Transmetalation

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This literature discussion is based on a communication from *Organometallics* (**2011**, *30*, 3457 https://dx.doi.org/10.1021/om200360q). This was developed for use at the start of a course-based undergraduate research experience (CURE) focused on transmetalation from gold to iron and as such, will ignore the ruthenium compounds presented in this paper.

1) The title of this paper is "Effective Transmetalation from Gold to Iron or Ruthenium". What is transmetalation? It is likely that you will look this up, be certain to cite your source.

2) What is a ligand?

3) The authors begin their introduction by stating why they are exploring gold chemistry and so we shall start there too. Draw the structure of PPh_3 and as a reminder, Ph represents a phenyl ($-C_6H_5$) group.

4) There are a number of different gold compounds used in this study, with most of them having some sort of aromatic group. Let's consider the least complex aromatic group, phenyl. Draw the structure of a NEUTRAL phenyl group and just a reminder, that is $-C_6H_5$.

5) In the abstract and in Table 1 the authors present R-Au-PPh_3 as one of the reagents in this study. The authors mention in the introduction that gold catalysts can either be Au(I) or Au(III) and that the reactions typically do not involve a change in the oxidation state of the gold. The compound of interest in this study is an Au(I) compound. Using your answers to the previous two questions, how do you justify this?

6) Let's now consider the other starting material, the iron compound. First off, what is going on with the five-membered ring. This is a cyclopentadienyl ligand (Cp for short). Based on the name, propose a formula and draw the structure of a cyclopentadienyl molecule (not bonded to a metal). The challenging part of the name is the -yl. Think about other organic groups that have that ending.

7) Consider your answer to question 4 and your structure in question 6. Do you think the cyclopentadienyl ligand will impact the valence of the iron? Why or why not? You might consider what is implied by the five-membered ring having a circle inside of it.

8) The bond from the iron seems to be going to the middle of the ring. What do you think is meant by this representation and how can you possible rationalize it?

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9) Draw the structure of a neutral CO ligand. Would you expect this ligand to impact the valence of the iron? Why or why not?

10) Draw the structure of a neutral iodide ligand. Would you expect this ligand to impact the valence of the iron? Why or why not?

11) The authors describe the iron compound as being a three-legged piano stool. Approximately, what do you think the C-Fe-C angle would be?

12) A reaction is shown at the top of Table 1. What product(s) are missing from this reaction?

13) The reactions are monitored by $^{31}P\{^{1}H\}$ NMR spectroscopy. Consider the starting material Ph-Au-PPh_3. How many phosphorus atoms are in this molecule? How many unique phosphorus signals would you see in the NMR for this molecule? What is the significance of the $\{^{1}H\}$? Answer these same questions considering your answer to question 12. Why might the authors have used this technique to monitor the reactions?

14) The supporting information provides the NMR data for several of the compounds in Table 1. Consider compound **3b** for which the following NMR data was reported. What is DEPT? It tells you how many hydrogen atoms are bonded to the carbon. If there is no signal there are no hydrogen atoms bonded to the carbon. If it is positive there are either 1 or 3 hydrogen atoms bonded to the carbon. If it is negative there are two hydrogen atoms bonded to the carbon. To the best of your ability assign these peaks.

^{1}H NMR		**$^{13}C\{^{1}H\}$ NMR**	
7.35 (d, *J* = 7.5 Hz, 2H)		216.2 (s, No DEPT)	
7.02 (d, *J* = 7.5 Hz, 2H)		145.6 (s, No DEPT)	
4.86 (s, 5H)		144.4 (s, No DEPT)	
1.27 (s, 9H)		139.9 (s, DEPT +)	
		124.8 (s, DEPT +)	
		85.7 (s, DEPT +)	
		33.8 (s, No DEPT)	
		34.1 (s, DEPT +)	

15) From your experience in organic, is there another spectroscopic technique you might consider using to characterize the iron compound? How might your answer to question 9 impact that?

16) What information can be gathered from Figure 1?

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17) In comparing the reactions to form **3f** and **3h** the authors do not provide much insight. They state that the aromatic ring with the strongly electron withdrawing *p*-NO_2 group was transferred "easily". With the *m*-NO_2, the reaction went to completion within an hour. In comparing Figures 1 and 2, it certainly seems that the reaction with the *m*-NO_2 is much slower. On page 3458 the authors state that this result was 'expected'. Why would this result be expected?

18) Based on your knowledge/intuition, propose a mechanism for this reaction that would be consistent with the data.