Literature discussion of “The Scandium(II) Carbonyl Complex (C5H2tBu3)2Sc(CO) and Its Isocyanide Analog (C5H2tBu3)Sc(CNC6H3Me2-2,6)”

W. Evans and co-workers, *J. Am. Chem. Soc.* **2024**, *146*, 24770-24775.

*Prior to class, please read through the paper and answer the first two questions. Be ready to discuss and answer the remaining questions in class.*

1. Transition metal (TM) carbonyl complexes are involve both significant s-donation and p-acceptance of electron density by the CO ligand. Use the Dewar-Chatt-Duncanson model and draw a general example depicting each of these M-CO orbital interactions.
2. TM carbonyl complexes typically utilize the IR stretching frequency of CO to observe and characterize bonding of the CO to the metal center, as well as detect changes in electron density at the metal. How would you expect the *n*CO to shift when there is significant p-acceptance? Why does this occur?
3. In the paper, the authors mention no stable carbonyl complexes of Sc(III) or rare-earth metals have been isolated. What drives the lack of stability of these compounds?
4. The authors cite several papers which report IR evidence for Ln(II) metallocenes binding CO ligands. What is the range of IR stretching frequencies observed for *n*CO in these compounds, and how do they compare to *n*CO of free CO? What does that imply about the degree of p back-donation in these compounds?
5. Looking at the data in Table 1, what is the *n*CO reported for the new Sc(II) compound? Does this imply that Sc(II) behaves more like a transition metal or a rare-earth metal?
6. The authors ascribe the difference in back-bonding between transition metals and rare-earth metals to a difference in the ground state electron configuration. What are the ground state configurations of Sc(II) versus Sm(II), Eu(II), and Yb(II)?
7. How might the difference in ground state configurations result in a difference in the metal center’s ability to p back-donate to a ligand?