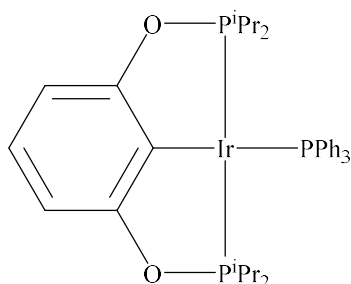


One-figure literature discussion: Addition of H₂ to four-coordinate Ir

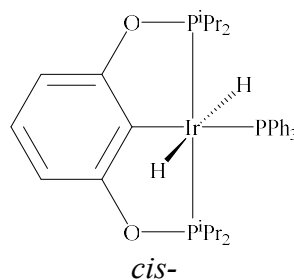
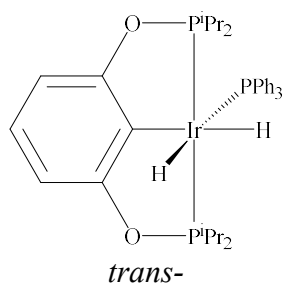
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This paper (*J. Organomet. Chem.* **2022**, 965-966, 122317) describes the synthesis and reactivity of four-coordinate iridium compound with a tridentate ligand. This ligand is referred to in the paper as a pincer ligand which are a general class of tridentate ligands that coordinate in a *mer*- arrangement. More specifically, this is called a POCOP ligand with the P and C representing the atoms coordinating to the metal center and the O representing that there is an oxygen atom between the atoms that coordinate. The carbon atoms are ignored in this shorthand method. While there is certainly lots more that can be unpacked from this paper, Figure 2 and reaction 3 of the paper are the focus of this literature discussion.

- 1) Classify the compound shown below. Determine the electron count, valence number, ligand bond number and dⁿ count for the iridium.



- 2) The addition of H₂ to the compound in the previous question results in the formation of a product that can exist as two different isomers which are shown below. Briefly describe how you could differentiate the two different isomers by NMR spectroscopy.



- 3) Classify the compounds in question 2. Determine the electron count, valence number, ligand bond number and dⁿ count for the iridium.
- 4) What type of reaction is taking place upon the addition of H₂? How did you draw this conclusion?

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- 5) The NMR spectrum of this reaction mixture varies over time. Shown below is a partial spectrum over the course of three hours. Referring back to your answer to question 2, how might you assign the peaks observed in this spectrum at 5 minutes?

[Insert Fig. 2 from the paper here]

- 6) One of the isomers could be described as the kinetic product and the other as the thermodynamic product. Describe what is meant by kinetic and thermodynamic products and how the NMR data allows you to decide which isomer is the kinetic product and which is the thermodynamic product.
- 7) Based on the reaction that is taking place, why is the kinetic product the isomer you chose in the previous question?
- 8) What factor(s) of the other isomer makes it the thermodynamic product?