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SYNTHESIS OF 30-MEMBERED AZAMACROCYCLES AS HOSTS FOR POLYOXOANION GUESTS

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The long term goal of this project is to create a capsule-shaped host molecule through the linkage of two macrocyclic compounds. This capsule is to be built around a polyoxometallate, a large, anionic cluster. Since most polyoxometallates decompose under basic condition, it may be possible to break down the polyoxoanion scaffold after the capsule is assembled. Size compatibility of the polyoxometallate and the macrocycles is essential, as these components must preferentially complex each other. Previous work on this project utilized fourteen membered macrocycles, which proved somewhat small to effectively complex with the polyoxometallate. Current work involves synthesis of much larger 30-membered macrocycles with the hope that they are more likely to provide a proper fit. In addition to steric factors, charge also plays an important role in determining whether the macrocycle and polyoxoanion will form an inclusion complex. Two different 30-membered rings are being investigated currently, one with four amine groups and the other with six. In acidic solution, the amine groups should form positive ammonium ions ideal for binding to the negatively charged polyoxometallate.

[Diagram showing steps a, b, and c, and labels for macrocyclic hemicage, polyoxometalate (POM), reactive functional group, polycyclic molecular cage, and fragments of POM (e.g., MO₄²⁻).]