Kinetic Analysis of Hexose Conversion to Methyl Lactate by Sn Beta: Effects of Substrate Masking and of Water

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Supporting Information

Catalysts characterization

X-Ray Powder Diffraction (XRPD)

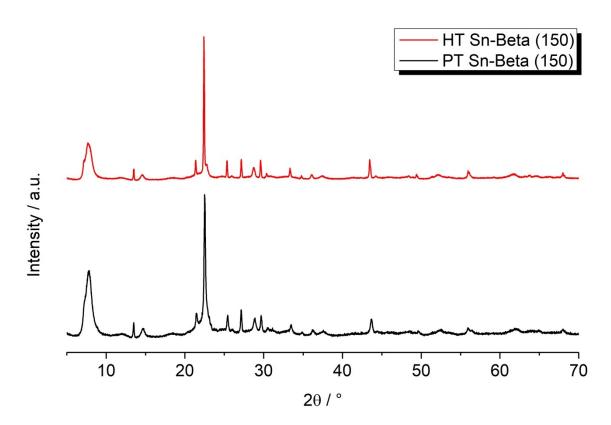


Figure S1- XRD patterns of the hydrothermal synthesized Sn-Beta (150) (red) and the post treated Sn-Beta (150) (black). The data are consistent with the reference *BEA crystal structure.

NH₃-Temperature Programmed Desorption (TPD)

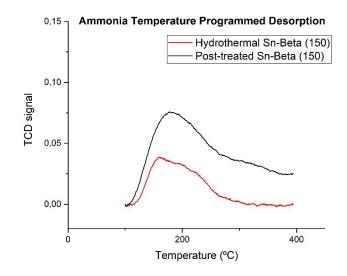


Figure S2- NH₃-TPD profiles of the hydrothermal (red) and post-treated (black) Sn-Beta (150) zeolites.

| | Hydrothermal Sn-Beta (150) | Post-treated Sn-Beta (150) |
|--|----------------------------|----------------------------|
| Cristallinity (%) ^a | 93,66 | 59,60 |
| Sn (wt %) ^b | 1,189 | 0,977 |
| Si/Sn ^b | 130,36 | 152,8001 |
| S _{BET} (m²/g) ^c | 602 | 722 |
| V _{micropore} (mL/g) ^d | 0,24 | 0,30 |
| Total acid sites (mmol/g) ^e | 5,57 | 10,84 |

 Table S1- Physicochemical properties of the hydrothermal and post-treated Sn-Beta (150) zeolites.

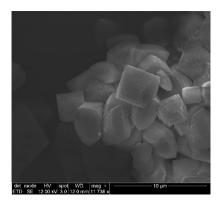
a. XRD measurements

b. ICP analysis

c. BET surface aread. Micropore volume

e. NH_3 -TPD analysis

HT Sn-Beta



PT Sn-Beta

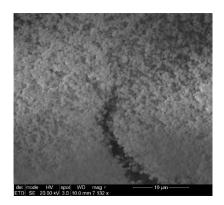


Fig. S3 Scanning electron microscope pictures of HT Sn-Beta (top) and PT Sn-Beta (bottom). The hydrothermal synthesis results in a large-crystal, defect-free material.

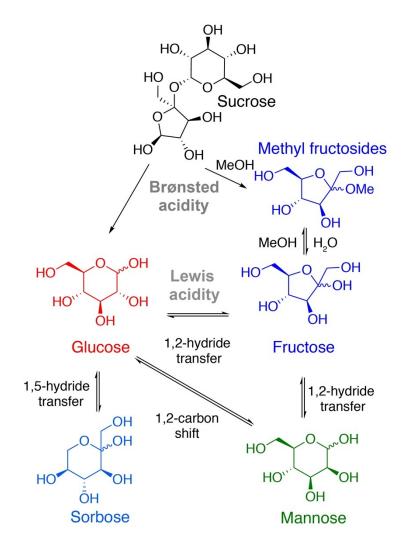


Fig. S4 Schematic overview of Sn-Beta catalyzed interconversions of carbohydrates. Only one isomer is displayed per monosaccharide for clarity. Glycosides of glucose, sorbose and mannose formed due to reaction with methanol are omitted for clarity.

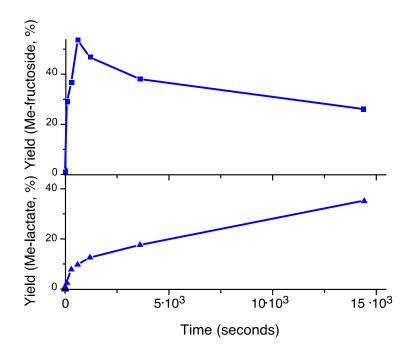


Fig. S5 Yields of methyl fructoside and methyl lactate in time resolved experiments starting from sucrose. Conditions: 108 mg substrate, 50 mg HT Sn-beta (150) catalyst, MW reactor for the indicated time at 160 °C.

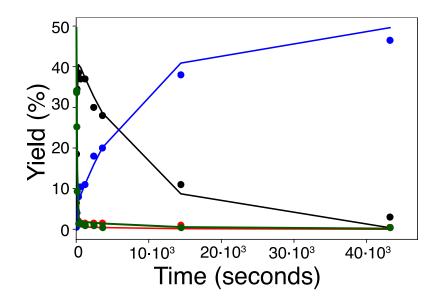


Fig. S6 Fit of experimental data to the kinetic model of main text Fig. 6 displayed on a linear time scale axis.

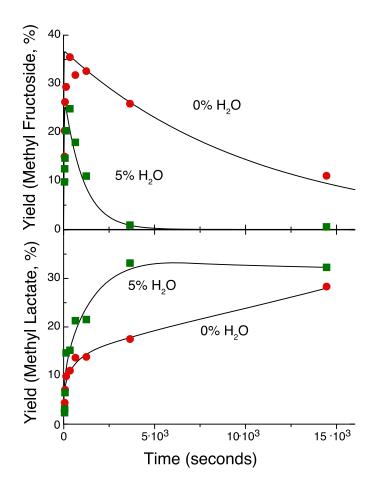


Fig. S7 Formation of methyl fructoside and methyl lactate using fructose substrate in the absence and in the presence of 5% (v/v) added water. Conditions: 120 mg substrate, 50 mg HT Sn-Beta (150) catalyst, MW reactor for the indicated time at 160 °C with or without addition of 5% water (v/v).