

**Supplementary Material**

**Direct synthesis of [B,H]ZSM-5 by solid-phase method: Al<sub>F</sub> siting and catalytic performance in MTP reaction**

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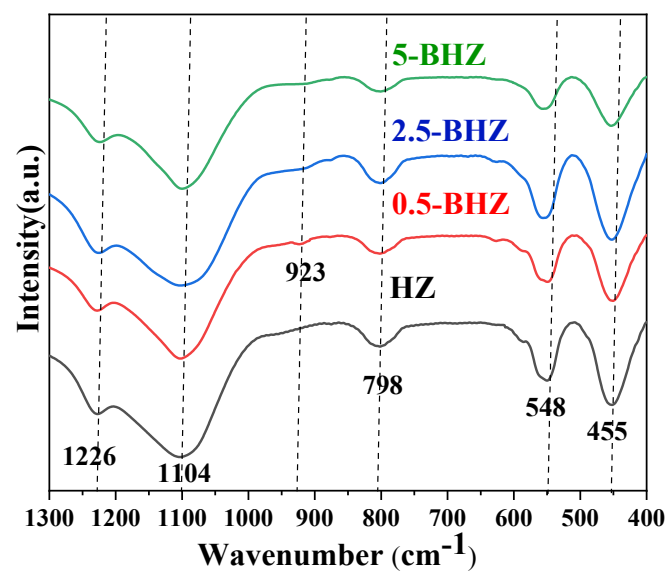


Fig. S1. FT-IR spectra of  $x$ -BHZ with different B/Al ratios

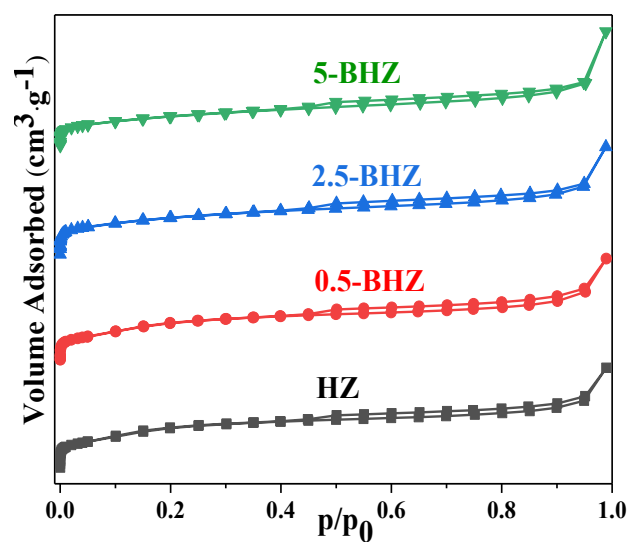


Fig. S2. N<sub>2</sub> adsorption/desorption isotherms of  $x$ -BHZ with different B/Al ratios

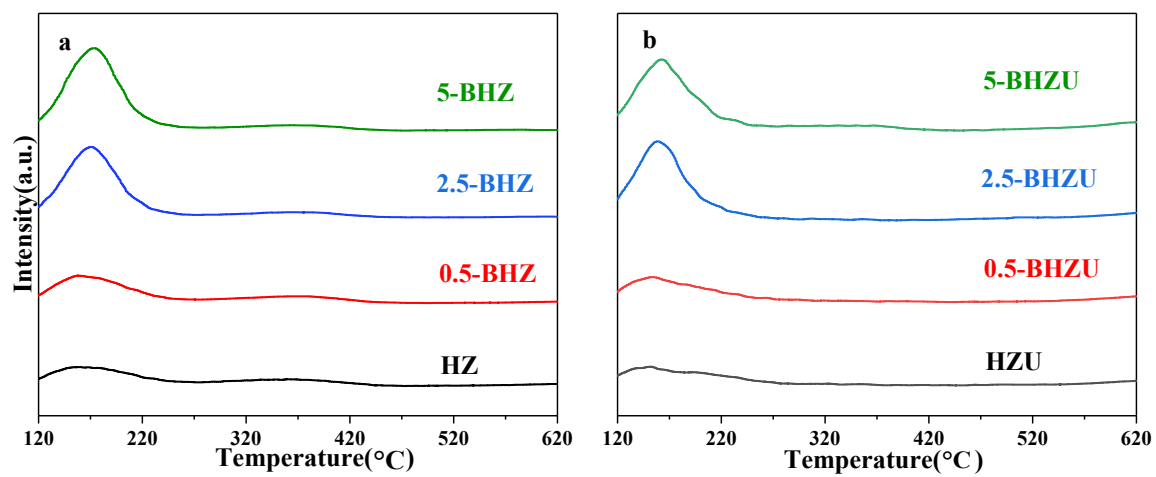


Fig. S3.  $\text{NH}_3$ -TPD profiles of different samples before (a) and after reaction (b)

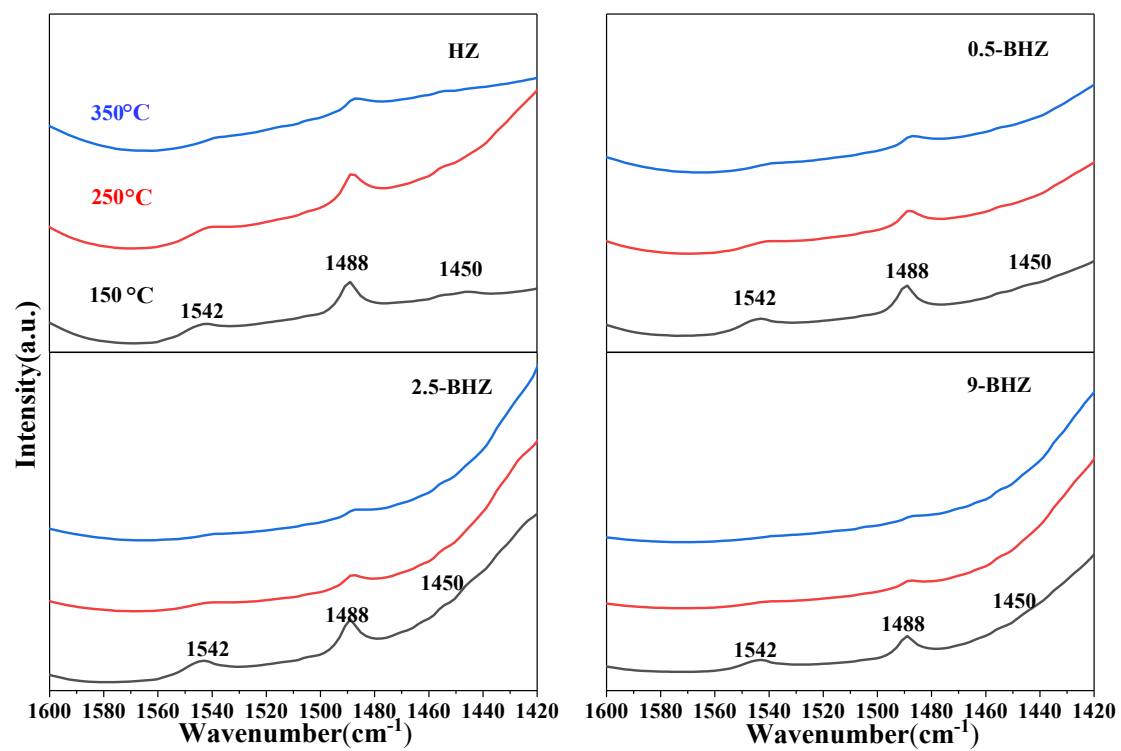


Fig. S4. py-IR spectra of *x*-BHZ with different B/Al ratios

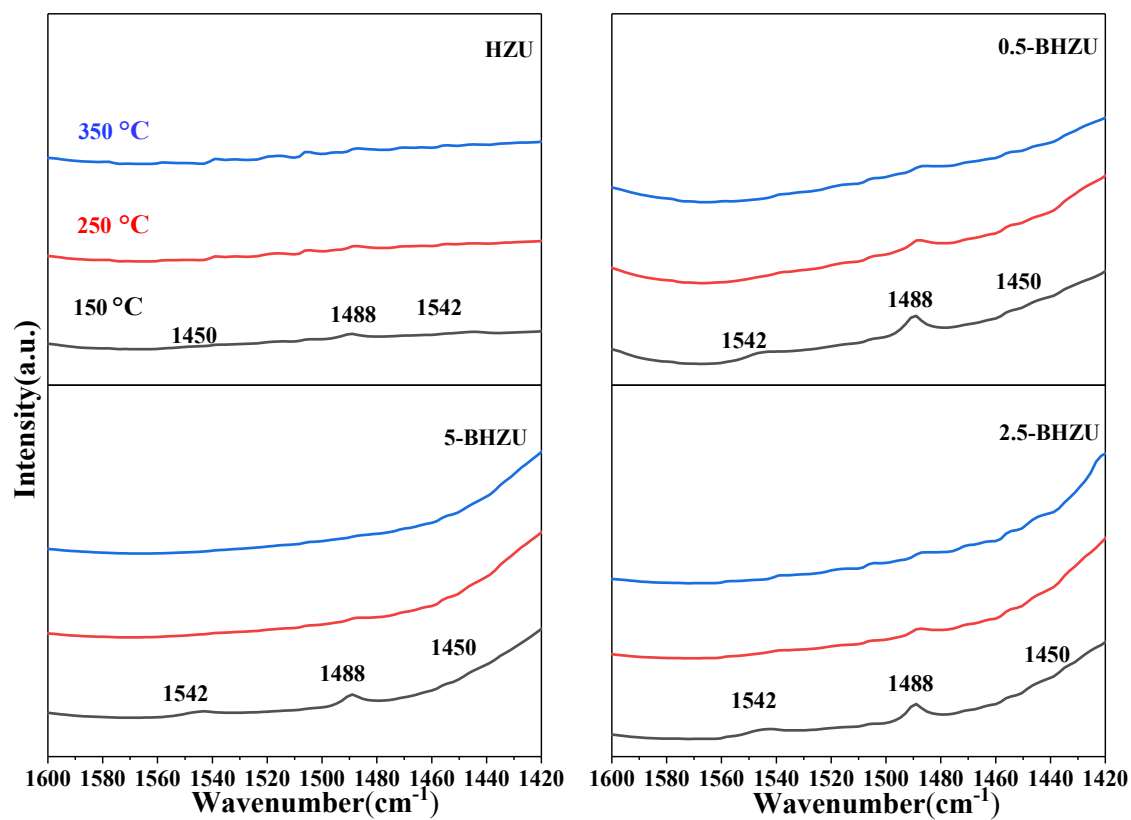


Fig. S5. py-IR spectra of *x*-BHZU with different B/Al ratios

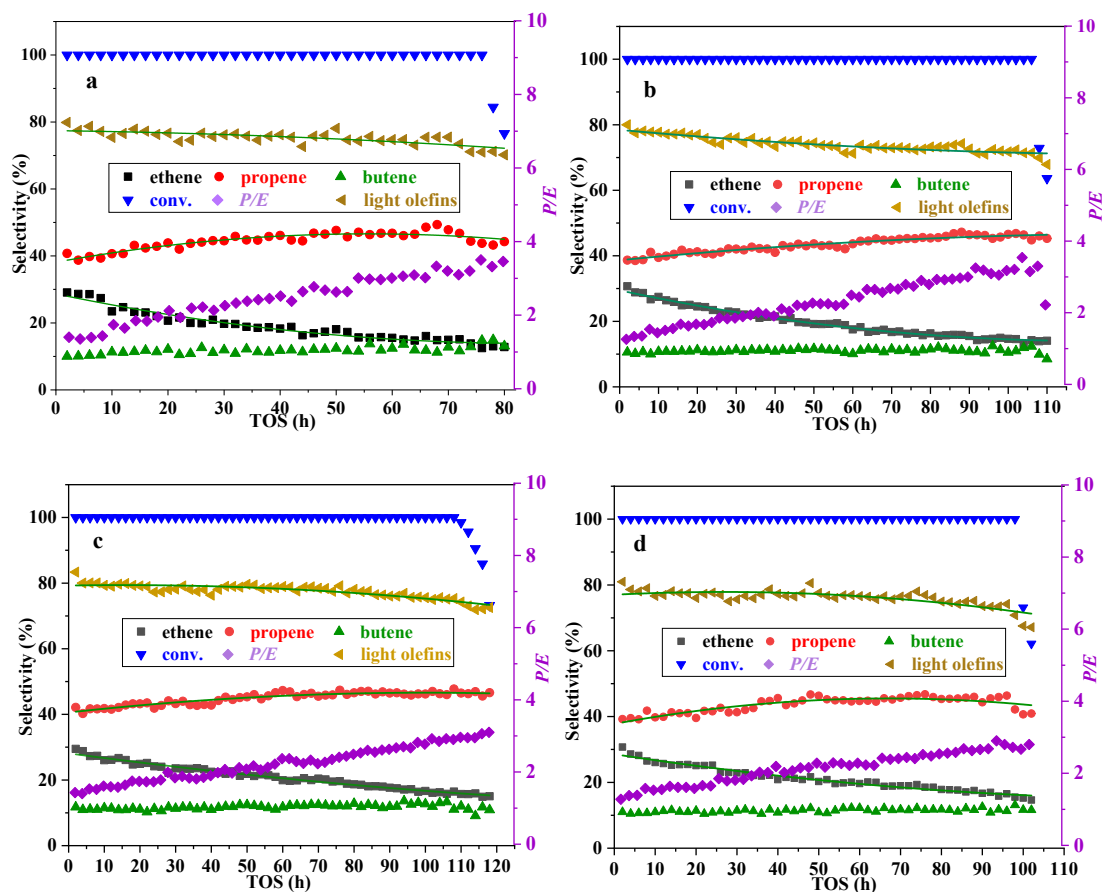


Fig. S6. Product distribution in the MTP reaction with time on stream (TOS) over catalysts (a. HZ, b. 0.5-BHZ, c. 2.5-BHZ, d. 5-BHZ)

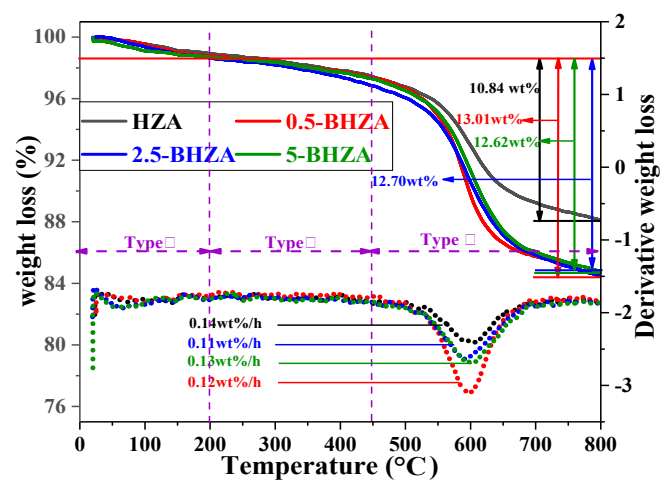


Fig. S7. TG analysis of BHZU samples toward MTP reaction



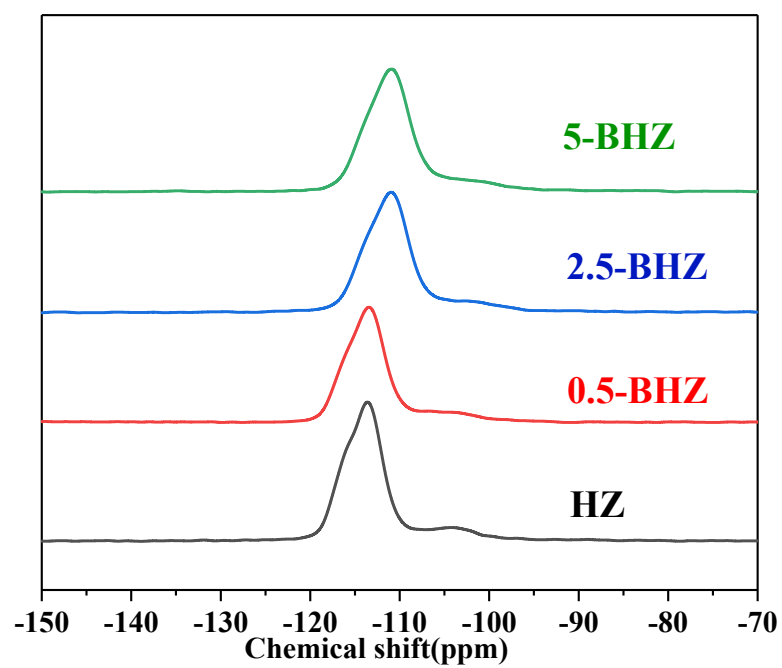


Fig. S8. The  $^{29}\text{Si}$  MAS NMR spectra of BHZ samples with different B/Al ratios

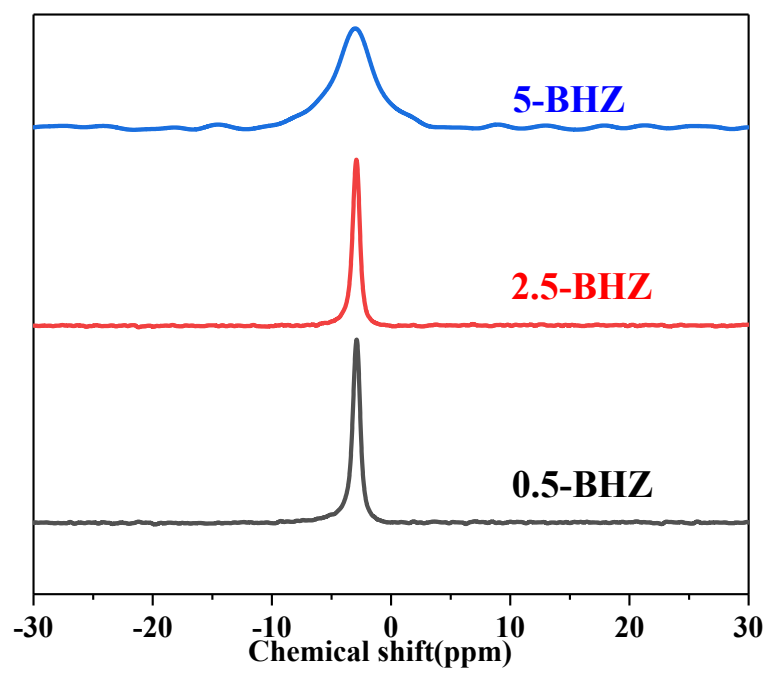


Fig. S9.  $^{11}\text{B}$  MAS NMR spectra of  $x$ -BHZ with different B/Al ratios

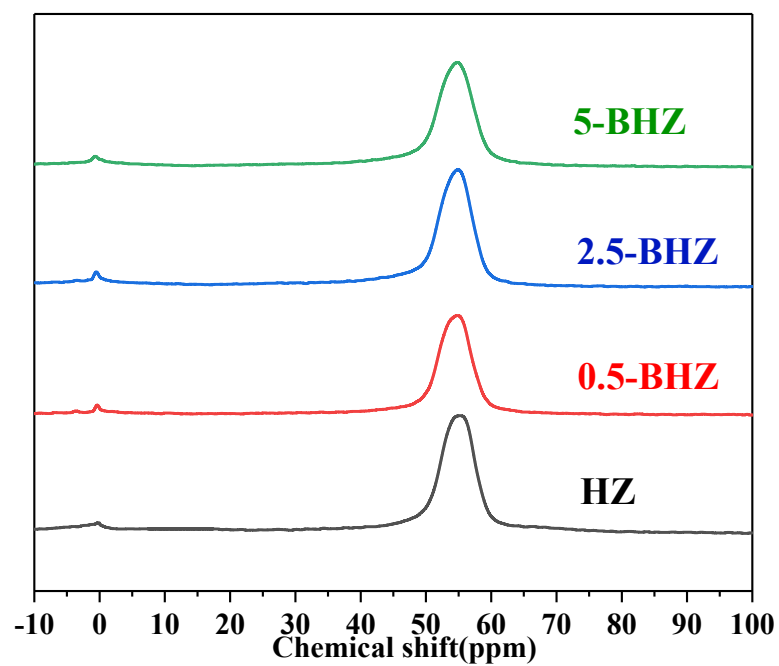


Fig. S10.  $^{27}\text{Al}$  MAS NMR spectra of  $x$ -BHZ with different B/Al ratios

Table S1. Relative percentages of Si species calculated from the  $^{29}\text{Si}$  MAS NM spectra for *x*-BHZ with

different B/Al ratios

| Sample         | Si[OSi] <sub>4</sub><br>(ppm) | Si[OSi] <sub>4</sub><br>(%) | Si[OSi] <sub>4</sub><br>(ppm) | Si[OSi] <sub>4</sub><br>(%) | Q <sup>4</sup> [1Al]<br>(ppm) | Q <sup>4</sup> [1Al]<br>(%) |
|----------------|-------------------------------|-----------------------------|-------------------------------|-----------------------------|-------------------------------|-----------------------------|
| <b>HZ</b>      | -116                          | 21                          | -113                          | 53                          | -108                          | 26                          |
| <b>0.5-BHZ</b> | -116                          | 18                          | -113                          | 57                          | -108                          | 25                          |
| <b>2.5-BHZ</b> | -114                          | 19                          | -111                          | 54                          | -107                          | 27                          |
| <b>5-BHZ</b>   | -114                          | 17                          | -111                          | 55                          | -107                          | 28                          |