

Supplementary Materials: Title Exploring Promising Catalysts for Chemical Hydrogen Storage in Ammonia Borane: A Density Functional Theory Study

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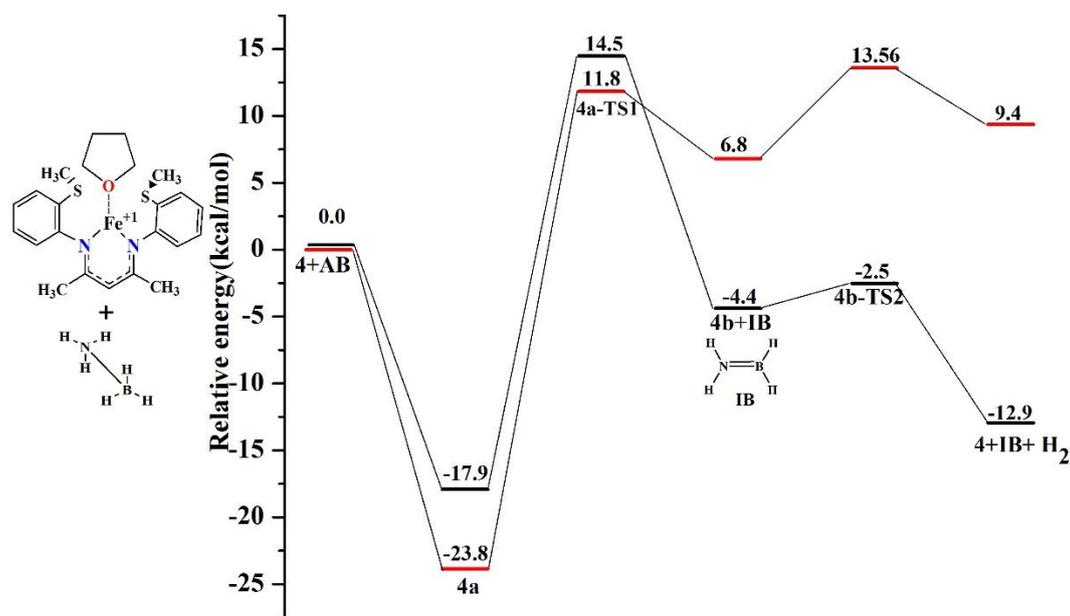


Figure S1. (a) Reaction-coordinate profile of addition of catalyst "4" to "AB" via 4-TS1 to form "4b" and (b) H₂ release from the dihydrogenated product "4b." Gas-phase relative free energies (kcal/mol) and relative free energies in THF solvent are also indicated (by red bars).

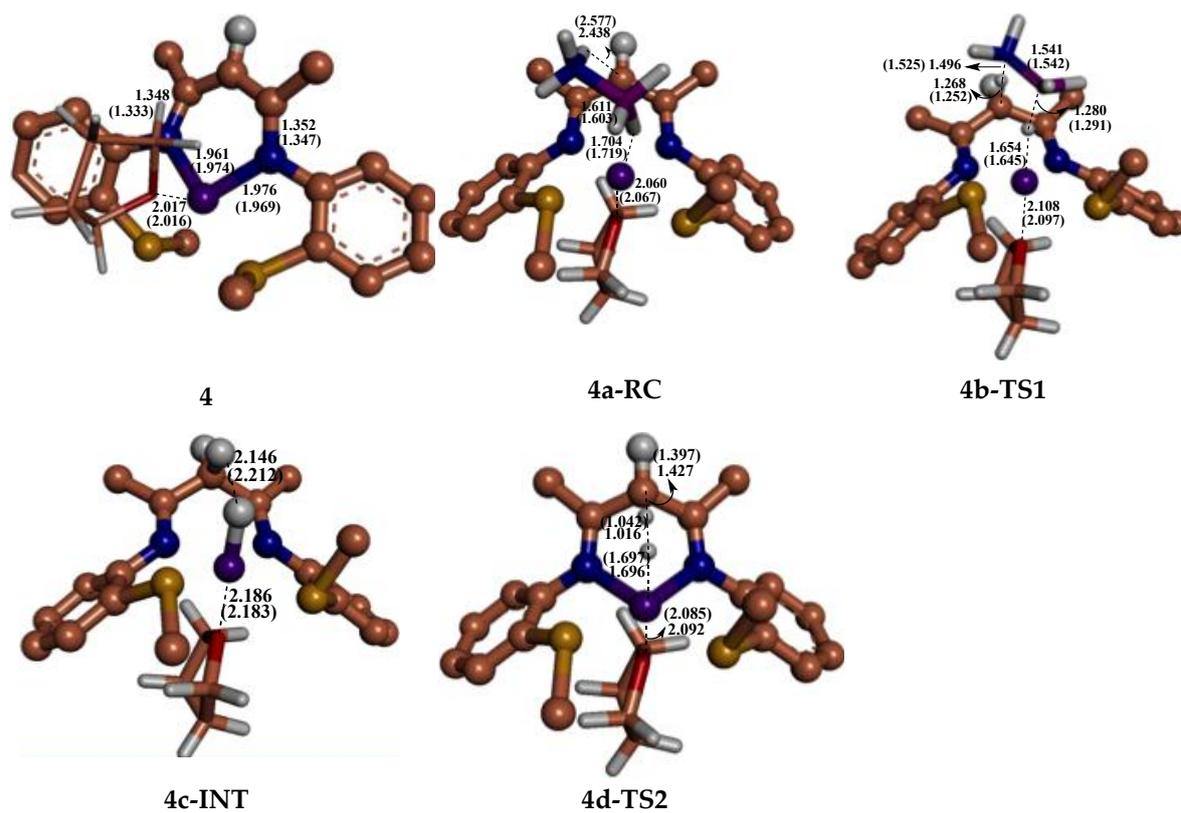


Figure S2. Significant optimized geometries of important stationary points for the reaction coordinate of AB addition to Fe metal catalyst **4**. Important hydrogen atoms are shown for clarity.