Project Title: Investigation of the Mechanism of Nucleophilic Attack on the [B20H18]2- Anion
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Project summary: Our laboratory has isolated and characterized a unique solvent-coordinated anion, [B20H17O (CH2)5]3-, resulting from the combination of the [B20H18]2- anion, a sterically demanding nucleophile, and the solvent, tetrahydropyran. Although the anion is clearly the product of the reaction of the [B20H18]2- anion with the solvent, the role of the nucleophile was unclear. Therefore, the goals of the grant were**:** 1) Determine the role of the nucleophile and the solvent in the reaction mechanism, 2) Complete a series of reactions using solvents with the same basic structure, but with varying nucleophilic atoms, and 3) Complete the reactions with the sterically demanding nucleophiles in a solvent, which does not inhibit the desired reaction. Although the role of the nucleophile has not been completely determined, we have eliminated several possibilities. Replacement of the nucleophile with a strong base (NaH), does not yield the product. Introduction of only a catalytic amount of the nucleophile does not yield complete reaction. Completion of the reaction in stoichiometric amounts of each of the reactants in a different solvent system does not yield the product. Therefore, the nucleophile is not acting as a base in the reaction nor is it a catalyst. The coordination of the solvent is a result of mass action. Goal 2 has been completed; however, the compounds have not been completely characterized. An undergraduate student will be completing this portion of the project during the summer, 2007. Goal 3 has been completed and final characterization of the resulting compounds is underway. We anticipate that the project will ultimately yield three publications in Inorganic Chemistry.