

EXAMINING THE IMPACT OF LIGAND BASICITY ON THE REACTIVITY OF TRANSITION METAL SYSTEMS THROUGH COMPUTATIONAL METHODS. John T. York, Department of Chemistry, Stetson University, 421 N. Woodland Blvd. DeLand, FL 32723

The electron-donating properties of supporting ligands can have a dramatic impact on the properties and observed reactivity of transition metal complexes. Indeed, gaining the ability to “tune” the properties of metal complexes is a primary goal in inorganic and organometallic chemistry. Unfortunately, a detailed understanding of the fundamental impact of ligand basicity on a metal center is often lacking. Presented herein is a discussion of several important computational (DFT) methods that can be used to elucidate the fundamental nature of metal-ligand interactions, including natural bond orbital (NBO) analysis, energy decomposition analysis (EDA), and molecular orbital analysis. By exploring their application in understanding the bonding in a number of important transition metal systems, we describe how these methods can provide useful insight into the rational design of metal complexes.