

Supplementary Materials: Development of FTIR Spectroscopy Methodology for Characterization of Boron Species in FCC Catalysts

Claire Chunjuan Zhang, Xingtao Gao and Bilge Yilmaz*

BASF Corporation, 25 Middlesex-Essex Tpk., Iselin NJ 08830, USA; claire.c.zhang@basf.com (C.C.Z.); xingtao.gao@basf.com (X.G.)

* Correspondence: bilge.yilmaz@basf.com

1. X-Ray Photoelectron Spectroscopy (XPS) characterization

Figure S1 shows the B1s XPS plot along with P2s region. P2s and B1s peaks are overlapping with each other. Hence, B surface concentration cannot be observed.

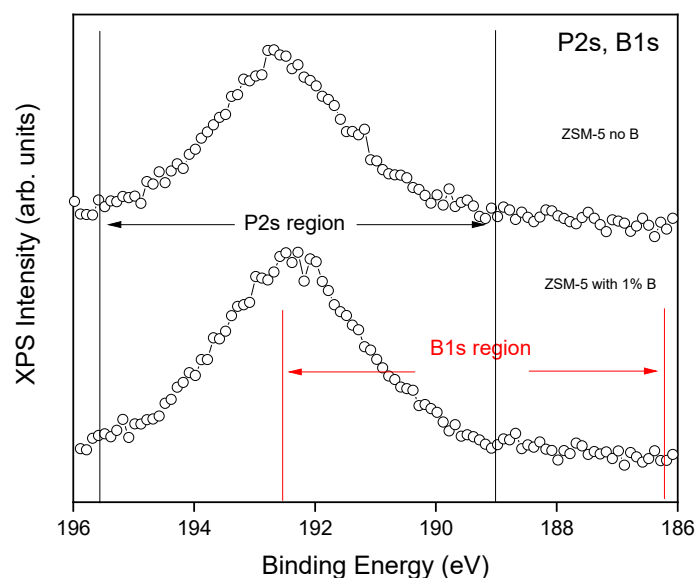


Figure S1. XPS P2s and B1s spectra for FCC ZSM-5 additive samples without boron (top) vs with 1 wt. % B_2O_3 (bottom). B1s region is overlapping with P2s region.

2. Nuclear Magnetic Resonance (NMR) spectroscopy characterization

^{11}B NMR spectroscopic analysis was also performed on an FCC ZSM-5 additive with 1% B_2O_3 , as shown in Figure S2 below. Due to quadrupolar aspects of the ^{11}B nucleus, precise peak fitting is challenging. Quadrupole lineshape distortion causes splitting and ambiguity in individual peak assignments. However, there is a large ppm shift which allowed us to separate the general BO_3 region from the more negative BO_4 region. For reference, ^{11}B NMR spectra of Al-borate, B-phosphate and boron oxide are also shown in Figure S3. As it can be seen the peaks for Al-borate and boron oxide are overlapping, which makes ^{11}B NMR not suitable as a stand-alone technique for EHS classification of boron species. As it was discussed in the manuscript using FTIR and Raman methods, there was no boron trioxide present in these samples after calcination. Therefore the NMR peak assignment can be stated as described in Figure S2, indicating the possible formation of B-phosphate and Al-borate, suggesting the interaction between Boron and Al and P.

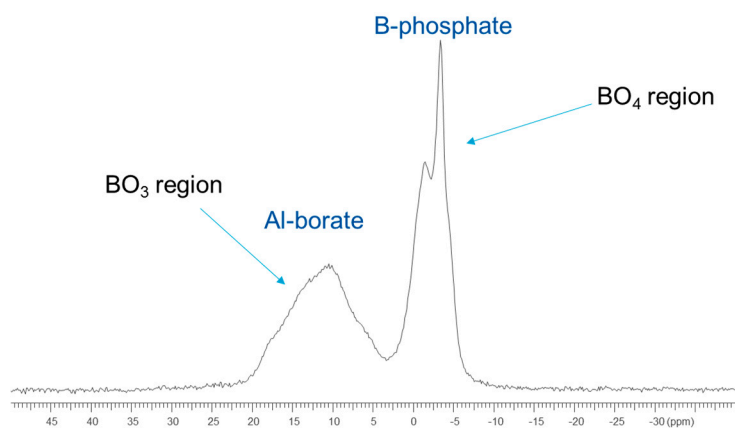


Figure S2. ^{11}B NMR spectrum of ZSM-5 additive with 1 wt.% B_2O_3 .

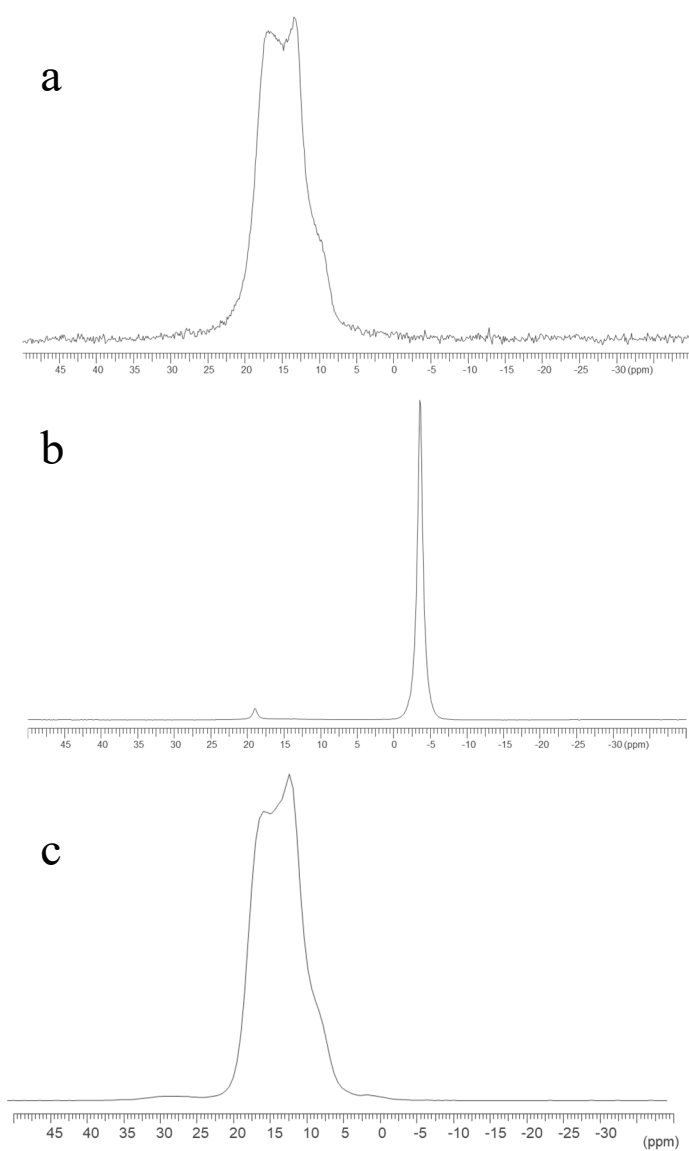


Figure S3. ^{11}B NMR spectra for (a) Al-borate and (b) B-phosphate (c) Boron trioxide.