Structural Chemistry and Organic Reactions of Ate Complexes: A Heterobimetallic Chemistry

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Aromatic structures are the basic architectures for building functionalized materials, such as medicines. However, the tools for the chemoselective, regioselective and stereoselective introduction of various functional groups onto aromatic rings are still limited in their applicability.

Our approach capitalizes on the high chemoselectivity of ate complex reagents, which allows flexible design and fine-tuning by modifying the ligation environment. They can be used to open new windows onto benzene architecture chemistry. We are developing a novel approach to functionalizing aromatic compounds using newly designed ate complexes, which should allow for highly efficient controlled functionalization of a wide range of aromatic rings. We recently found that chemoselective halogen-metal exchange, direct deprotonative metalation, and benzyne formation reactions can be performed on functionalized benzene rings using ate complexes. Furthermore, some of the dianion-type ate complexes created by our group are effective for the chemoselective anionic polymerization of multi-functionalized monomers and for the construction of multisubstituted olefins.

In this presentation, I shall present some of our recent work on organoate complex-mediated organic transformations and discuss them together with structural chemistry obtained from quantum calculations and spectroscopic studies. In particular, I'll describe how we have designed ate complexes and improved their function.