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Literature Discussion of Perhalogenated Carba‐closo‐dodecaborate Anions as Ligand Substituents: Applications in Gold Catalysis

This guided literature discussion explores  the 2013 paper by Lavallo and coworkers reporting the synthesis and hydroamination activity of a carba-*closo*-dodecaborate ligated gold catalyst. Lavallo, V.; Wright II, J. H.; Tham, F. S.; Quinlivan, S. *Angew. Chem. Int. Ed.* **2013**, *52*, 3172. DOI: <https://doi.org/10.1002/anie.201209107>.

This guided discussion examines the synthesis and structure of the ligand and catalyst complex. For a deeper exploration of the catalytic data, see the 1FLO on the same paper.

This LO was developed at the 2022 VIPEr workshop at Cal Poly Pomona in Pomona, CA.

Structural Questions

1. It is noted that in figure 1 the bond length between the phosphorous atom and the carborane cage carbon atom is significantly longer than those between the phosphorous atom and the isopropyl groups.  What are those bond lengths and why is this the case?

1. Using the structure of compound (3LiCl) presented in Figure 2, draw the van der Waals interaction between the weakly coordinating chloride and gold using a dotted line.

1. Why does the peak for phosphinein compound (3LiCl) in the 31P NMR spectrum shift downfield from the starting material (2)?

1. What is a Tolman cone angle? How does the angle of ligand (2) compare to the angle for P*t*BU3? Why is this significant?

1. What is a pendant weakly coordinating anion? Find another example of this type of anion in the literature.

Synthetic Questions

1. In Figure 2, the same starting material can be turned into 2 different products depending on the choice of solvent. Why is this the case?

1. Find a literature procedure for the synthesis of compound 1.

1. The authors screened ClAu(THT) and ClAu(THT) + [HCB11Cl11][Cs] as potential catalysts. Why did the authors do that? What were the results and what do you think that demonstrated? Are there other catalysts that one could screen to better answer that question?