Theoretical Insights to Novel Beryllium Reactivity

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Recent reports have found beryllium to facilitate the activation of relatively inert chemical bonds. Therefore, interest in beryllium chemistry has grown significantly in recent years with a number of beryllium compounds stabilised by N-heterocyclic carbene (NHCs) and cyclic (alkyl) (amino) carbene (CAACs). We report results of theoretical investigations for a series of novel beryllium carbodicarbenes (CDC) in collaboration with synthetic studies.[1-3] We have utilized Atoms in Molecules (AIM) calculations and Energy Decomposition Analysis (EDA) to determine the local electronic environment of **1** and **2**. Further we have undertaken mechanistic studies to understand different reactivity to form **3** and **4**.[4]

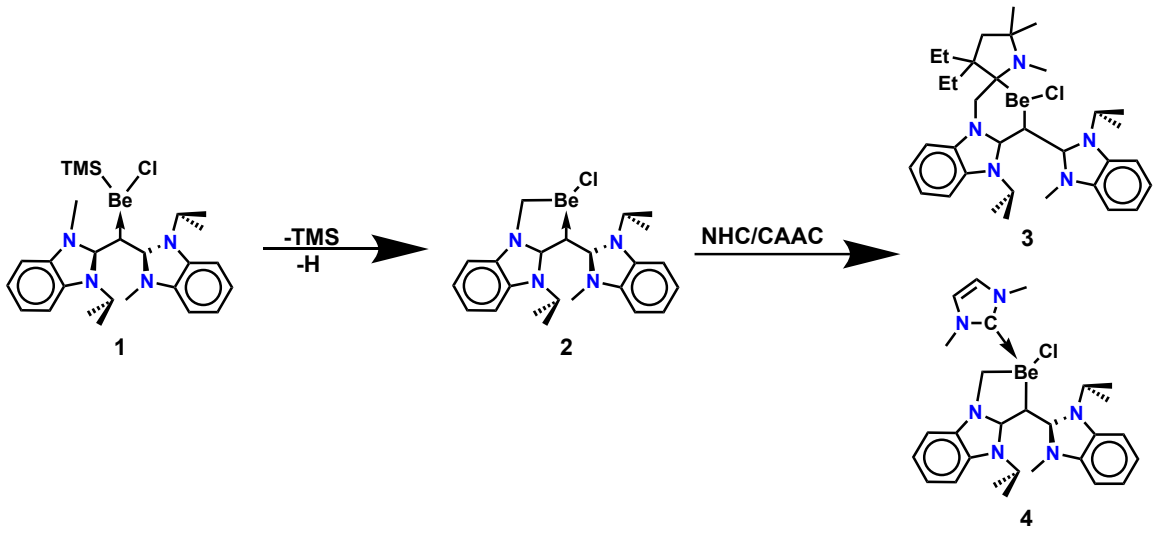

Figure 1: CAAC-promoted ring expansion of beryllium.

References

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