

Supporting information for

Tailoring of the properties of amorphous mesoporous titanosilicates active in acetone condensation

Vera R. Bikbaeva ¹, Anna S. Artem'eva ¹, Sergey V. Bubennov ¹, Alexander I. Nikiforov ², Viktor Y. Kirsanov ^{1,3}, Dmitry V. Serebrennikov ¹, Lubov F. Korzhova ³, Stanislav G. Karchevsky ³, Leonard M. Khalilov ¹, Boris I. Kutepov ¹, Nellia G. Grigoreva ^{1,*}

¹ Institute of Petrochemistry and Catalysis of the Ufa Federal Research Center of the Russian Academy of Sciences, Ufa 450075, Russia

² Department of Chemistry, Lomonosov Moscow State University, Moscow 119991, Russia

³ Joint stock company "Institute of petrochemical processing" (JSC "INHP"), Ufa 450065, Russia

*Correspondence: ngg-ink@mail.ru

Figures

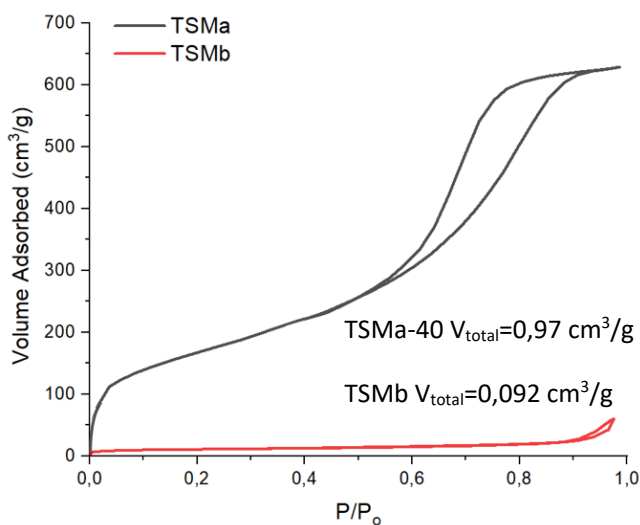


Figure S1. N₂ adsorption-desorption isotherms of amorphous titanosilicates TSMa-40 and TSMb.

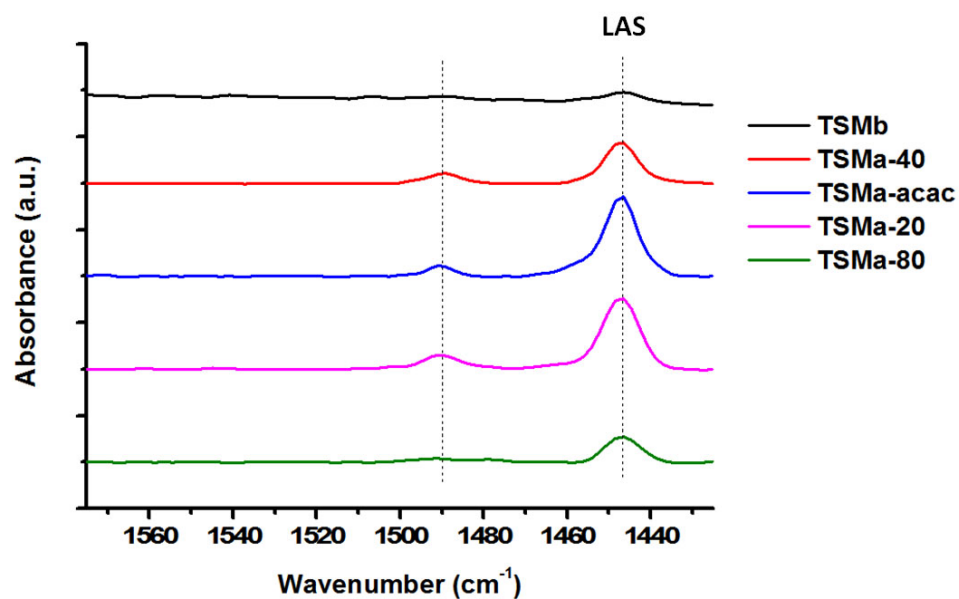


Figure S2. FTIR spectra of adsorbed pyridine for the titanosilicates

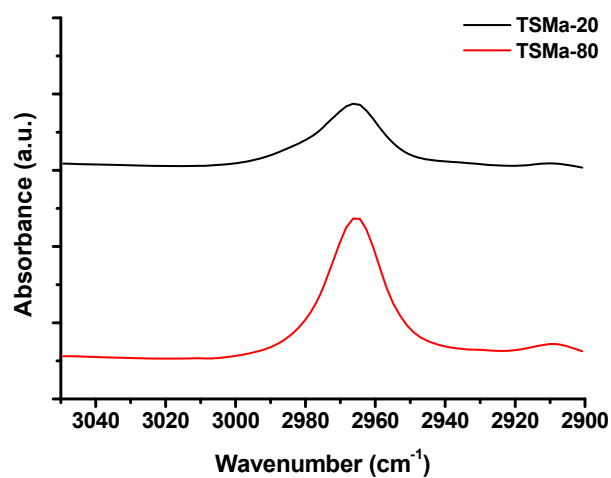


Figure S3. FTIR spectra of adsorbed chloroform for the titanosilicates

Effect of Si/Ti molar ratio

The influence of Si/Ti molar ratio on the catalytic properties of titanasilicates in acetone condensation was studied using samples with different ratios of framework atoms: Si/Ti= 20; 40; 80. The results are shown in Fig.S4.

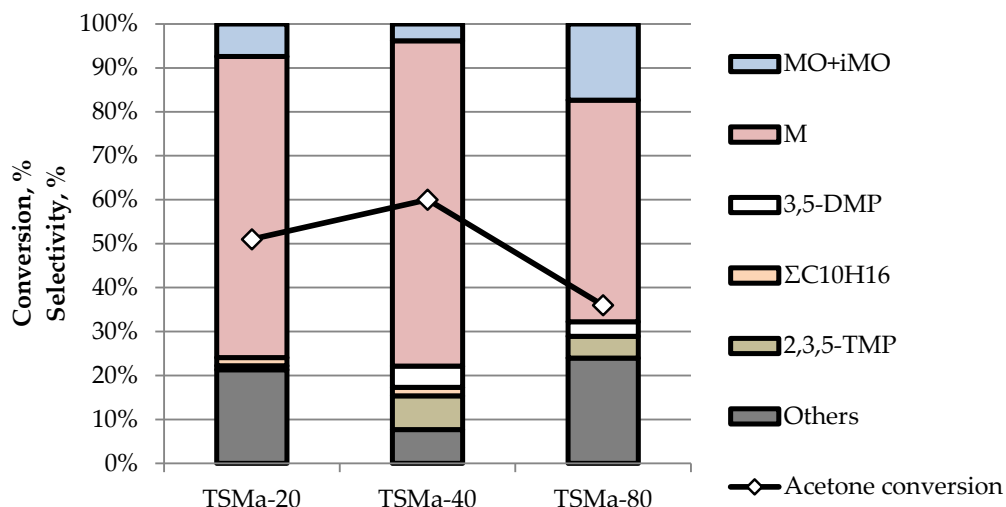


Figure S4. Effect of Si/Ti molar ratio on acetone conversion and selectivity of products (350 °C, 1 h⁻¹, TOS = 1h)

The acetone conversion curve has an extreme character, the maximum conversion were reached on sample TSMa-40 (60%), the minimum conversion on sample TSMa-80 (36%).

The most selective (77%) mesitylene is formed on sample TSMa-40, a close value of 74% was achieved on sample TSMa-20. It should be noted that the amount of mesitylene oxides and products of side reactions ($\Sigma C_{12}H_{16}$, $\Sigma C_{15}H_{20}$, ΣC_7H_{12} , $\Sigma C_{13}H_{20}$) increases in the reaction products as the amount of titanium in the structure of titanasilicates decreases.

The obtained results (maximum activity and selectivity in the reaction of sample TSMa-40) are obviously due to the structural characteristics of the samples. In TSMa samples with Si/Ti ratios from 20 to 80, tetracoordinated titanium Ti(IV) is predominantly present. As it was found (Figure 3), the content of hexacoordinated titanium increases with decreasing Si/Ti ratio.