

Unusual Products Arising from the Tandem Dehydrogenation of $\text{Mg}(\text{BH}_4)_2$ and Pyrrolidine

Supplemental Information

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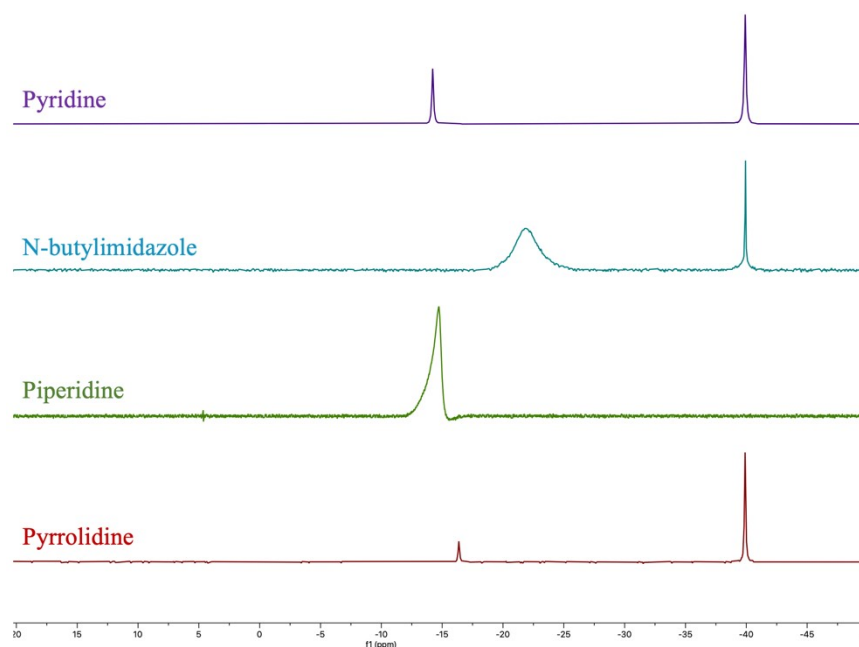


Figure S.1. The $^{11}\text{B}\{^1\text{H}\}$ NMR spectra (160.45 MHz, neat unless otherwise noted) of the reaction of $\text{Mg}(\text{BH}_4)_2$ (upfield signal) with pyridine, N-butylimidazole, piperidine and pyrrolidine at room temperature. From top to bottom, purple: (CD_3CN) Pyridine- BH_3 complex at -14.2 ppm.¹ blue: N-butylimidazole- BH_3 complex at -21.9 ppm.² green: The NMR spectrum of $\text{Mg}(\text{BH}_4)_2$ in piperidine after room temperature reaction. All of the $\text{Mg}(\text{BH}_4)_2$ has been converted to the known borane pyridine complex seen with the broad peak at -13 ppm.¹ red: The NMR spectrum (C_6D_6) of $\text{Mg}(\text{BH}_4)_2$ and pyrrolidine, pyrrolidine- BH_3 is at -16 ppm.³

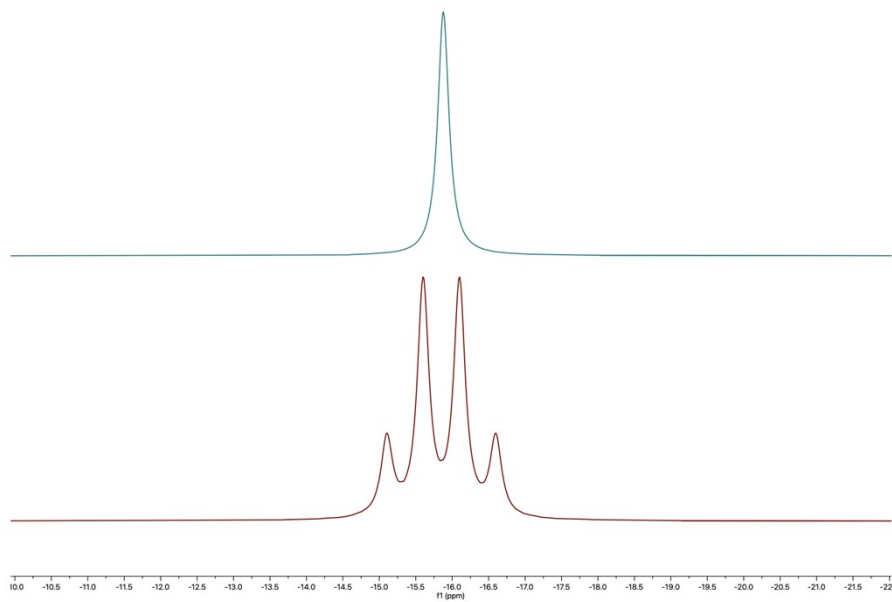


Figure S2. The ^{11}B NMR (Bottom) and $^{11}\text{B}\{^1\text{H}\}$ NMR (Top) (192.5 MHz, C_6D_6 , $\delta = -16$ (q) ppm) of alternatively synthesized pyrrolidine- BH_3 .³

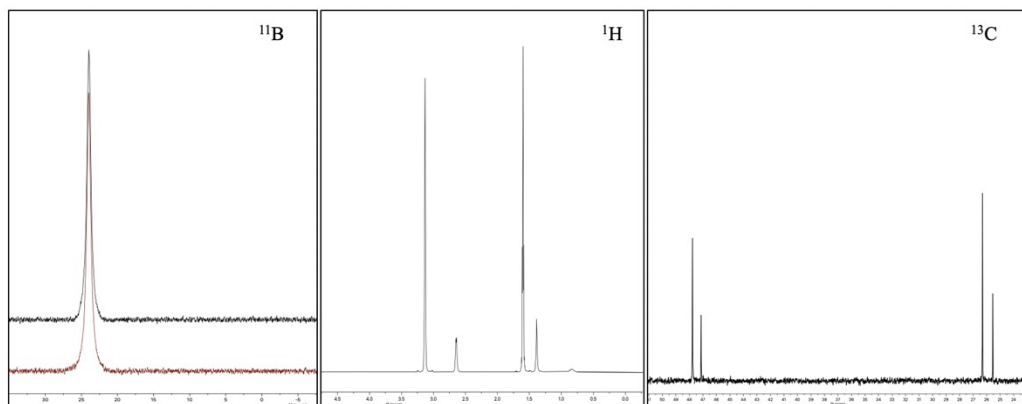


Figure S3. The ^{11}B NMR (192.5 MHz, C_6D_6), ^1H NMR (600 MHz, C_6D_6) and ^{13}C NMR (150 MHz, C_6D_6) spectra of 1 to 10, $\text{Mg}(\text{BH}_4)_2$ to pyrrolidine heated to 180 °C for 24 h. There is only tris(pyrrolidino)borane and free pyrrolidine observable (pyrrolidine: ^1H $\delta = 2.6, 1.4$ ppm, ^{13}C $\delta = 47.1, 25.5$ ppm).

References

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