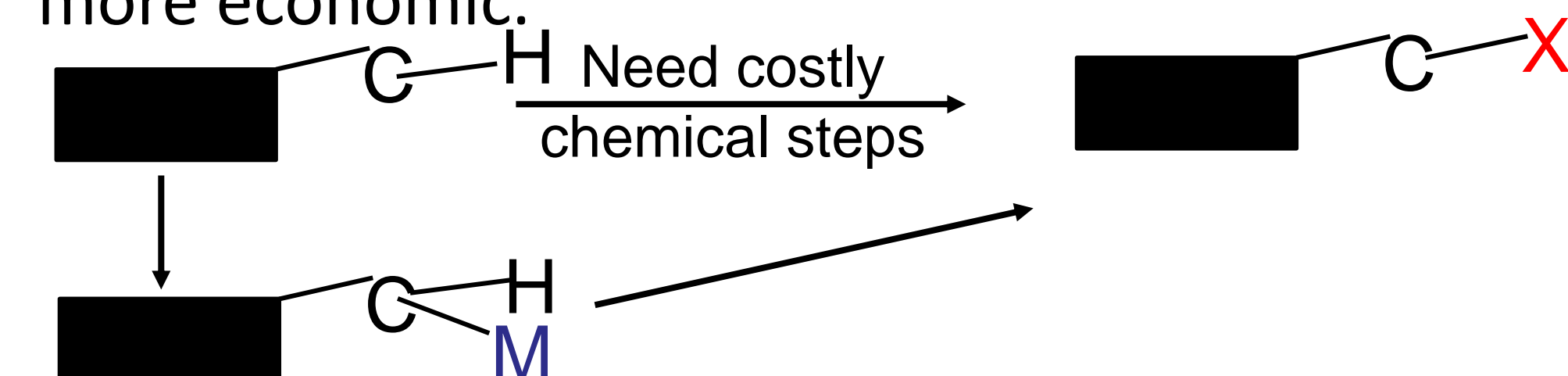


Research Question

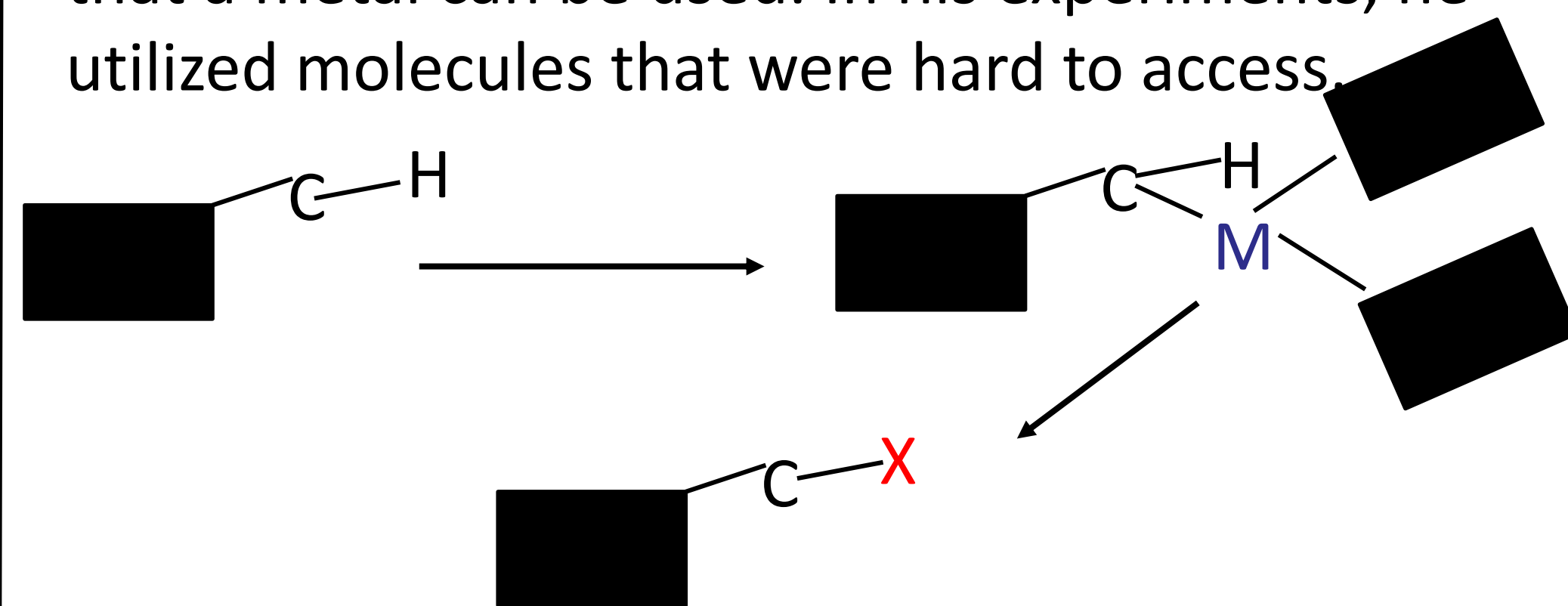
What can be used to mediate Carbon Hydrogen bond activation?

Background

In order for Carbon-Hydrogen bond activation to occur, Sanford introduces the ideas of using a metal catalyst to try and help weaken the C-H bond. In this discovery, Sanford has enabled us to have a synthesis that consists of less steps and thus is more economic.



While Cocco, furthered this research confirming that a metal can be used. In his experiments, he utilized molecules that were hard to access.



Predictions

From prior research that has been conducted, I want to investigate a new structure. This new structure consists of a metal catalyst with much more easy access to it. This structure will help me in the study of the Carbon Hydrogen breaking process.

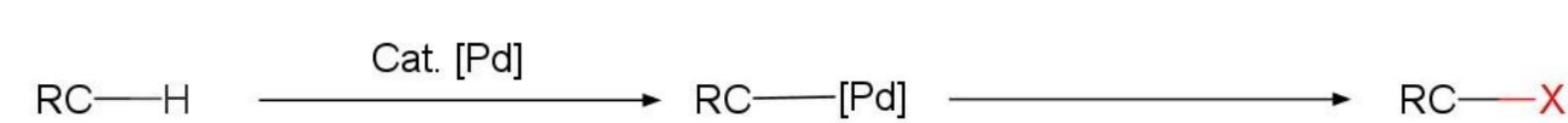
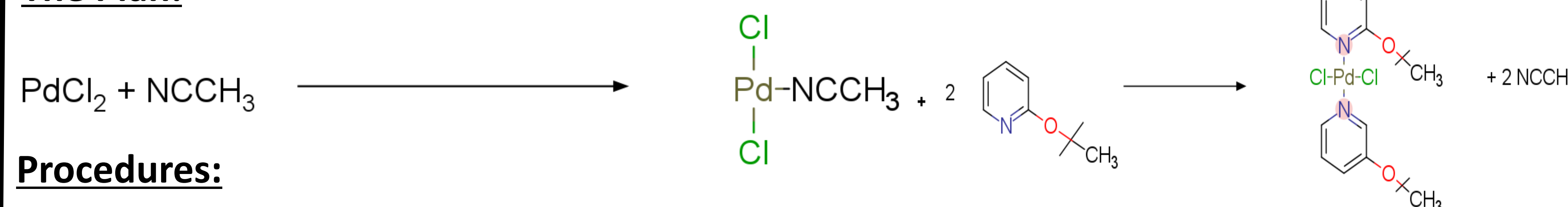


Figure 3: Transformation of C-H bonds into several functional groups by using a Palladium Catalyst

Method

The Plan:



Procedures:

Synthesis of $Pd(NCCH_3)_3Cl_2$:

- React 0.0252 grams of $PdCl_2$ into a 25 mL round bottom flask
- Add 3 mL of acetonitrile
- Heat for 30 minutes and stir at a temperature of 200 °C
- Precipitate the complex with 2 mL of hexane
- Vacuum filter the precipitate and wash with hexane then collect to dry (0.0093g)
- After a week, 10 drops of DCM were added to the compound to check the solubility
- The procedure above was done twice

Synthesis of $PdCl_2TBP_2$:

- After, with the compound that was soluble, 0.035 grams of $Pd(NCCH_3)_3Cl_2$ was added to 20 microliters into a beaker
- In that beaker, 3 mL of DCM was added into it
- Let the mixture stir for 4 days at room temperature
- After the 4 days collect this solid (0.0245 grams) with vacuum filtration
- Conduct NMRs on solid complexes that were collected

Discussion

Recap of Findings:

Despite there being prior research that shows the ability of using a metal catalyst to activate the Carbon-Hydrogen bond, in my research I was not able to do so. I was not able to synthesize $PdCl_2TBP_2$. Thus, it was not possible to investigate if a palladium molecule with more access can be used to activate the Carbon-Hydrogen bond.

Future Research:

- $Pd(NCCH_3)_3Cl_2$: Conduct NMR on this complex to make sure that it is a pure product.

Results

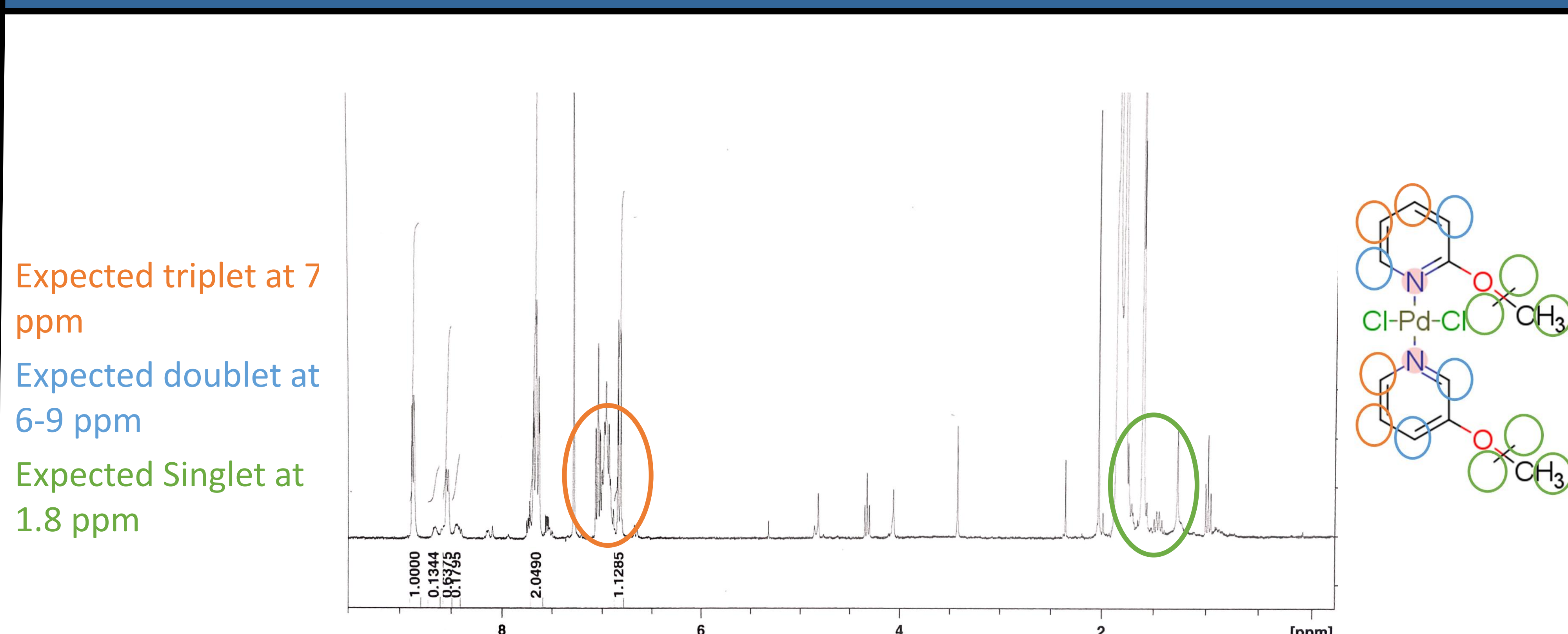


Figure 12 An NMR spectrum.

References

Cocco, F.; Zucca, A.; Stoccoro, S.; Serratrice, M.; Guerri, A.; Cinellu, M. A. Synthesis and Characterization of Palladium(II) and Platinum(II) Adducts and Cyclometalated Complexes of 6,6'-Dimethoxy-2,2'-Bipyridine: C(Sp³)-H and C(Sp²)-H Bond Activations. *Organometallics* **2014**, *33* (13), 3414–3424. <https://doi.org/10.1021/om5003057>.

Neufeldt, S. R.; Sanford, M. S. Controlling Site Selectivity in Palladium-Catalyzed C-H Bond Functionalization. *Acc. Chem. Res.* **2012**, *45* (6), 936–946.

<https://doi.org/10.1021/ar300014f>.