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Editorial: <https://pubs.acs.org/doi/10.1021/acs.inorgchem.2c00729>

Special Issue: <https://pubs.acs.org/page/inocaj/vi/out-inorganic-chemistry-2022?ref=vi_collection>

The questions below refer to the following 2020 publication by Dr. Jonathan Kuo and Dr. Karen Goldberg

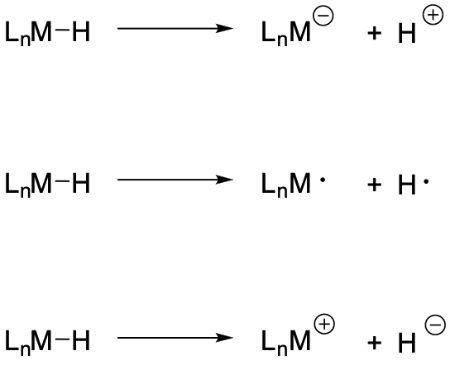
“Metal/Ligand Proton Tautomerism Facilitates Dinuclear H2 Reductive Elimination”

Jonathan L. Kuo and Karen I. Goldberg\*

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1. Describe the ligands on compound **[3-LH]+** and **[4-LH]+** in terms of their denticity (e.g. κ1) and their L and X character (see Reaction 1). Also, do the same for [**1-MH·***t***BuPy**]+ from Figure 1.
2. Why are Ir(II) monomeric species paramagnetic, but compounds **72+** and **8** are diamagnetic?
3. What is the definition of a conformer? Of a tautomer?
4. Metal-hydride bonds can form and break via several methods. What happens to the metal’s oxidation state for each of the following cases of breaking a M-H bond?



5) Solutions of [**1-MH·***t***BuPy**][PF6] are noted to be thermochromic (Figure 8).

1. What does “thermochromic” mean?
2. Draw the equilibrium that is responsible for thermochromicity.
3. Why is the position of this equilibrium affected by temperature?
4. In the paper, equation 7 simplifies to equation 6 when k–1[tBuPy] ≫ k2[IrIII–H]. What would equation 7 simplify to if the opposite were true (k2[IrIII–H] ≫ k–1[tBuPy])?
5. For the interconversion between [**2-LH**]+/*t*BuPy to [**1-MH**]+,
6. Which order of events is more reasonable: (1) slow ligand association followed by fast tautomerism or (2) slow tautomerism followed by fast ligand association?
7. How could you distinguish between these two possibilities using kinetic experiments, assuming that accessing the reactive intermediate is the rate determining step (hint: check out Figure 13)?
8. NMR data provides valuable information for this dynamic system. Answer the following questions:
9. Why do the chemical shifts in Figure 6 move in the upfield direction upon incremental additions of *t*BuPy?
10. How many Ir(III)-Hs are present in solution in total?
11. Write a mathematical expression for the observed chemical shift δobs as a function of the mole fraction (χ) of the various Ir(III)-Hs. Think of it as a weighted average of the true chemical shift for each species multiplied by their mole fraction.