**Guided Literature Reading and Discussion: Synthesis & Characterization of Reduced Borafluorene Monoanions**

Please complete these guiding questions to *Angew. Chem. Int. Ed*. **2021**, *60*, 13065-13072. <https://onlinelibrary.wiley.com/doi/10.1002/anie.202103628>

**Part I: Preparing to read the article**

*Optional:* Before reading the paper, review section 8.5.2 (*Other chemistry of the group 13 elements*) in Miessler, Fischer, and Tarr or other relevant material. (This can be removed at the professor’s discretions; the reading is not strictly necessary.)

1. What is the electron configuration (full or condensed) of boron?
2. Many compounds have similar names but very different structures.
   1. Draw the Lewis dot structure of a single atom of fluorine.
   2. Draw the Lewis dot structure of difluorine.
   3. Draw the line structure of fluorene.
   4. Draw the line structure borafluorene.
3. Draw the Lewis dot structures of BCl3 and NH3. Identify the Lewis acid and the Lewis base.
4. Define reduction and oxidation.
5. In 1-2 sentences, describe the relationship between bond order, bond length, and bond strength?

**Part II: Reading the introduction**

The introductions of scientific articles typically possess a funnel structure. They provide broad context and progressively narrow to the specific topics of the paper. Keep this in mind as you are reading the introduction and answering the following questions.

1. Using only the information from reading the abstract, describe in 1-2 sentences what this paper is about.
2. Write one sentence to explain the major takeaway from the first paragraph of the introduction.
3. One of the most important paragraphs of the introduction is paragraph 3 on page 13066 beginning with, “Recently, we have utilized carbenes…”. What is the purpose of paragraph 3? What are the authors trying to convey?
4. Consider the abbreviations NHC and CAAC.
   1. Define the abbreviations.
   2. Draw the structure of the uncoordinated NHC ligand and the uncoordinated CAAC ligand used in this paper.
   3. What do both of these structures have in common?
   4. What is a key difference in the electronic properties of the two?
5. NHC is a common ligand class for both main group and transition metals. Draw a generalized skeleton of an NHC compound.

**Part III: Analyzing Results & Discussion** 

In the results and discussion section, the authors reported a series of different NHC and CAAC-containing complexes. Through the following questions use the author’s data to compare these compounds. 

1. What are the orbitals that overlap to form the boron-carbon bonds between the carbene ligands and the boron?
2. Which compound do the authors report as more stable, compound **3** or **6**? Explain the difference in stability and how it connects to reactivity in 1-2 sentences.
3. The authors use lithium naphthalenide (LiNp), sodium metal, and potassium graphite (KC8) as reducing agents.
   1. Define the term reducing agent.
   2. What are the characteristic properties of good reducing agents?
4. Look up the carbon-boron (C1-B1) bond lengths in compounds **1**, **2**, **3**, and **6** and write them down. What do these differences imply about bond order and strength?
5. Consider the electron donating abilities (Lewis base properties) of the NHC and CAAC ligands.
   1. Describe and compare the - and - donating properties of the NHC and CAAC compounds. Refer to the crystallographic data you used to answer question 4.
   2. How does these properties affect how they act as ligands?
6. The authors performed Density Functional Theory (DFT) calculations, which are a type of quantum mechanics calculation.
   1. According to the authors’ explanation, did the results of the DFT calculations support or contradict the crystallography data?
   2. Why did the authors choose to include this information in the paper?
7. Figure 4a on page 13068 shows compound 3 with yellow and blue areas which have been determined using DFT calculations. [Insert figure 4 here for color]
   1. What do the yellow and blue areas on the figure describe?
   2. How is this information useful to the researchers?

1. In Scheme 2 the reactivity of **5** and **8** with several complexes is shown.
   1. Is the boron center acting as a Lewis acid or a Lewis base in these reactions?
   2. Draw an arrow-pushing mechanism to describe the movement of electrons in one of these bond forming reaction.
2. Up to page 13070, the authors’ focused on the synthesis and characterization of new borafluorene compounds. After this point, the focus of the paper shifts.
   1. In one sentence, what is the focus of the remainder of the paper?
   2. Why do you think the authors’ include this?
   3. Imagine that you were a student working on this project. In a meeting with Dr. Gilliard, you are discussing next steps. What would you propose as a next experiment or project?