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Inert Bond Activation Using a Pentanuclear Nickel Hydride Cluster

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The activation and cleavage of inert bonds, such as C-C, C-H, and C-O bonds, in cheap and abundant chemical feedstocks provides a hypothetical alternate route to essential chemicals and fuels. Through the development of cost-efficient catalysis for these difficult bond transformations, presently unusable waste materials could become future feedstocks. The bonds in lignins and hydrocarbons are considered inert due to the thermodynamic and/or kinetic barriers of activation. The pentanuclear nickel hydride cluster, $[(^i\text{Pr}_3\text{P})\text{Ni}]_5\text{H}_6$ (**1**), has recently demonstrated the ability to activate and/or cleave typically inert bonds under mild conditions due to cooperative reactivity between the five Ni centres, reminiscent of surface catalysis. Studies into the mechanisms of C-C, C-H and C-O bond activation by **1** are underway, in the hopes of better understanding how these species dismantle and remake typically inert bonds under extremely mild conditions, with the potential to discover new reactivity. In previous work, it has been suggested that the electron deficient intermediate $[(^i\text{Pr}_3\text{P})\text{Ni}]_5\text{H}_4$ (**2**) in the reactive intermediate in bond activation. The current goal is to develop a synthetic route to species **2**, which is likely highly reactive, and study its interactions and reactivity with inert-bond containing substrates.

The proposed intermediate, **2**, has been briefly observed in proton NMR at low temperature when one equivalent of isobutylene is exposed to **1**. Since the suggested intermediate **2** has been observed in solution simultaneously with **1**, we proposed that it was possible to produce **2** by first abstracting a hydride from **1** using trityl tetrakis[3,5-bis(trifluoromethyl) phenyl]borate, followed by a mild base to remove the remaining proton. Initial attempts to abstract a hydride from **1** using this approach resulted in a paramagnetic intermediate $[(^i\text{Pr}_3\text{P})\text{Ni}]_5\text{H}_6^+$ (**3**), and attempts to transform **3** into the proposed intermediate **2** are currently underway.

