

## Prediction of $^{13}\text{C}$ NMR Chemical Shifts of Organic Species Adsorbed on H-ZSM-5 Zeolite by ONIOM-GIAO Method

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### Electronic Supplementary Information

#### Samples preparation<sup>1</sup>

A H-ZSM-5 sample was dehydrated at 673 K under pressure below  $10^{-3}$  Pa for 5 h on a vacuum line. A known amount of ethyl iodide-1, 2- $^{13}\text{C}$  ( $^{13}\text{C}$ , 99%, Cambridge Isotope Inc.) was introduced and frozen on the activated catalyst with liquid  $\text{N}_2$ . The loading of ethyl iodide-1, 2- $^{13}\text{C}$  was estimated to be 0.2 mol/g. The sealed samples were transferred into a  $\text{ZrO}_2$  rotor (sealed by Kel-F cap) under a dry nitrogen atmosphere in a glove box prior to NMR measurement.

#### NMR measurements

$^{13}\text{C}$  NMR experiments were carried out at 9.4 T on a Varian Infinityplus-400 spectrometer using a 5 mm double-resonance probe. The resonance frequencies are 400.12, and 100.5 MHz for  $^1\text{H}$  and  $^{13}\text{C}$ , respectively. The  $\pi/2$  pulse lengths for  $^1\text{H}$  and  $^{13}\text{C}$  were measured to be 4.0 and 4.4  $\mu\text{s}$ , respectively.  $^1\text{H}$ - $^{13}\text{C}$  CP/MAS spectrum was recorded at ambient temperature with a 3 ms contact time and a 3 s recycle delay. The  $^{13}\text{C}$  chemical shifts were referenced to TMS. The MAS spinning speed was set to be 8 kHz.

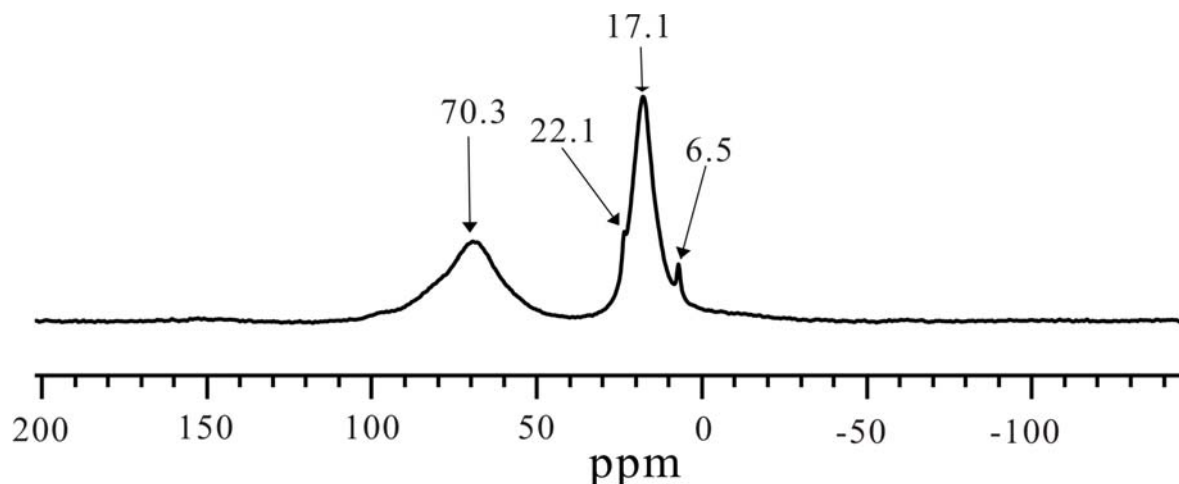


Figure.  $^{13}\text{C}$  CP/MAS NMR spectrum of ethyl iodide-1, 2- $^{13}\text{C}$  adsorbed on H-ZSM5 zeolite. The two intense signals at 70.3 and 17.1 ppm can be assigned to  $\text{CH}_2$  and  $\text{CH}_3$  groups of the framework-bound ethoxy species, respectively. The other two small peaks (at 22.1 and 6.5 ppm) are due to unreacted ethyl iodide-1, 2- $^{13}\text{C}$  adsorbed on the zeolite surface.<sup>1</sup>

1. D. K. Murray, J.W. Chang, and J. F. Haw, *J. Am. Chem. Soc.*, 1993,115, 4732.