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Activity: Advanced ChemDraw

Learning objectives:

Students will be able to:

1. Convey 3-D structure of a molecule in a drawing.
2. Recreate molecular drawings found in the literature.
3. Create digital drawings of molecules using ChemDraw
4. Create digital drawings of reaction schemes & cycles

Activity:

Part A: Each of the following structures was found in recently published papers. For each,

1. Determine the molecular formula of the complex.
2. Determine the approximate geometry around the metal center (ie. Octahedral, square planar...)
3. Recreate the drawing as best you can using Chemdraw.

Complex 1: Na, H.; Lai, P. -N.; Cañada, L. M.; Teets, T. S. "*Photoluminescence of Cyclometalated Iridium Complexes in Poly(methyl methacrylate) Films,*" *Organometallics*, **2018**, DOI: 10.1021/acs.organomet.8b00446

(insert figure of molecule in top left of Chart 1)

Complex 2: Yamamoto, N.; Sato, Y.; Kayaki, Y.; Ikariya, T. "*Synthesis and Reactivity of Cp*Ir^{III} Complexes with a C-S Chelate Displaying Metal/Sulfur Bifunctionality,*" *Organometallics*, **2018**, DOI: 10.1021/acs.organomet.8b00562

(insert figure of molecule D from Chart 2)

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Part B: Each of the following reactions was found in recently published papers. For each,

1. Recreate the reaction scheme in Chemdraw
2. Be sure to watch out for everything being lined up, font types, colors
3. Use templates to help speed up drawing

Reaction 1: Xiong, Y.; Sun, Y.; Zhang, G. "Copper-Catalyzed Synthesis of β -Azido Sulfonates or Fluorinated Alkanes: Divergent Reactivity of Sodium Sulfinates," *Org. Lett.* **2018**, DOI: 10.1021/acs.orglett.8b02735

(insert figure of reaction scheme in TOC graphic, only showing the first product)

Reaction 2: Bowes, E. G.; Pal, S.; Love, J. A. "Exclusive Csp^3-Csp^3 vs Csp^2-Csp^3 Reductive Elimination from Pt^{IV} Governed by Ligand Constraints," *J. Am. Chem. Soc.* **2015**, *137*, 16004-16007.

(insert figure of Scheme 1)

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Challenge (5 points extra credit): Draw the following structure from the paper:

Palumbo, C. T.; Darago, L. E.; Dumas, M. T.; Ziller, J. W.; Long, J. R.; Evans, W. J.

Structure, Magnetism, and Multi-electron Reduction Reactivity

of the Inverse Sandwich Reduced Arene La₂+ Complex

$[\{[C_5H_3(SiMe_3)_2]_2La\}_2(\mu-\eta^6:\eta^6-C_6H_6)]^{1-}$, *Organometallics*, 2018,

10.1021/acs.organomet.8b00523

(insert figure of the product from Scheme/Reaction 6)

Part D: Upload your Chemdraw file to blackboard by the end of the weekend.