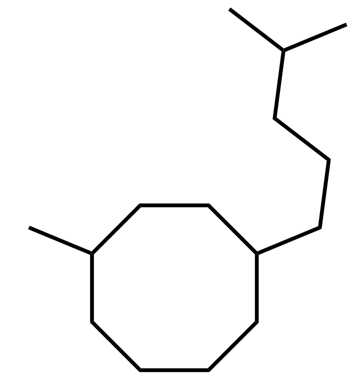
Rosenkoetter, K. E.; Kennedy, C. R.; Chirik, P. J.; Harvey, B. G., *Green Chemistry* **2019,** *21*, 5616-5623. Woodroffe, J.-D.; Harvey, B. G. *Energy & Fuels* **2022,** *36*, 2630-2638.

[4+4] Cycloaddition Products in Bioderived Fuels

	Jet A		 *	 *
density (g/mL)	>0.775	0.827	0.84	0.783
NHOC (MJ/kg)	>42.8	43.82	43.63	43.68
Kinematic Viscocity (mm^2/s)	<8	4.17	10.8	3.8

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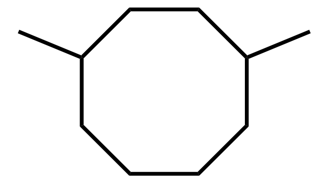
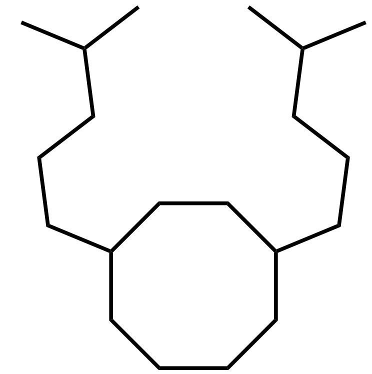
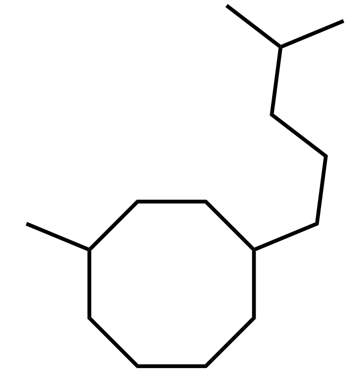
Rosenkoetter, K. E.; Kennedy, C. R.; Chirik, P. J.; Harvey, B. G., *Green Chemistry* **2019,** *21*, 5616-5623. Woodroffe, J.-D.; Harvey, B. G. *Energy & Fuels* **2022,** *36*, 2630-2638.

[4+4] Cycloaddition Products in Bioderived Fuels

	Jet A		 *	 *
density (g/mL)	>0.775	0.827	0.84	0.783
NHOC (MJ/kg)	>42.8	43.82	43.63	43.68
Kinematic Viscocity (mm^2/s)	<8	4.17	10.8	3.8
Freezing Point (°C)	<-40	<-78	—	—

*** Main product in mixture**

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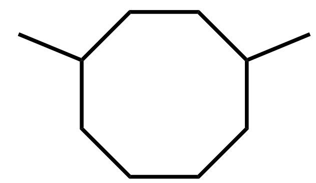
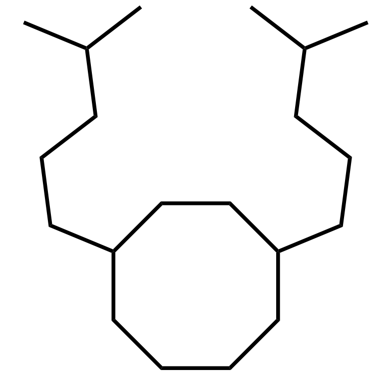
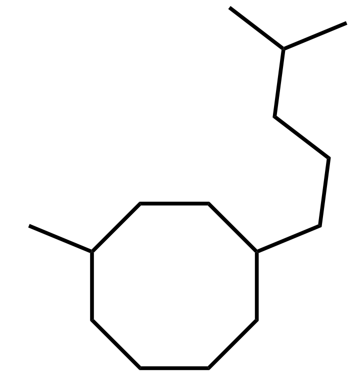
	Jet A		 *	 *
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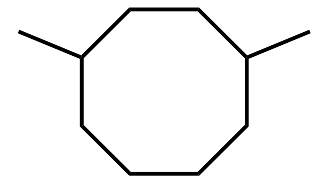
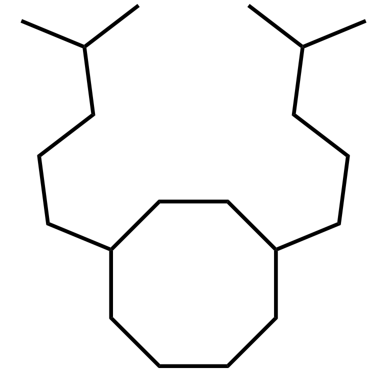
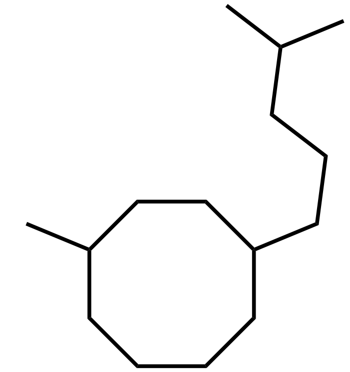
[4+4] Cycloaddition Products in Bioderived Fuels

	Jet A		 *	 *
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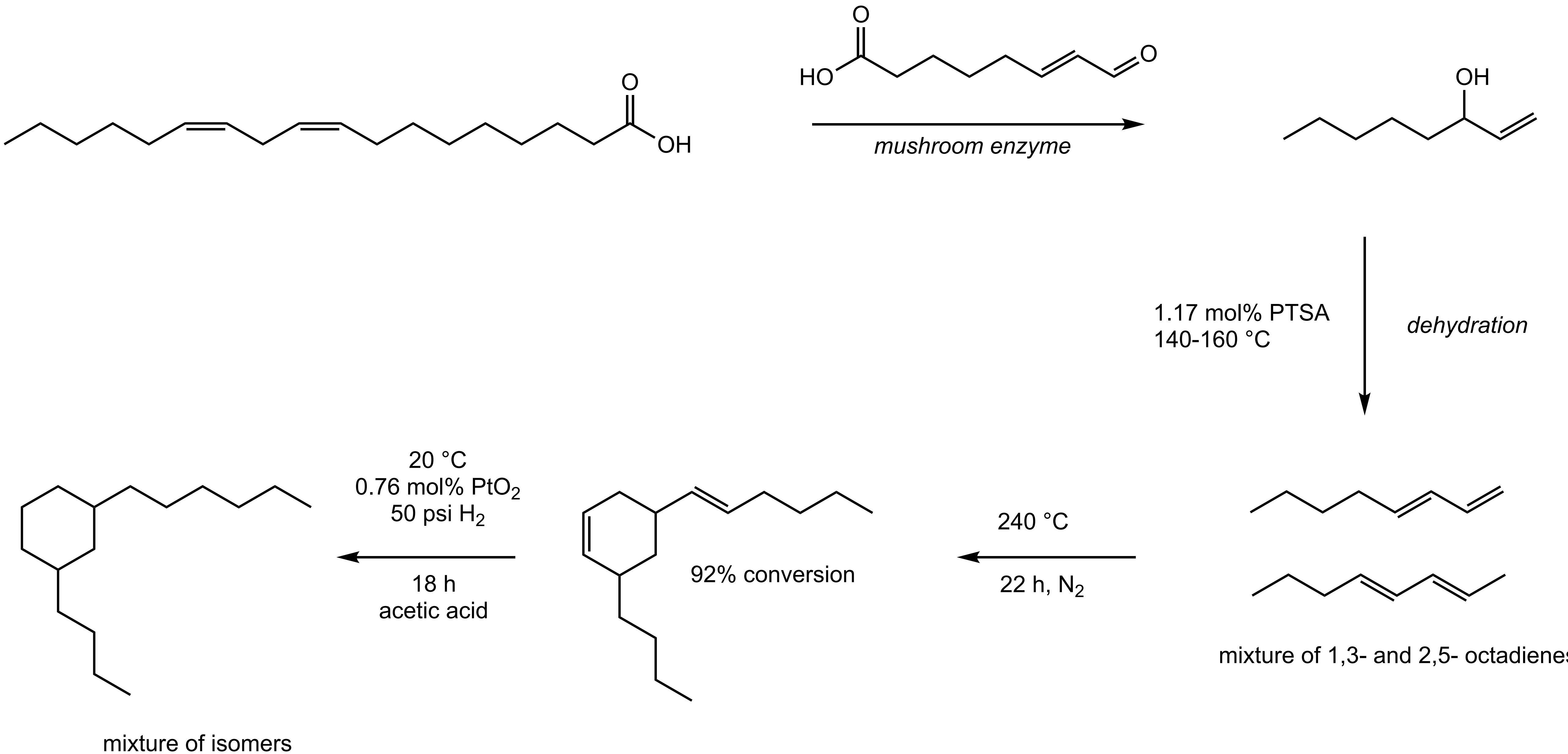
*** Main product in mixture**

Fuels Exhibit Optimal Properties when Blended

Rosenkoetter, K. E.; Kennedy, C. R.; Chirik, P. J.; Harvey, B. G., *Green Chemistry* **2019,** *21*, 5616-5623. Woodroffe, J.-D.; Harvey, B. G. *Energy & Fuels* **2022,** *36*, 2630-2638.

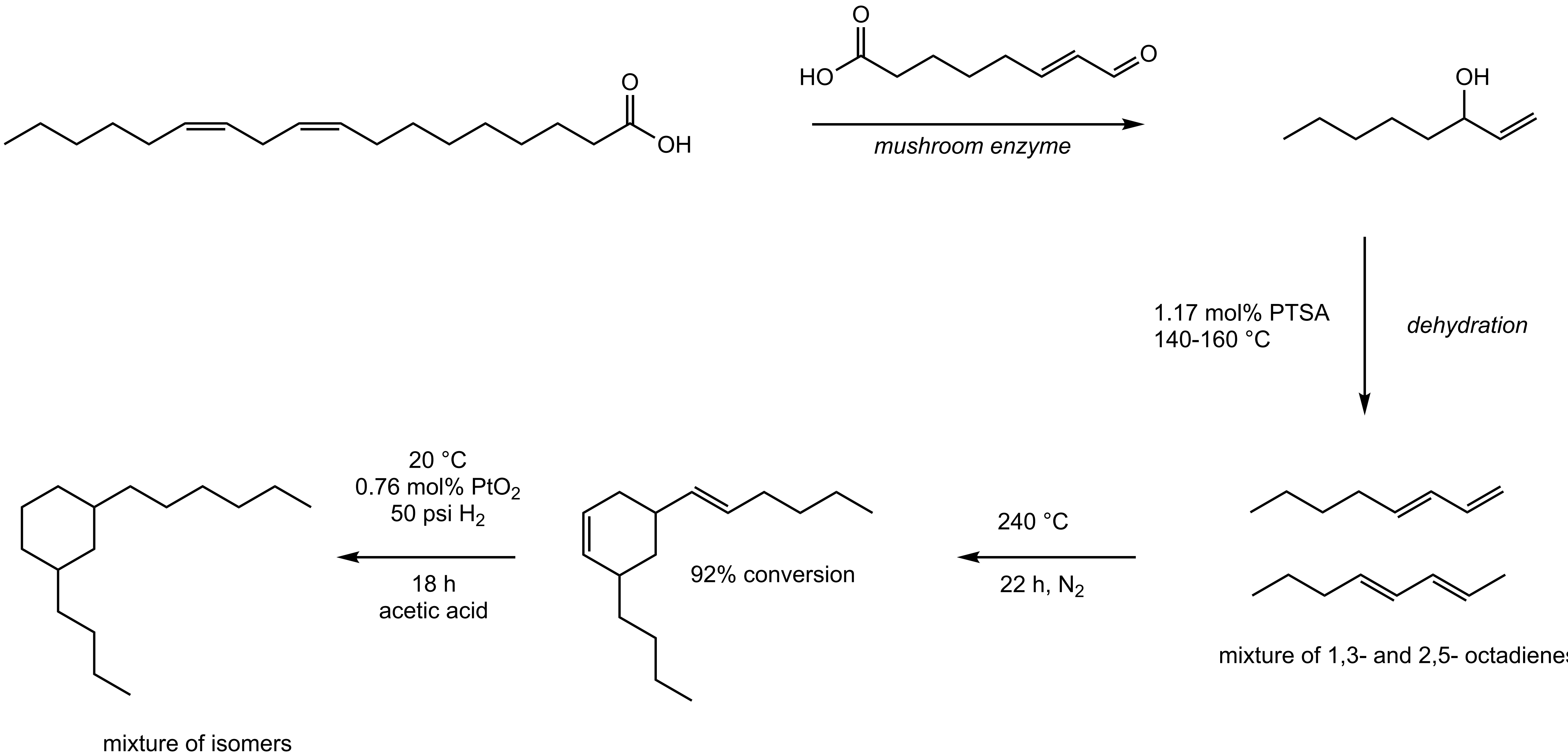
Hydrogenated Octadiene Dimers Derived from Linoleic Acid



Density: 0.835 g/mL (15 °C) - too high

Siirila, M. J.; Zeng, M.; Woodroffe, J.-D.; Askew, R. L.; Harvey, B. G. *Energy & Fuels* **2020,** *34*, 8325-8331.

Hydrogenated Octadiene Dimers Derived from Linoleic Acid

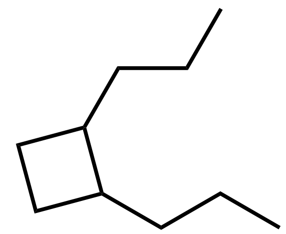


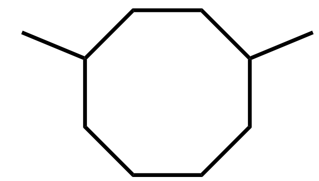
Density: 0.835 g/mL (15 °C) - too high

Do less strained cycloalkanes make less optimal fuels?

Siirila, M. J.; Zeng, M.; Woodroffe, J.-D.; Askew, R. L.; Harvey, B. G. *Energy & Fuels* **2020,** *34*, 8325-8331.

Conclusions and Outlooks

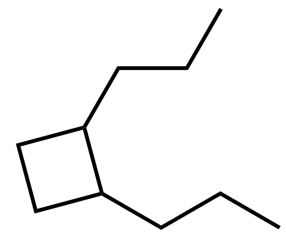


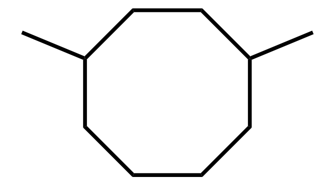


[2+2] and [4+4] products made from bio-based alkenes had properties competitive with or better than Jet-A

Baral, N. R.; Yang, M.; Harvey, B. G.; Simmons, B. A.; Mukhopadhyay, A.; Lee, T. S.; Scown, C. D. *ACS Sustainable Chemistry & Engineering* **2021,** *9*, 11872-11882.

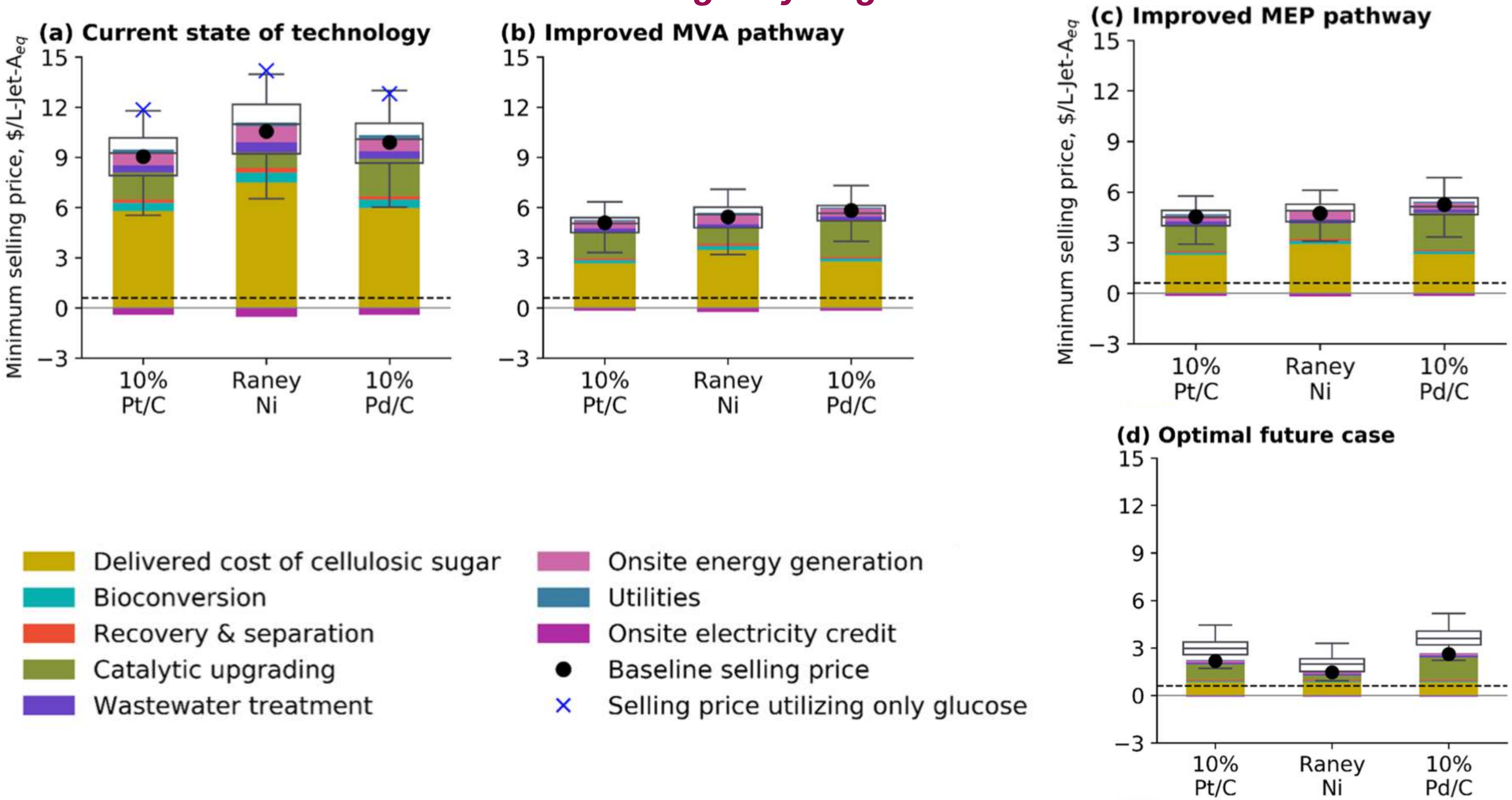
Conclusions and Outlooks





[2+2] and [4+4] products made from bio-based alkenes had properties competitive with or better than Jet-A

Challenge: Hydrogenation



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