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# Computational Investigation of the Mechanism of an Octahedral Ni(II) Proton Reduction Catalyst and Importance of Intramolecular Hydrogen Bonding

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Bhattacharjee, Avik; Brown, Dayalis S.V.; Virca, Carolyn N.; Ethridge, Trent E.; Mendez Galue, Oreana; Pham, Uyen T.; and McCormick, Theresa M., "Computational Investigation of the Mechanism of an Octahedral Ni(II) Proton Reduction Catalyst and Importance of Intramolecular Hydrogen Bonding" (2022). *Student Research Symposium*. 15.

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**Presenter Information**

Avik Bhattacharjee, Dayalis S.V. Brown, Carolyn N. Virca, Trent E. Ethridge, Oreana Mendez Galue, Uyen T. Pham, and Theresa M. McCormick

# Computational investigation of the mechanism of an octahedral Ni(II) proton reduction catalyst and importance of intramolecular hydrogen bonding

Avik Bhattacharjee

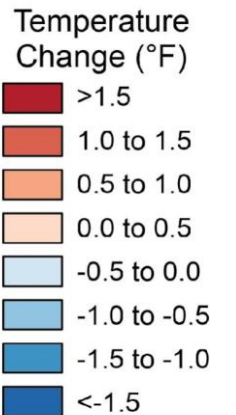
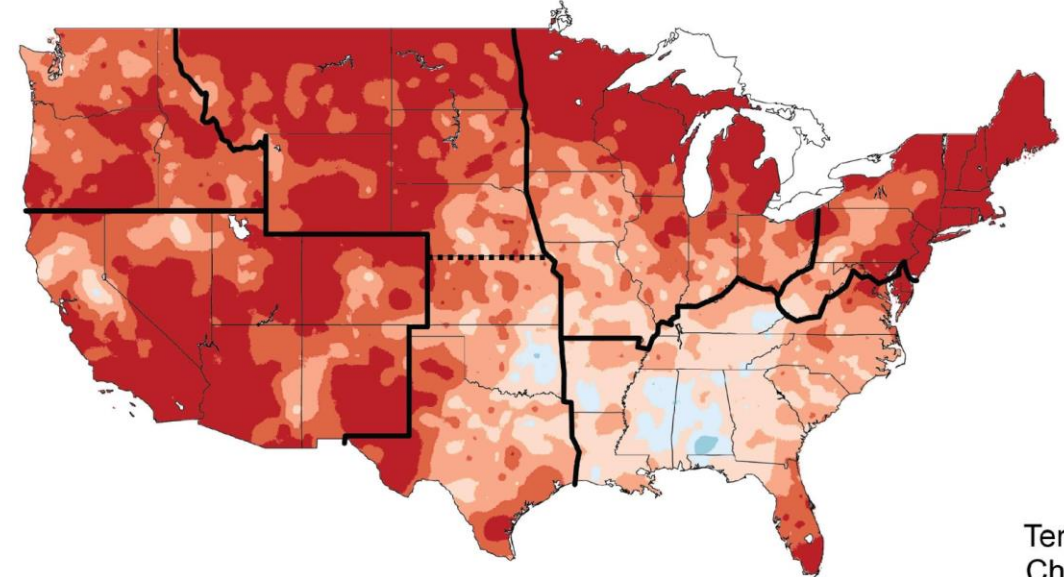
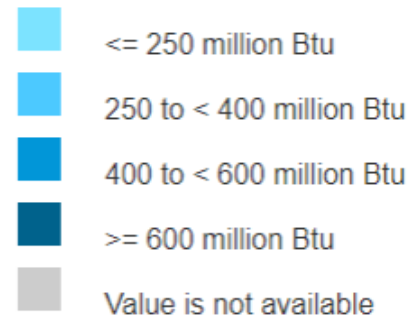
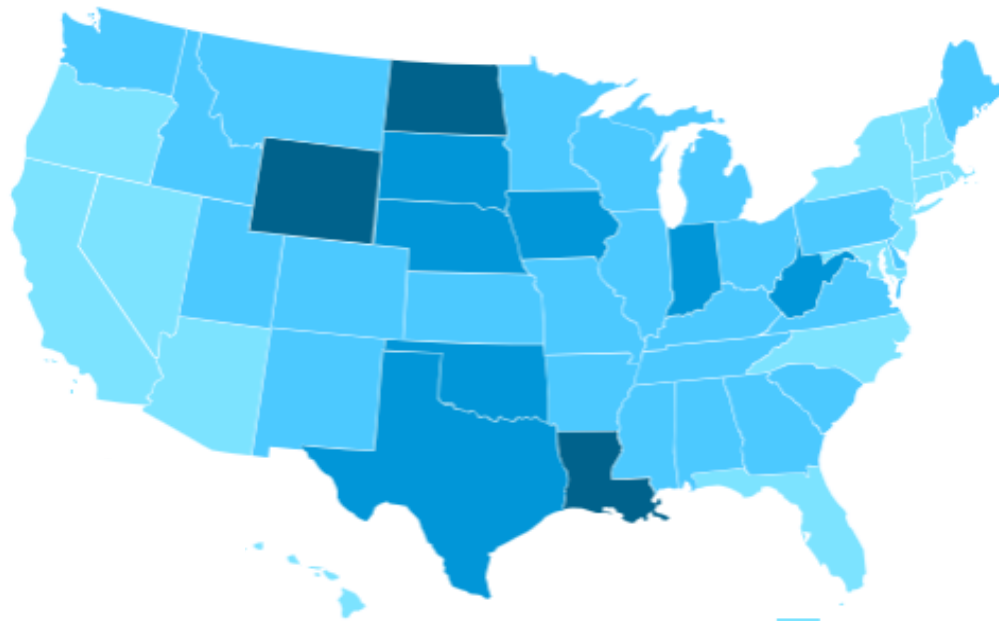
McCormick Group

Oral presentation

Student Research Symposium

05/04/2022

# Use of fossil fuel and Climate Change



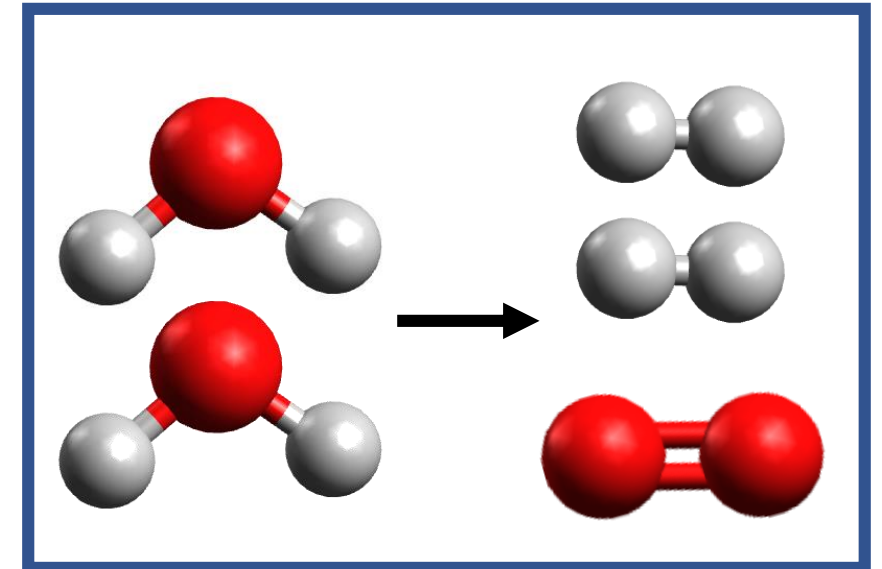
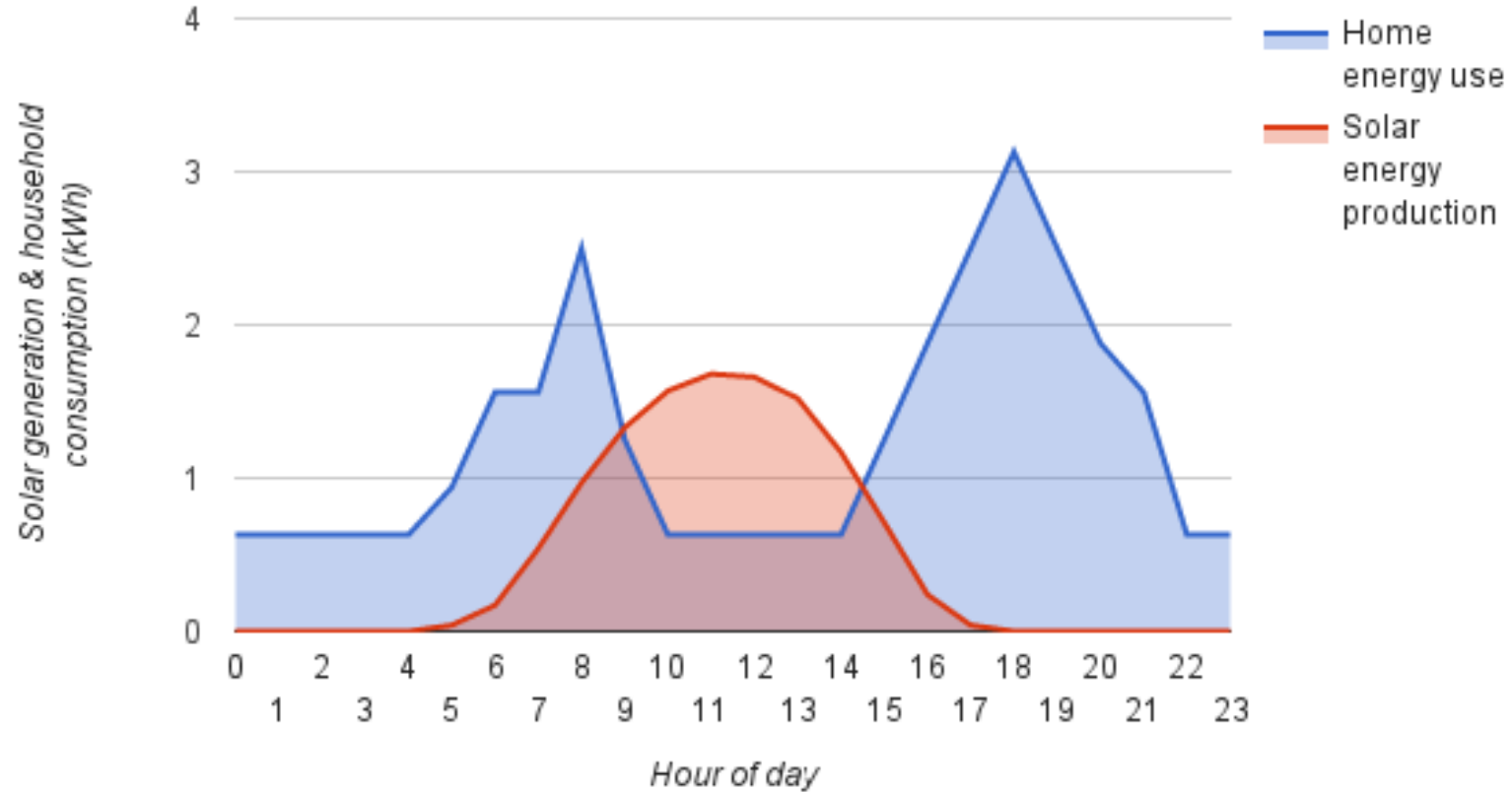
World Energy Council Congress – Enerdata ([Global energy Statistical Yearbook 2019](#))

United States Energy Information Administration ([eia.gov/state/rankings/](https://eia.gov/state/rankings/))

United States Environmental protection Agency (<https://www.epa.gov/ghgemissions/sources-greenhouse-gas-emissions>)

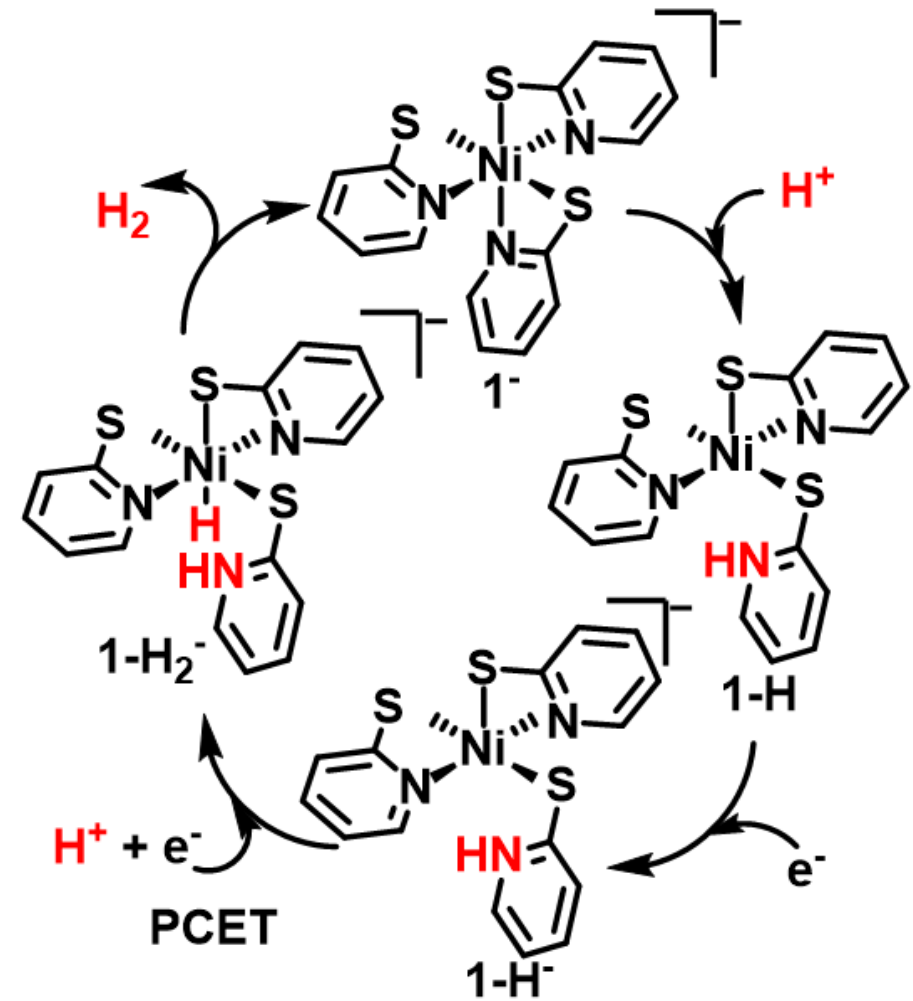
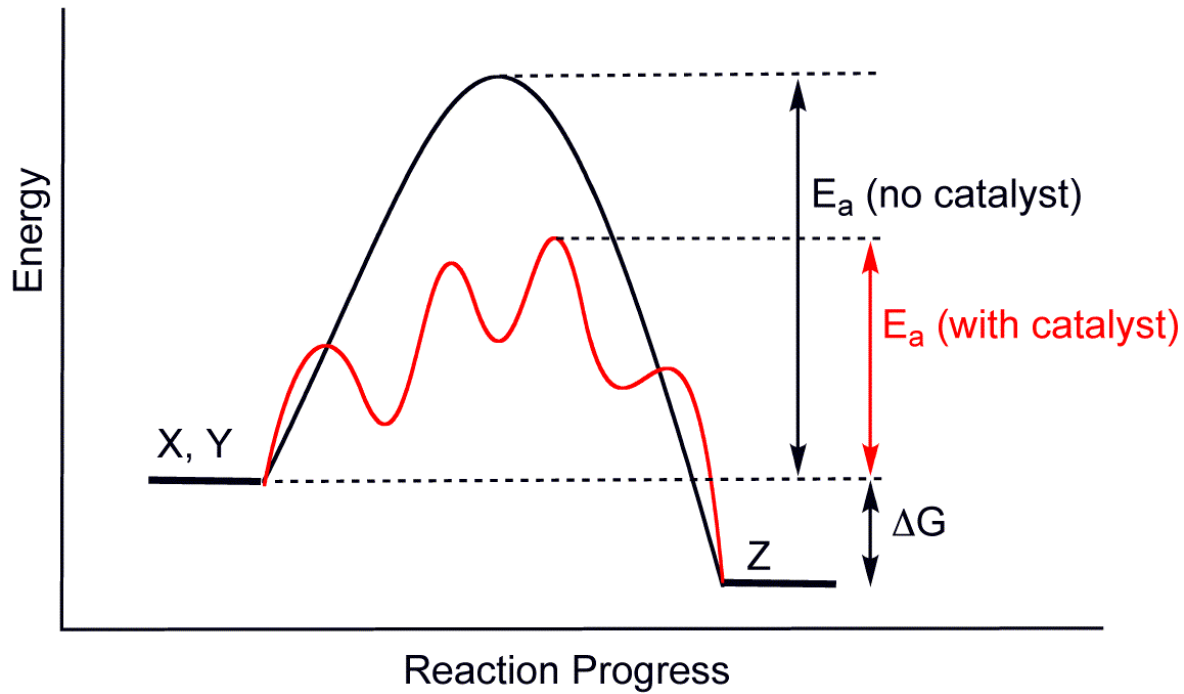
Climate changes in the United States: NASA earth observatory (<https://earthobservatory.nasa.gov/images/83624/climate-changes-in-the-united-states>)

# Solar energy use and practical challenges



<https://www.solarchoice.net.au/blog/solar-self-consumption-overview/>

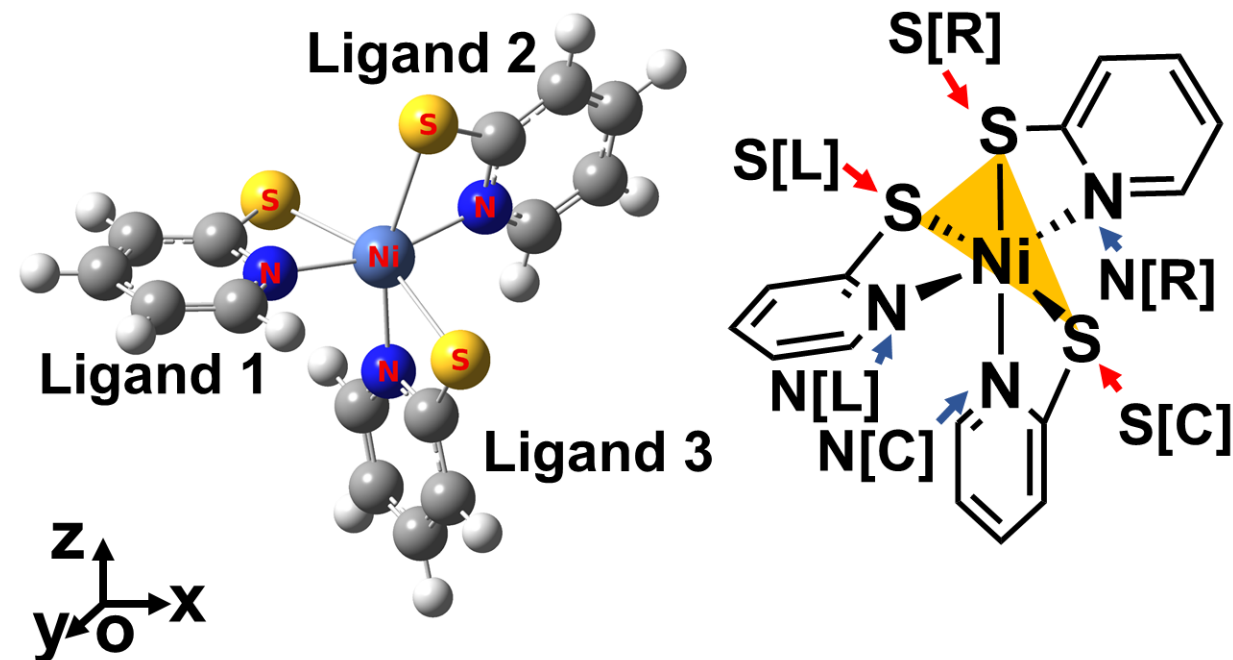
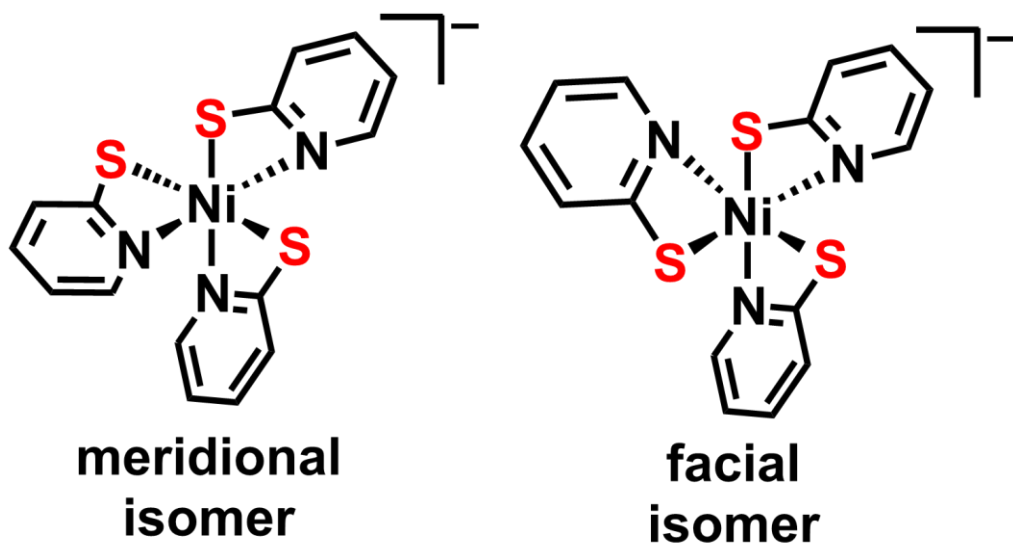
# Catalysis and hydrogen production



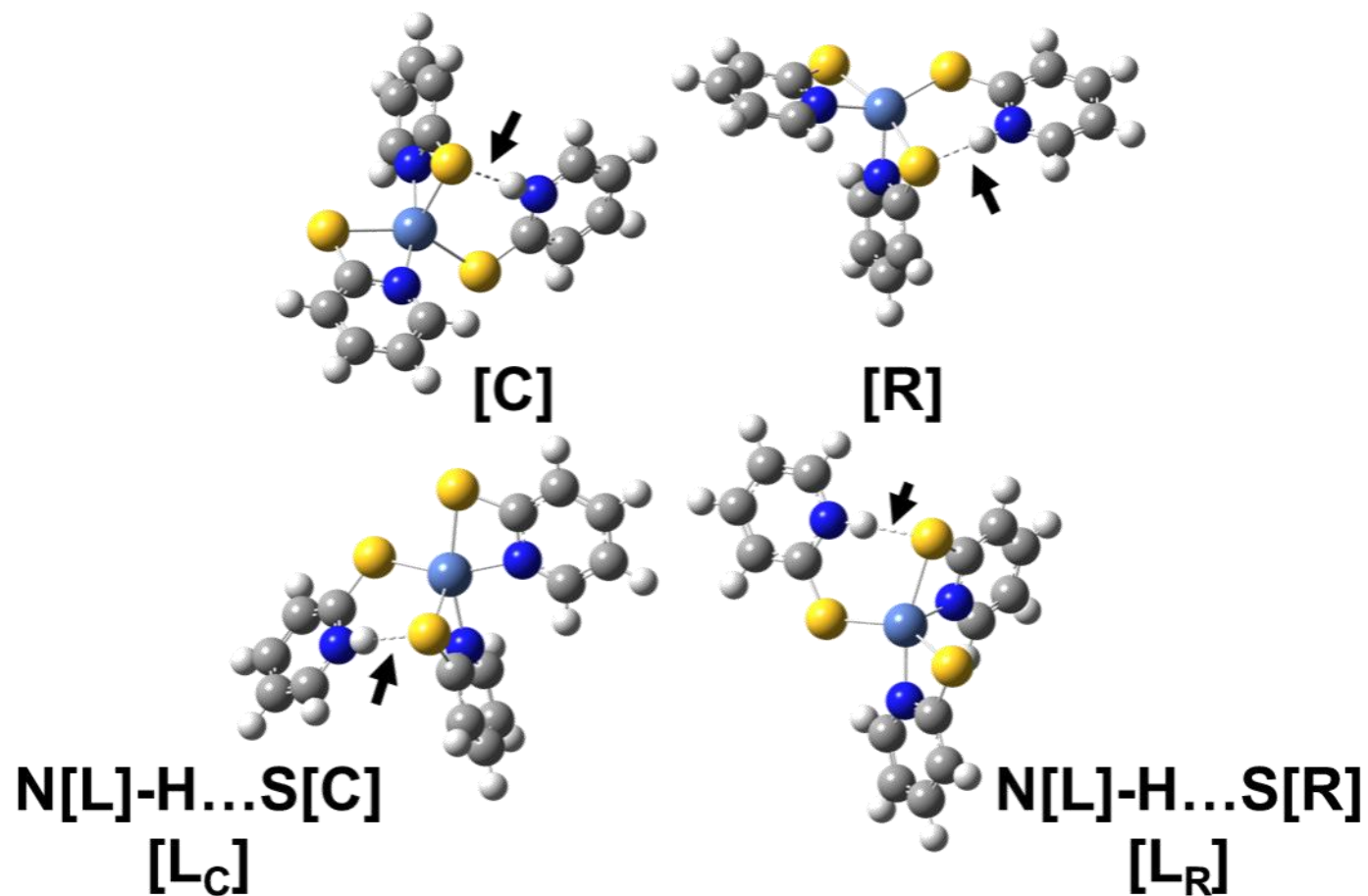
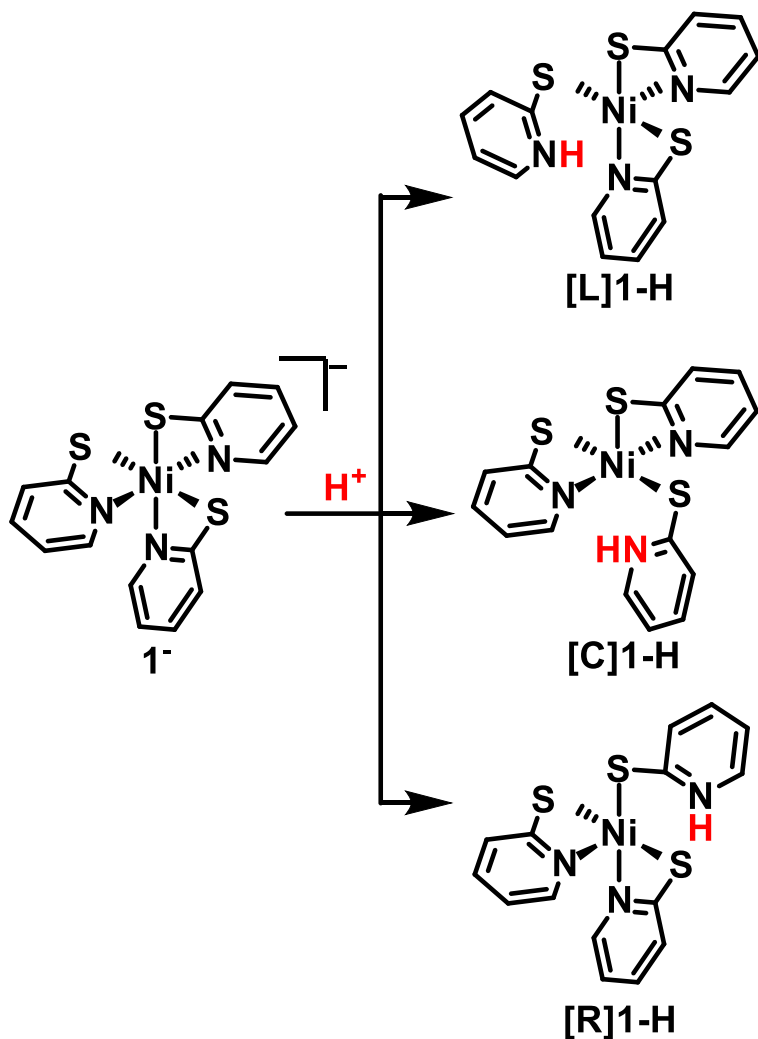
<https://en.wikipedia.org/wiki/Catalysis#/media/File:CatalysisScheme.png>

*Dalton Trans.* **2015**, *44*, 14333–14340.

# Structure and isomers of Ni(II) catalyst

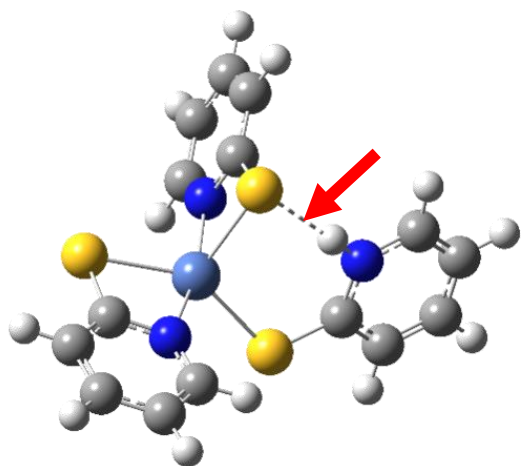


# Protonation of Ni(II) catalyst: *Expectation v. Reality*





# Difference in isomer stability and property

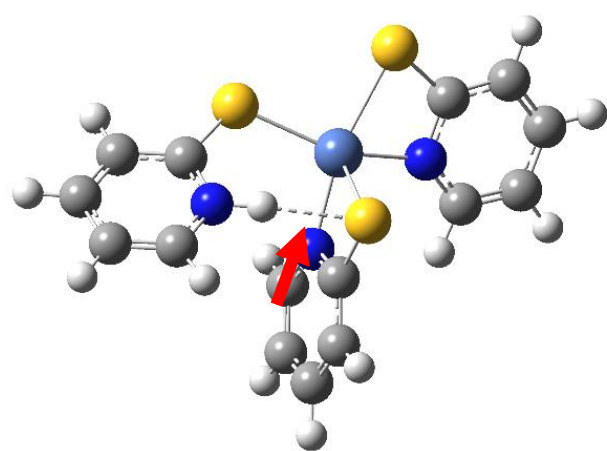


[C]

$pK_a = 11.4$

$\%x = 5.27$

$E^{HB} = -6.32$  kcal/mol



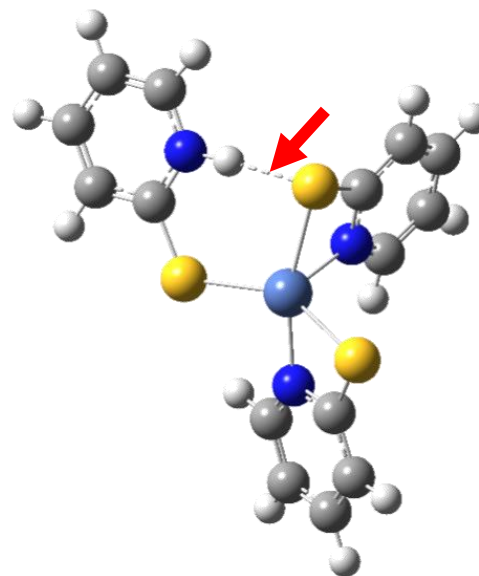
N[L]-H...S[C]

[L<sub>C</sub>]

$pK_a = 11.1$

$\%x = 2.51$

$E^{HB} = -5.99$  kcal/mol



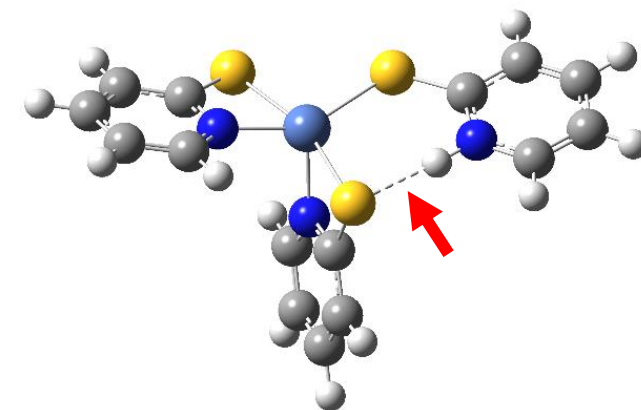
N[L]-H...S[R]

[L<sub>R</sub>]

$pK_a = 12.2$

$\%x = 31.93$

$E^{HB} = -7.36$  kcal/mol



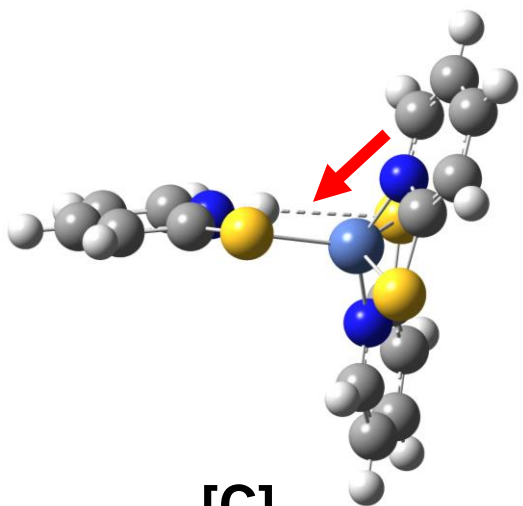
[R]

$pK_a = 12.4$

$\%x = 60.30$

$E^{HB} = -7.39$  kcal/mol

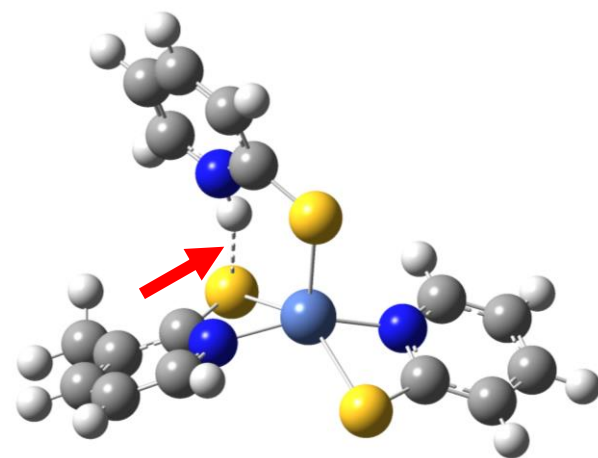
# Reduction step of the catalysis



[C]

%x = 44.29

$E^{\text{HB}} = -6.06 \text{ kcal/mol}$

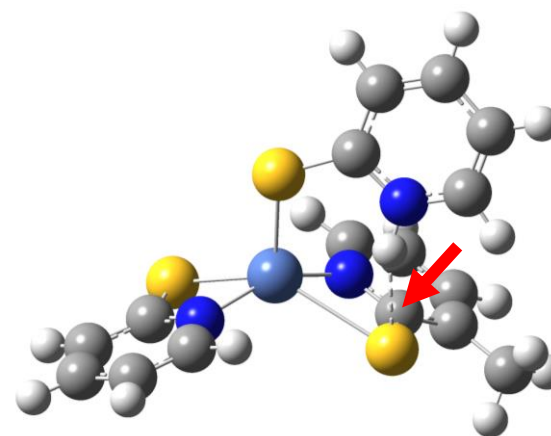


N[L]-H...S[C]

[L<sub>C</sub>]

%x = 8.39

$E^{\text{HB}} = -6.39 \text{ kcal/mol}$

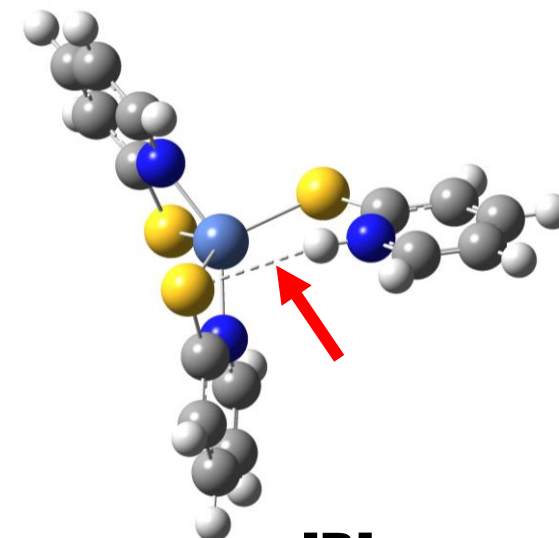


N[L]-H...S[R]

[L<sub>R</sub>]

%x = 3.72

$E^{\text{HB}} = -6.49 \text{ kcal/mol}$

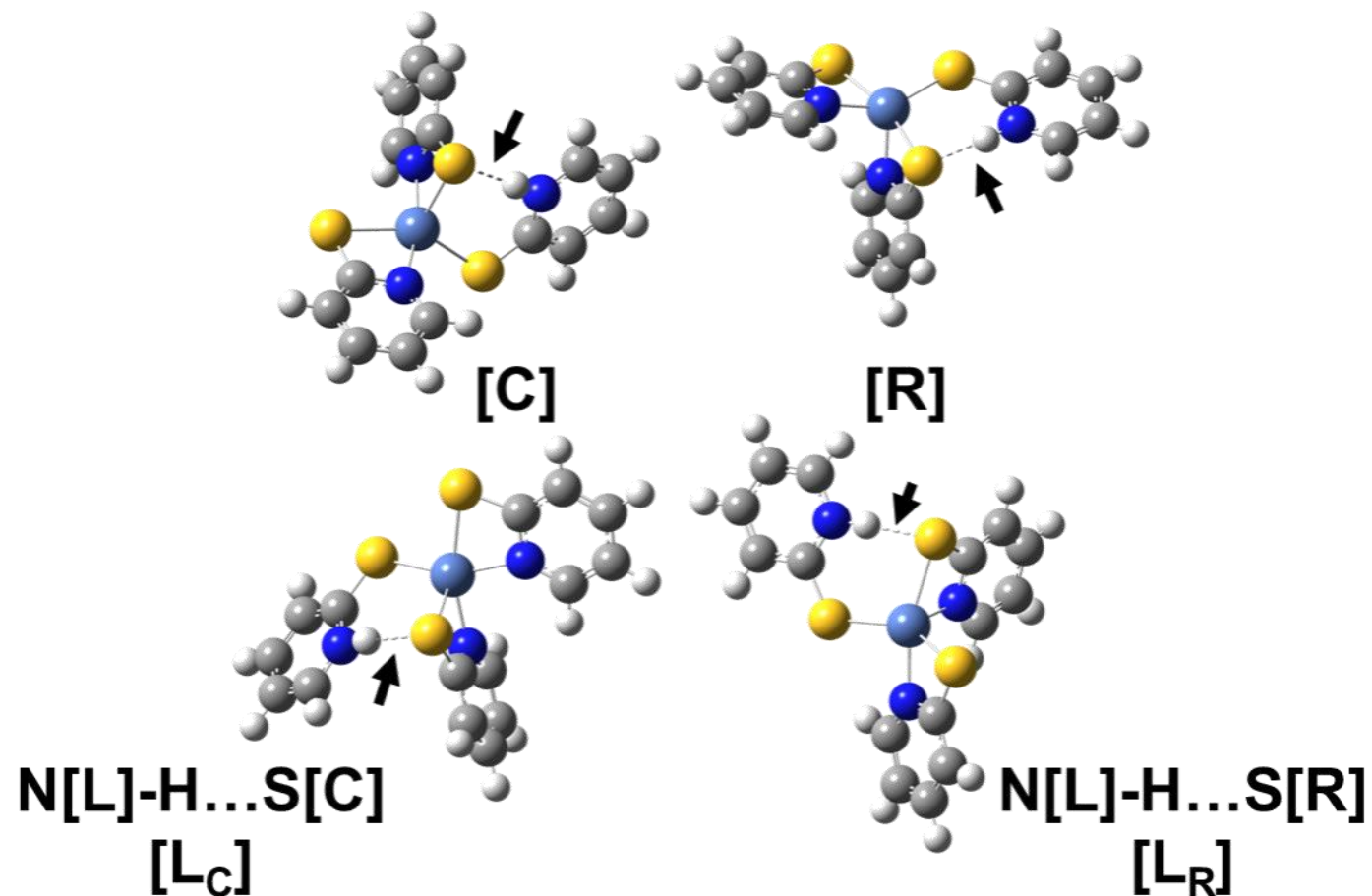
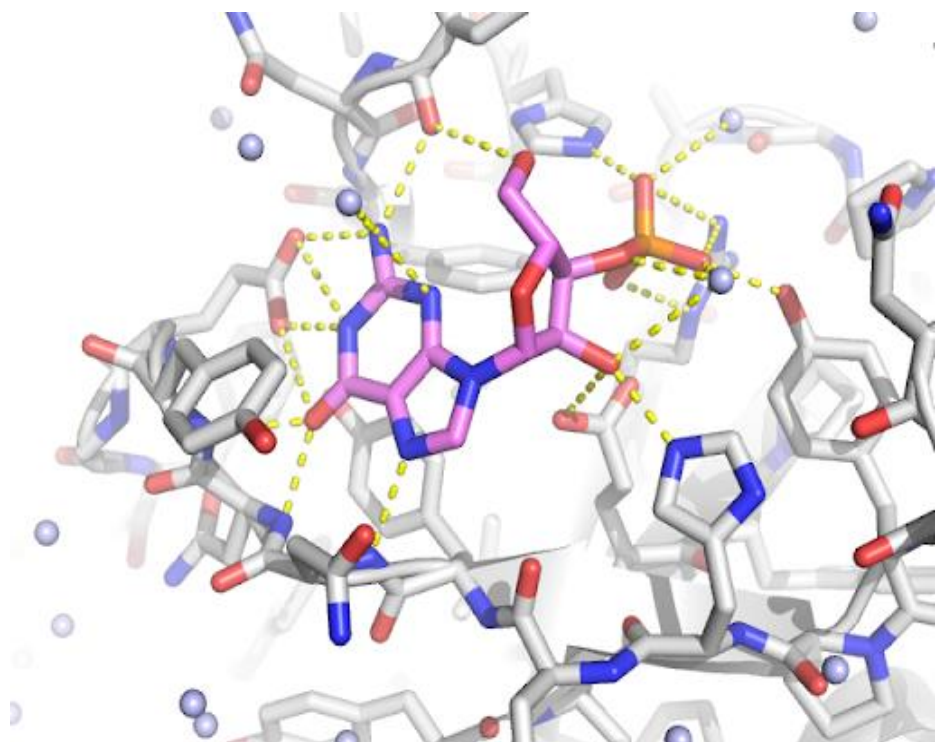


[R]

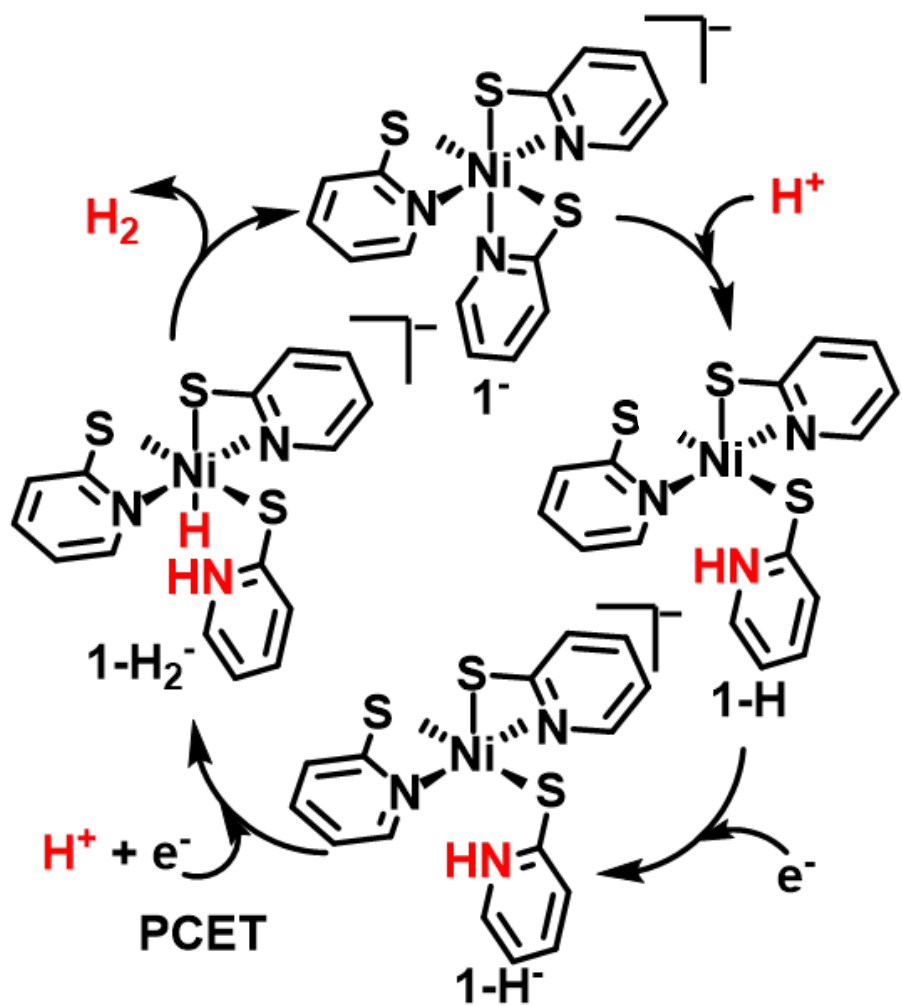
%x = 43.59

$E^{\text{HB}} = -6.06 \text{ kcal/mol}$

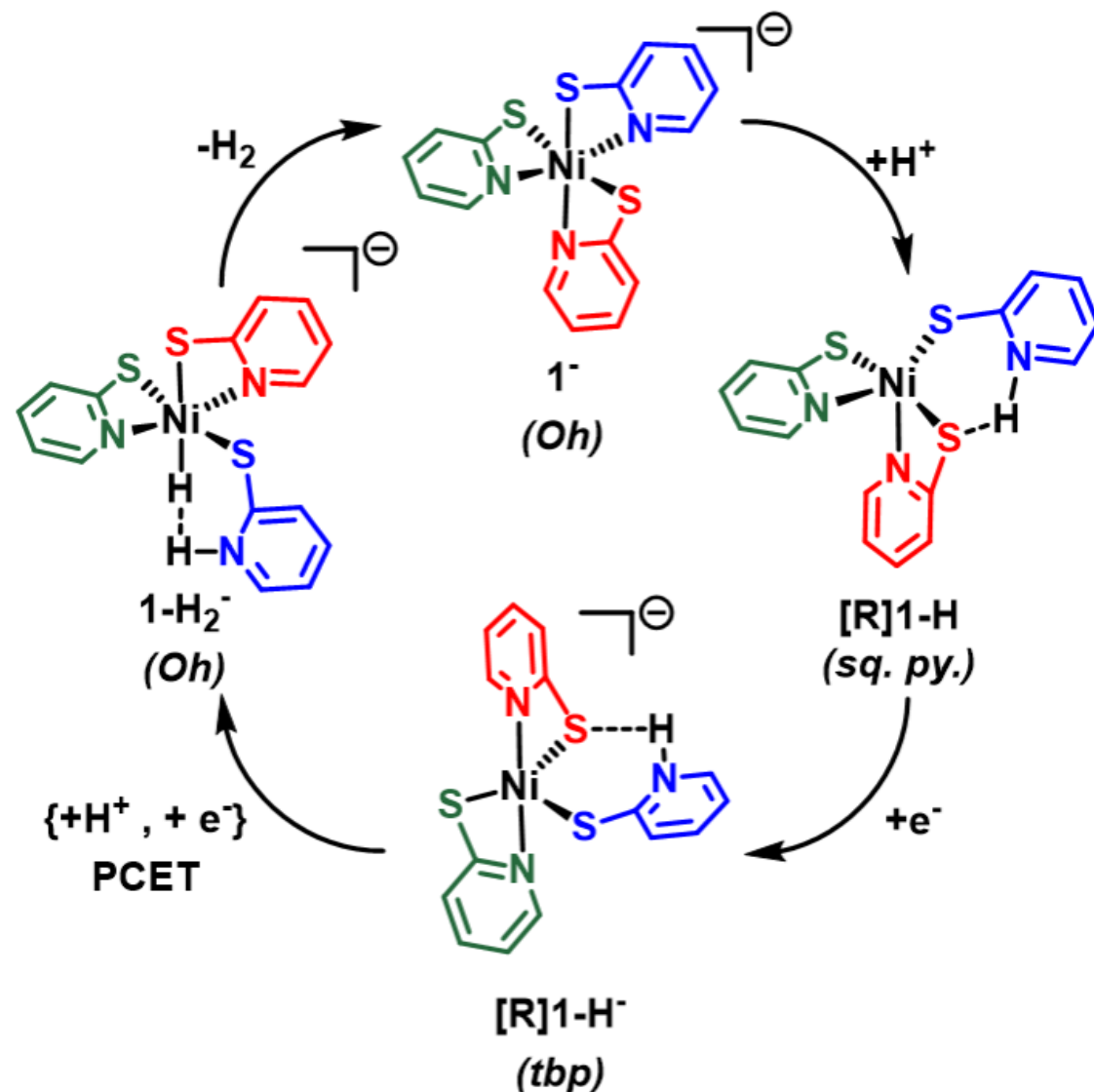
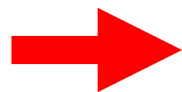
# Importance of intramolecular H-bonding in small molecules



# Effect of H-bonding on the catalytic cycle



*Dalton Trans.*, **2015**, *44*, 14333-14340



*Dalton Trans.*, **2022**, *51*, 3676-3685

# Thank you

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Uyen Pham  
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Dr. Austin Shigemoto  
Dr. Carolyn Virca  
Prof. Eric Rivard  
Dr. Kodi Beyeh  
Dr. David Stuart

