The following questions refer to the article “Crystal Structure Determination of the Pentagonal-Pyramidal Hexamethylbenzene Dication C6(CH3)62+” by Malischewski and Seppelt, published *Angewandte Chemie International Edition* in 2017, volume 56, pages 368-370 (DOI: 10.1002/anie.201608795). In this exercise you will use the skills you have learned to look at a purely organic molecule through the lens of Inorganic Chemistry. Complete this assignment prior to coming to class. We will do an in-class exercise related to the paper and discuss this paper in class as well.

**Question 1.** *Angewandte Chemie International Edition* is abbreviated *Angew. Chem. Int. Ed.* (sometimes written at ACIE) and is a very prestigious journal whose readership covers the entire field of chemistry in terms of specialization. Why do you think this article was suitable to be published in this journal?

**Question 2.** The authors crystallized a unique structure of the hexamethylbenzene dication. What is the point group for this dication? What is the point group of regular hexamethylbenzene? Breifly explain how you came to your point group assignments.

**Question 3.** If the title compound was [((CCH3)5)MCH3]2+ instead of [((CCH3)5)CCH3]2+, what would the oxidation state of the metal be? Describe each of the ligands as X or L (or a combination thereof), and described the coordination of *each ligand* in terms of η, κ, and/or μ. Also, what is the common abbreviation for the (CCH3)5 group when it is a ligand on a metal?

**Question 4.** Create a qualitative MO diagram of the important pi-orbital MOs in the Cp\*-1 ligand. Be sure to assign the point group to the fragment and label the MOs with the proper irreducible representation label. Sketch the MOs as well.

**Question 5.** A methyl anion (CH3-1) has the same symmetry and number of electrons as ammonia. Find the MO diagram for ammonia in your text book and use it to draw and label with appropriate symmetries the HOMO and LUMO of CH3-1.

**Question 6.** How many electrons are in C6H62+? What is the charge on the B6H6 species that would be isoelectronic with this compound? What is the structure of this charged boron compound according to Wade’s Rules?