Supporting Information

Dehydrogenation of Ammonia-Borane by Cationic Pd(II) and Ni(II) Complexes in Nitromethane Medium: Hydrogen Release and Spent Fuel Characterization

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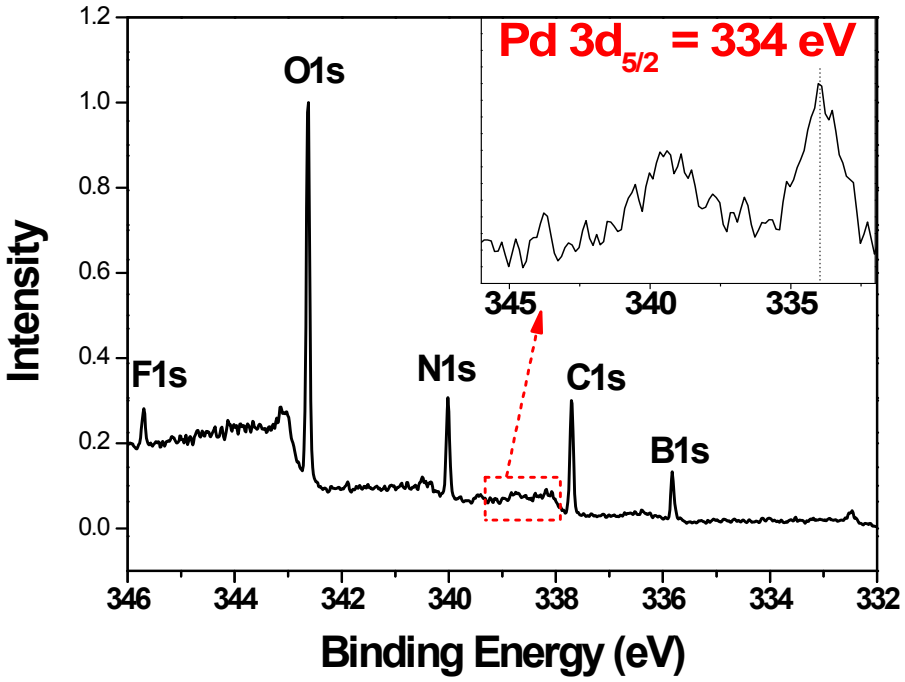

Fig. S1 X-ray photoelectron spectroscopy (XPS) of spent fuel.

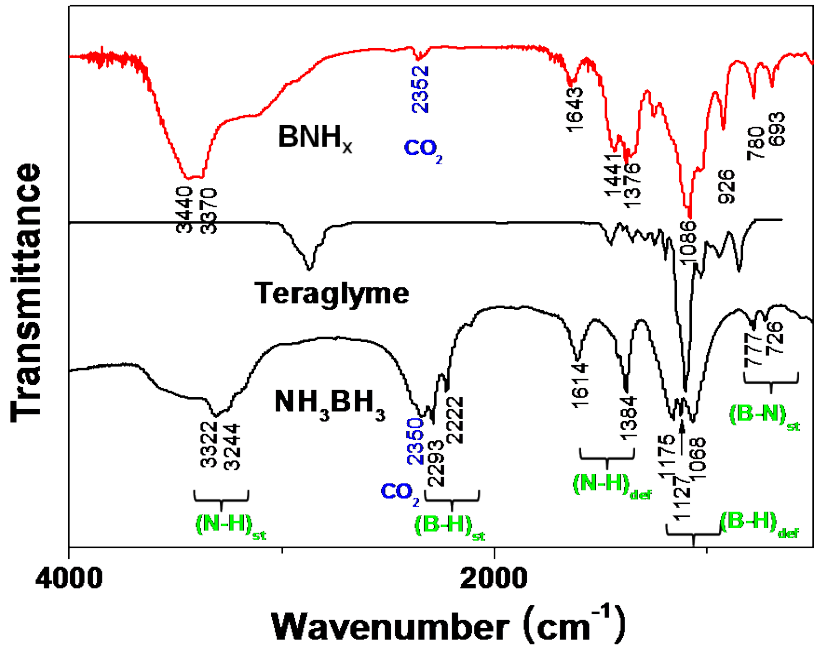

Fig. S2 IR spectra of AB and the spent fuel.

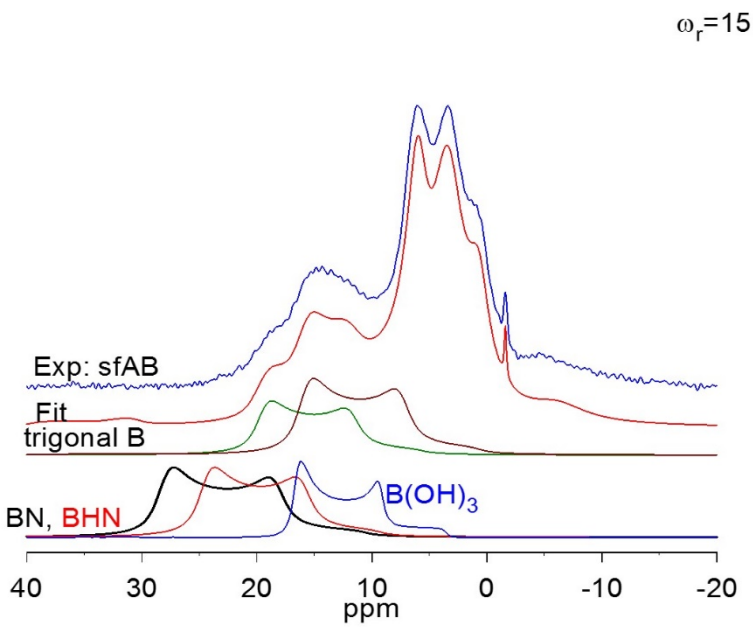

Fig. S3 Experimental ^{11}B MAS NMR spectrum of spent fuels and fit of the trigonal borons(sp^2 parts) (see Figure 1). Simulated spectra of BN, BN_2H using reported quadrupole parameters (ref), and experimental ^{11}B MAS spectrum of boric acid are provided for reference.

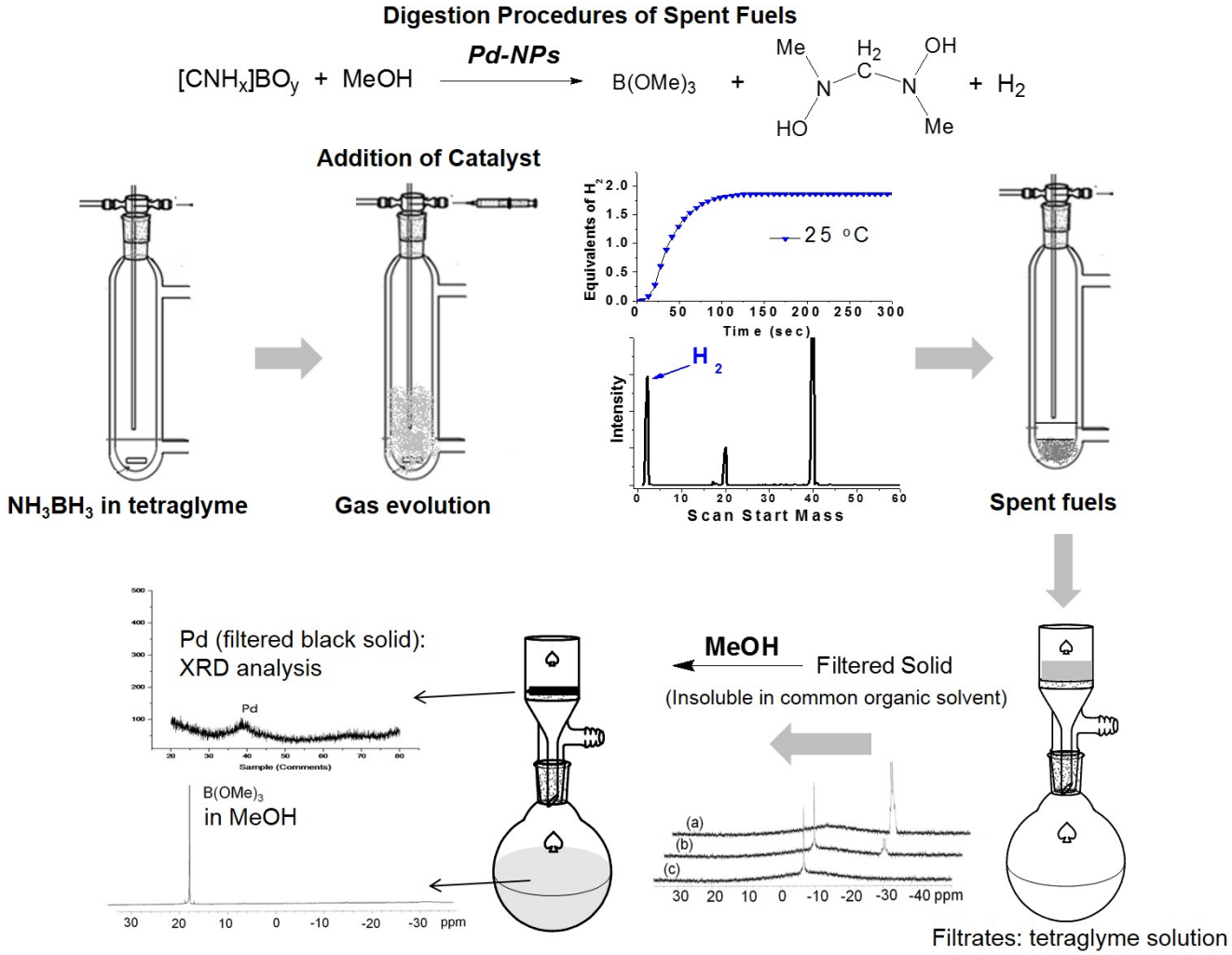

Fig. S4 Digestion procedures of spent fuels ($[CNH_x]BO_y$/PdNPs) remaining after AB dehydrogenation by Pd catalyst **1**.

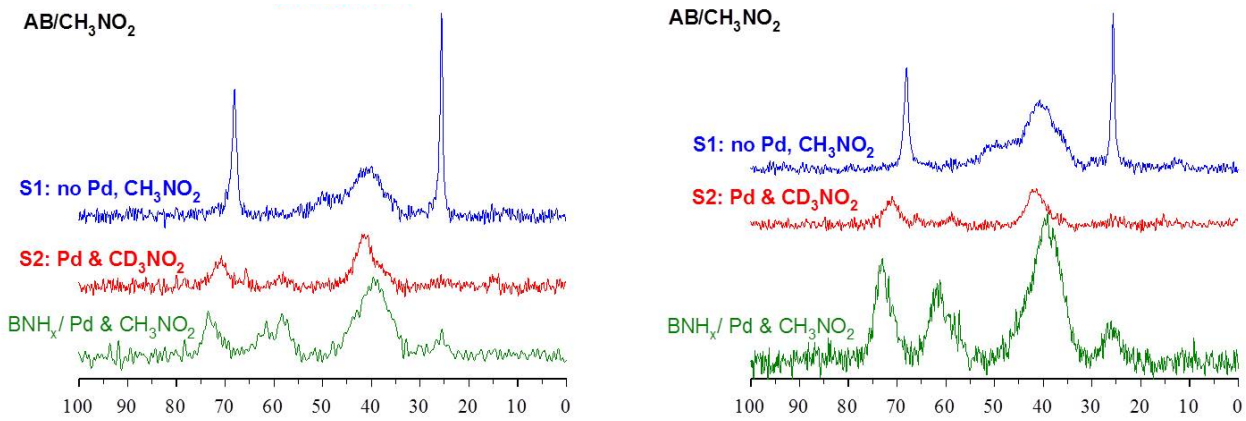

Fig. S5 ^{13}C MAS (left) and CPMAS NMR (right) spectra of the precipitates (S1, blue line) produced from AB dehydrogenation without **1** and TG, precipitates (S2, red line) generated with **1** in CD_3NO_2 solvent, and AB spent fuels ($[CNH_x]BO_y$/Pd NPs, green line) generated with **1** and TG in CH_3NO_2 solvent: ^{13}C MAS and CPMAS spectra comparison also provide additional information. TG and Pd particles are missing in S1, and in ^{13}C spectra present strong signal near 40 ppm while the two peaks at 60 and 75 ppm are missing as shown in Figure S5. The 40 ppm signal can then be attributed to the $MeNO_2$ precipitated in the solids. The rest 60 and 75 ppm peaks are believed to be originated from the TG.

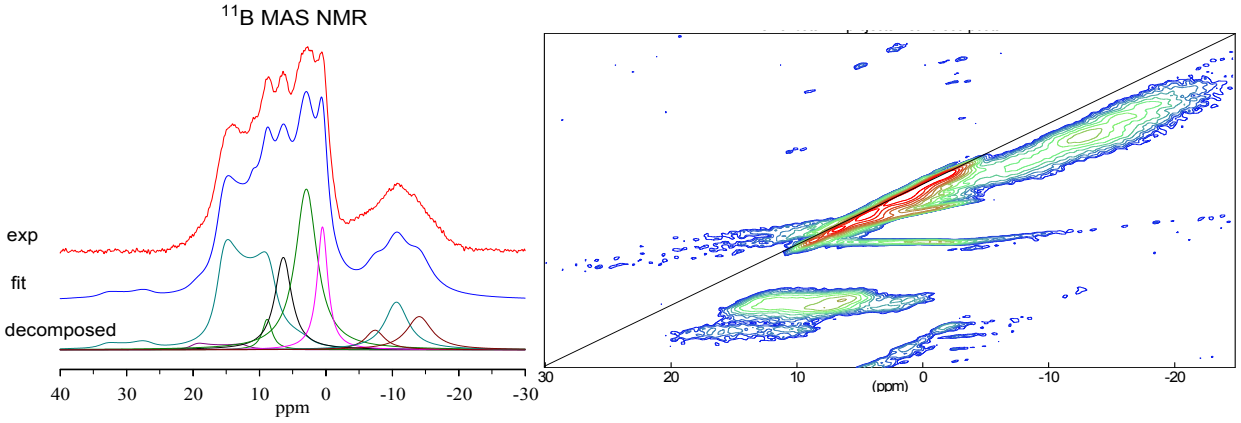

Fig. S6 1D ^{11}B MAS (left) and 2D ^{11}B MQMAS (right) NMR spectra of spent fuels from dehydrogenation of AB with $MeNO_2$ 80 °C