**The elusive tetrabenzylthorium compound (Bart)**

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D. M. Ramitha, Y. P. Rupasinghe, Makayla R. Baxter, Matthias Zeller, and Suzanne C. Bart “Isolation and Characterization of Elusive Tetrabenzylthorium Complexes” *Organometallics* **2023** *42* (15), 2079-2086 DOI: 10.1021/acs.organomet.3c00248

1. In 2-3 sentences, explain why tetrabenzylthorium is deemed “elusive” in the article’s title.

2. The authors use the term “homoleptic” to describe several tetrabenzyl metal complexes. Please provide a definition for the term homoleptic.

3. Some of the earliest reported homoleptic organometallic compounds contained either benzyl or t-butyl ligands. These ligands lent stability to the metal complexes because they did not contain beta-hydrogens. In words and diagrams, explain how the presence of a beta-hydrogen can lead to the decomposition of an organometallic complex.

4. **NMR spectra.** The authors were able to obtain the homoleptic tetrabenzylthorium complex, listed as complex 4 in the article, by using ThCl4(THF)3.5 as their thorium starting material. As evidence of the successful synthesis, they describe 4 resonances in the 1H NMR spectrum and 5 resonances in the 13C NMR spectrum. Using words and a sketch of the molecule, explain the number of resonances in the 1H and 13C NMR spectra. You may also look in the Supporting Information if you wish (Figures S7 and S8).

5. **Electron counting.** Using the CBC electron counting method, count the electrons in tetrabenzylthorium. Determine the electron number, ligand bond number, metal valence, and dn count.

6. **X-ray crystal structure.** Due to the electron-deficient nature of this complex, it is not surprising that the benzyl ligands distort to bring more electron density to the metal.

a) Define hapticity.

b) On p 2082 (left column), the authors describe several different models, or classification methods, that have been used in the literature to describe benzyl group hapticity. The authors say that two criteria must be met: “M−C bond distances should be within the sum of the van der Waals radii” and “there must also be electron density donated by the π system of the phenyl group to the metal ion.”

The authors use the Andersen and Zalkin (AZ) model to explore the hapticity of tetrabenzylthorium. Using this model, they found that the benzyl ligands were either η3 or η4, depending on the polymorph they examined. (Things get a little complicated here. Not only was the product isolated in different crystal forms, but it also underwent phase changes when it was cooled. Therefore, the authors report four different X-ray structures for tetrabenzylthorium.)

Use words and sketches to explain the difference between η3 and η4 hapticity in the tetrabenzylthorium complex. To help with your explanation, here are the labels of the pertinent carbon atoms.

