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Role of Secondary Interactions (π , agostic) as well as Solvent Influence on Alkali metal complexes

A Capstone Project Submitted in Partial Fulfillment of the Requirements of the Renée Crown University Honors Program at Syracuse University

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Honors Capstone Project in Biochemistry

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Abstract:

We here attempt to synthesize heterobimetallic alkali metal complexes with bulky phenolate ligands via solid state direct metallation. The solid state route may offer a facile method of producing these heterobimetallic species. Synthesis of heterobimetallic alkali metal compounds remains a challenge, as the homometallic complexes are generally favored over formation of the heterobimetallic species. Previous work has shown that the alkali metals have a strong solvent dependency; the recrystallization of heterobimetallic products from toluene yields the heterobimetallic, while recrystallization from THF yields the homometallic. However, the ability for phenolate ligands to stabilize metal centers through secondary interactions, such as $M \cdots \pi$ interactions, has also been observed to compete with solvents in saturating the coordination spheres of the metals.

A novel group of potassium-containing 1-D coordination polymers demonstrates the importance and role of K-C π interactions. [K(Odpp)]_{\$\omega\$}, **1**, (Odpp = 2,6-diphenylphenolate) forms a ladder-type polymer where extensive K-C π interactions provide additional coordinative saturation. {[K₂(Odpp)₂H₂O]₂}_{\$\omega\$}, **2**, consists of tetrameric cores of K₄O₆ polyhedra linked via a network of K-C π interactions. Compound **2** displays not only inter- and intramolecular K-C π contacts, but also several K-H agostic interactions that provide further coordinative saturation.

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