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Chalcogen Bond-Mediated Alkylation Catalysis: Selenoxide-Pillar[5]arene as a Recyclable Catalyst in Aqueous Solutions

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ABSTRACT

In this study, we introduce a novel strategy for catalyzing alkylation reactions via chalcogen bond interactions using a chalcogen-macrocyclestructure. Chalcogen bonding (ChB), involving elements like sulfur, selenium, and tellurium, is defined as the interaction between a positively polarized chalcogen atom and a Lewis base. This electrostatic attraction and charge-transfer component make ChB a powerful tool for achieving high yields and controlling selectivity.[1-3] Employing a macrocyclic pillar[5]arene decorated with organoselenium, we achieved efficient catalysis of benzyl bromide cyanation in water using only1.0 mol% selenoxide-pillar[5]arene (**P[5]SeO**) as the recyclable catalyst. Supported by control experiments and theoretical models, ^{1}H NMR analysis revealed that **P[5]SeO** facilitated inclusion complex formation, enabling nucleophilic displacement. The reaction protocol proved applicable to a broad range of nucleophiles and substrates, including aromatic, heteroaromatic, and alpha-carbonyl derivatives. Notably, the method is scalable, and the catalyst **P[5]SeO** can be effectively recovered and reused for multiple cycles, showcasing its sustainability.

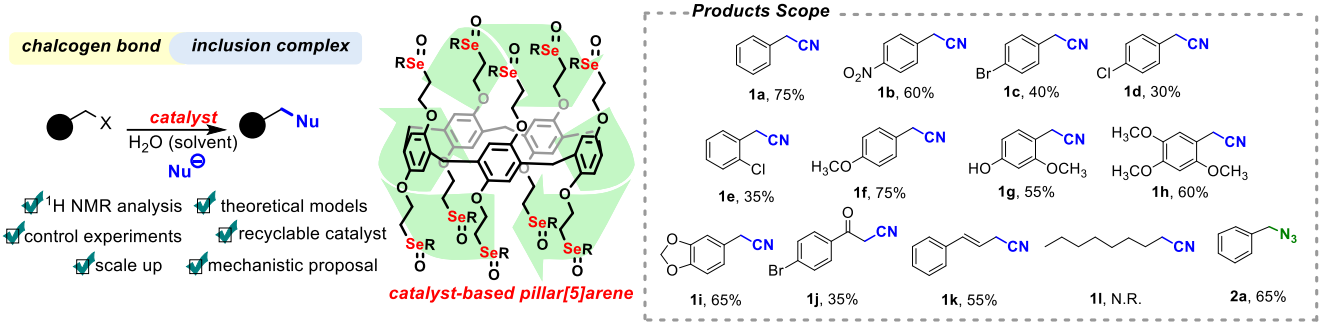

Figure 1. Representation of the work and achieved scope.

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