Viability of an Iron Complex for Reactivity

By: Ethan Estrada, Alan Lim, Maritza Vasquez, George Velasco

Mentor: Anthony Wong, PhD Student

Research Lab: Dr. Gabriel Ménard, Chemistry and Biochemistry
Carbon–Carbon Bonds are Difficult to Create Through Chemical Reactions
Carbon–Carbon Bonds are Difficult to Create Through Chemical Reactions

Methanol + Carbon Monoxide
Carbon–Carbon Bonds are Difficult to Create Through Chemical Reactions

\[ \text{Methanol} + \text{Carbon Monoxide} \rightarrow \] Rhodium
Carbon–Carbon Bonds are Difficult to Create Through Chemical Reactions

\[
\text{Methanol} + \text{Carbon Monoxide} \xrightarrow{\text{Rhodium}} \text{Acetic Acid}
\]
Carbon–Carbon Bonds are Difficult to Create Through Chemical Reactions

\[
\text{H}_3\text{C}-\text{O}-\text{H} + \text{C}≡\text{O} \rightarrow \text{H}_2\text{C}-\text{C}-\text{O}-\text{H}
\]

Methanol  Carbon Monoxide  Rhodium  Acetic Acid
Facilitation by Rare Elements can be Replaced by an Iron Complex
Facilitation by Rare Elements can be Replaced by an Iron Complex
Facilitation by Rare Elements can be Replaced by an Iron Complex

\[ \text{Rhodium Complex} \rightarrow \text{Iron Complex} \]
Iron Provides an Alternative to Forming C-C Bonds
Iron Provides an Alternative to Forming C-C Bonds
Iron Provides an Alternative to Forming C-C Bonds
X-Ray Crystallography Confirms 3D Structure of Synthesized Product
X-Ray Crystallography Confirms 3D Structure of Synthesized Product
X-Ray Crystallography Confirms 3D Structure of Synthesized Product
Mossbauer Complements X-ray Crystallography Results

Starting material

Absorbance (%) vs. Velocity (mm/s) for Fe$^{4+}$
Mossbauer Complements X-ray Crystallography Results

Starting material

Absorbance (%) vs. Velocity (mm/s)

Fe$^{4+}$
Mossbauer Complements X-ray Crystallography Results

Final Product

\[
\text{Absorbance (\%) vs. Velocity (mm/s)}
\]

Fe\(^{3+}\)

\[
\begin{array}{c}
\text{Fe(I)} \\
\text{Fe(II)} \\
\text{Fe(III)} \\
\text{Fe(IV)} \\
\text{Fe(VI)} \\
\end{array}
\]

- Fe(I) \(S=3/2\)
- Fe(I) \(S=1/2\)
- Fe(II) \(S=1\)
- Fe(II) \(S=0\)
- Fe(III) \(S=5/2\)
- Fe(III) \(S=3/2\)
- Fe(III) \(S=1/2\)
- Fe(IV) \(S=2\)
- Fe(IV) \(S=1\)
- Fe(VI) \(S=1\)

\[\delta/\text{mm s}^{-1}\]

-1.0, -0.5, 0, 0.5, 1.0, 1.5, 2.0

Final Product
Mossbauer Complements X-ray Crystallography Results

Final Product

Absorbance (%) vs. Velocity (mm/s) for Fe\(^{3+}\)

[Graph showing data points and curves for absorbance vs. velocity]

[Diagram showing different Fe states and their spin quantum numbers]

Fe(I) S=3/2, Fe(I) S=1/2, Fe(II) S=2, Fe(II) S=1, Fe(II) S=0, Fe(III) S=5/2, Fe(III) S=3/2, Fe(III) S=1/2, Fe(IV) S=2, Fe(IV) S=1, Fe(VI) S=1, Fe(VI) S=1/2

Final Product
Nuclear Magnetic Resonance Confirms Iron's Presence in the Molecular Structure
Nuclear Magnetic Resonance Confirms Iron's Presence in the Molecular Structure
Isolation of Organic Segments Requires Future Research
Isolation of Organic Segments Requires Future Research
Acknowledgements

**Mentor:** Anthony Wong

**SIMS Coordinator:** Rachel Alvelais

**RAs:** Trevor "Travis" Cohen,
Carina Motta, Madeline Allen,
Euclid Quirino

**Ménard Group**

*Clean Energy | Sustainable Chemistry*
Acknowledgements
Iron Provides an Alternative to Forming C-C Bonds