Reading Instructions for "Cyclometalated Iridium(III) Aquo Complexes: Efficient and Tunable Catalysts for the Homogeneous Oxidation of Water"

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Reading:

Read the first two paragraphs of the introduction (up to the paragraph beginning "Previously reported…") but skip the rest of the introduction. Pick up again at the results and discussion section on page 212. Thus half of the introduction section and all of the experimental section will not be read.

However, please pay attention to Figure 2 on page 211, as this is important to the discussion of the paper. (Figure 1, Scheme 1, and Table 1 may all be ignored).

Questions to consider while reading:

1. There are four different parameters that the authors test in relation to the Ir complex – rate studies, substitutions on the phenylpridine, stability of the catalyst, and density functional theory calculations. What information does each of these studies give and how does it relate to the oxidation process?

2. Table 2 and Figure 8 both present key results of this paper. What trends are observed in Table 2? What is causing these trends and why are they important? Do the trends in Table 2 agree with the information presented in Figure 8?

3. Figure 8 shows the relative energies of compounds 3 and 4. Based on this information, how would the relative energies of compounds 1, 2, and 5 compare? Why is this important?

4. The authors of the paper seem very excited about the electronic tunability of the Ir compound. Why do they care so much about this feature? How does it relate to the larger goal of the research?

Useful Information:

Sacrificial oxidant – a species that is used to activate the water oxidation catalyst, and is thereby reduced in the process (ceric ion, in the form of ceric ammonium nitrate, occupies this role)
Cyclometalated – a compound containing one or more metal atoms in a ring with the ligand
Cyclic Voltammetry (CV) – a technique that measures current as a function of an applied voltage and therefore used to determine oxidation and reduction potentials
NHE – normal hydrogen electrode, a common reference electrode

Water redox reactions –
Oxidation: $2H_2O \rightarrow O_2 + 4H^+ + 4e^-$
Reduction: $2H^+ + 2e^- \rightarrow H_2$