3.1: Ligand Field Theory and Frontier Molecular Orbital Theory

In this post, we'll begin to explore the molecular orbital theory of organometallic complexes. Some background in molecular orbital theory will be beneficial; an understanding of organic frontier molecular orbital theory is particularly helpful. Check out Fukui's Nobel Prize lecture for an introduction to FMO theory. The theories described here try to address how the approach of ligands to a transition metal center modifies the electronics of the metal and ligands. The last post on geometry touched on these ideas a little, but we'll dig a little deeper here. Notably, we need to address the often forgotten influence of the metal on the ligands —how might a metal modify the reactivity of organic ligands?

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