Electronic Supplementary Material (ESI) for Energy & Environmental Science

Kinetic and Thermodynamic Investigation of Hydrogen Release from Ethane 1,2-di-amineborane

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Supporting Information

Figure 1S and 2S show the ^{11}B and the ^{13}C NMR data for the as prepared sample.

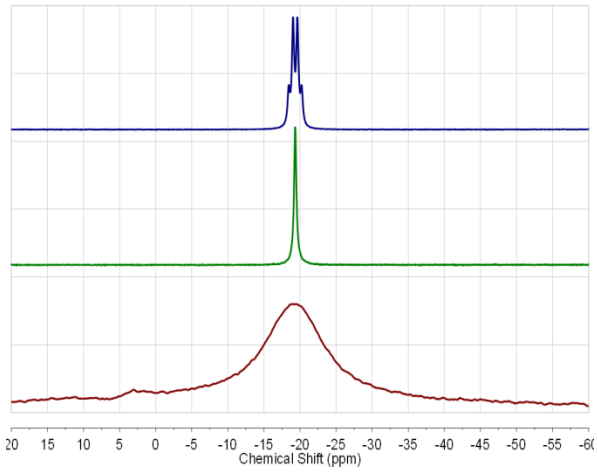

Figure 1S. ^{11}B NMR data for EDAB as prepared. Red line ^{11}B MAS NMR, green and blue lines are coupled and decoupled solution ^{11}B NMR.

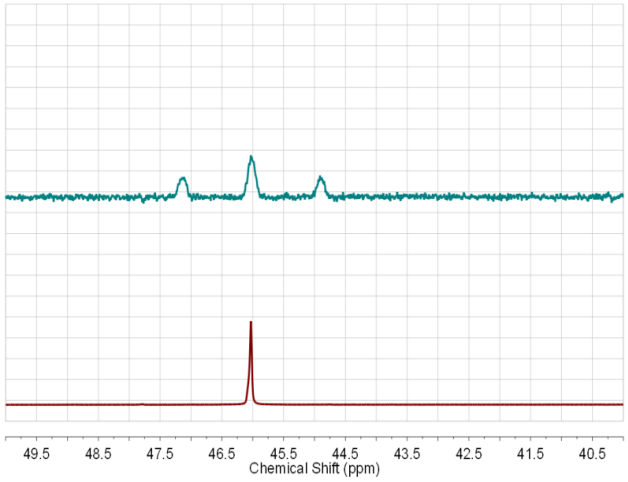

Figure 2S. ^{13}C NMR solution. Green ^{1}H coupled, red decoupled.

Figure 3 shows the heat profile from the decomposition of EDAB in a C80 Calvet calorimeter heated at a ramp rate of 1 K/min and the PCT data obtained under the similar conditions. Figure 4 shows the PCT data for EDAB obtained by heating under 1 bar H_2 from 25°C to 110°C, 120°C and 200°C with 13°C/min. Table 1S summarizes the raw gas burette and PCT data obtained for EDAB under different heating conditions.

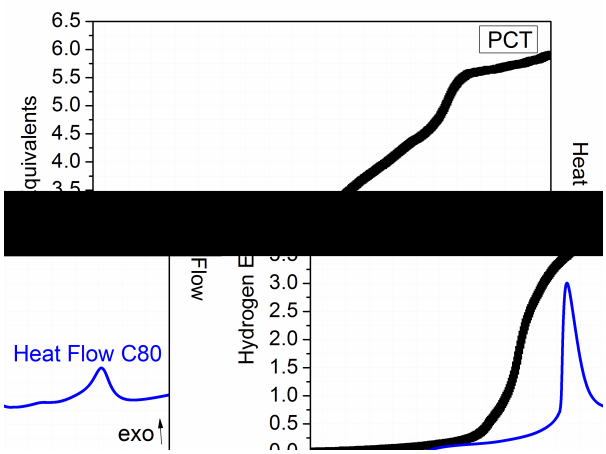

Figure 3S. Hydrogen equivalents (black curve) heat flow (blue curve) as a function of temperature for EDAB heated with 1°C/min from 25°C to 230°C.

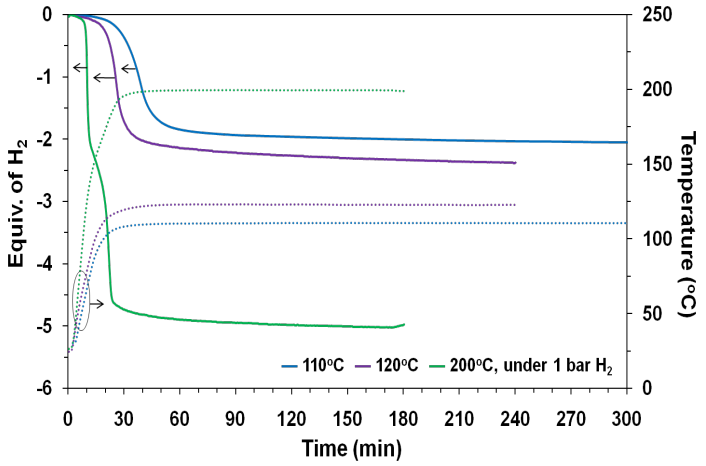

Figure 4S. PCT data obtained by heating EDAB under1 bar H_2, with 13°C/min to 110°C, 120°C and 200°C.

Table 1S. Raw calorimetry, volumetric gas burette and PCT data for EDAB.

C 80 calorimetry experiments	T (°C)	Burette H_2 equivalents	PCT H_2 equivalents	Heat (kJ/mol)	T_{onset} (°C)
Ramp 1°C/min 200 C	1st dehydrogenation step	Not determined	3	-20±1.5	130
	2nd dehydrogenation step	Not determined	3	-7.5±1.2	178
isothermal	99	1.94	2.1	-11	
isothermal	109	2.15	2.1	-21	
isothermal	120	2.15	2.4	-22	
isothermal	130	2.2	2.7	Not determined	
isothermal	85 – 33 hrs	Not determined	Not determined	none	none