Supplementary Information

Aromatisation of bio-derivable isobutyraldehyde over HZSM-5 zeolite catalysts

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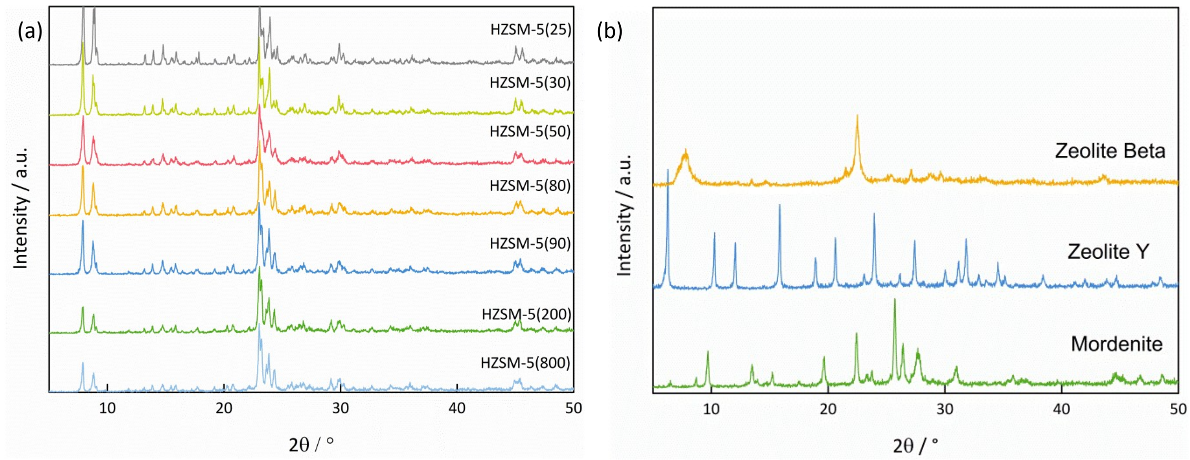
Table S1 Aromatic composition for the conversion of IBA over H-ZSM-5 (80). T = 400 °C, WHSV = $3h^{-1}$.

Table S2 Product composition over time for the conversion of IBA over HZSM-5(80) catalysts. T = 400 °C, WHSV = $3h^{-1}$.



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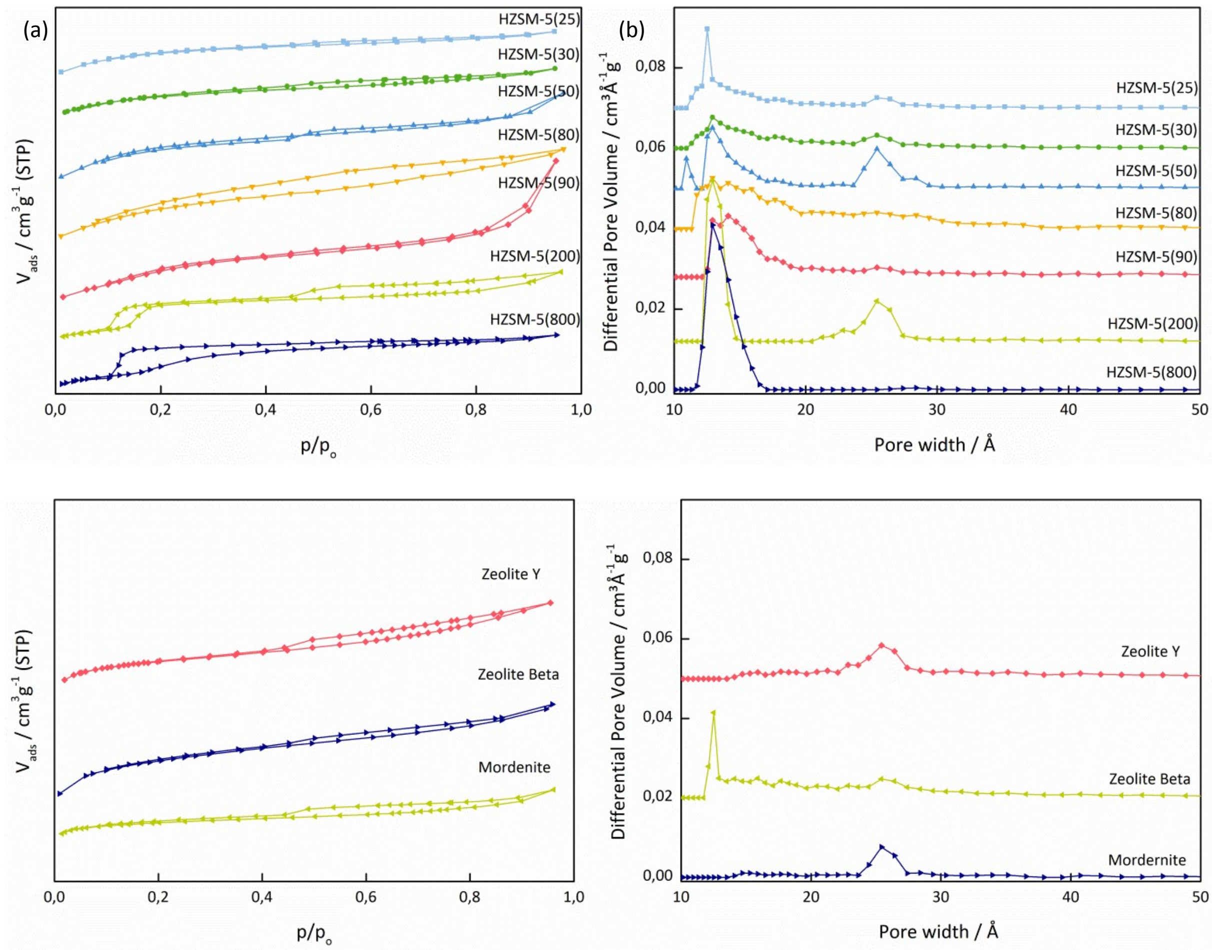

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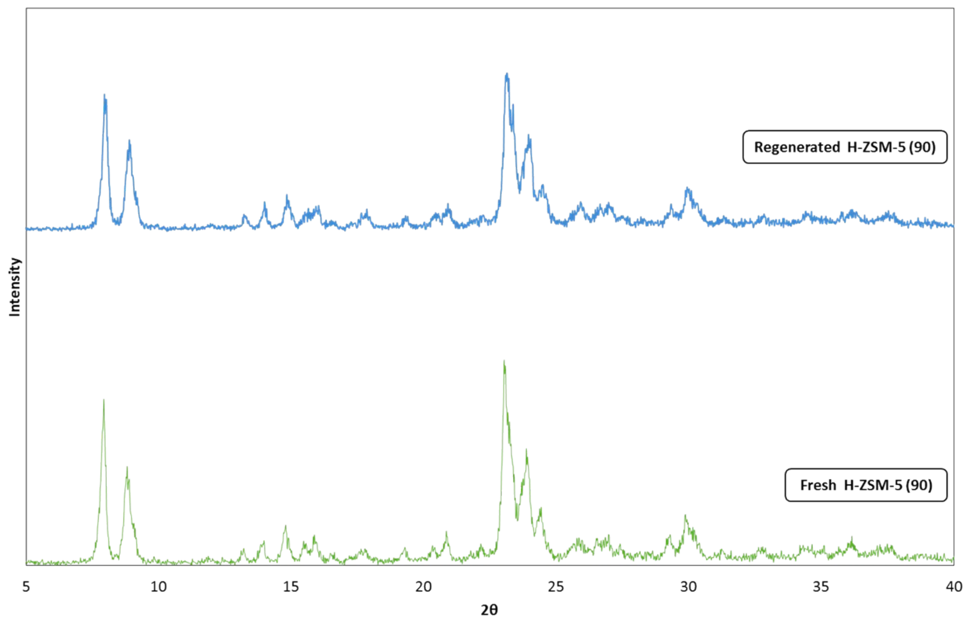

Fig. S3 XRD diffractograms of H-ZSM-5 (90) before and after calcination of spent catalyst.

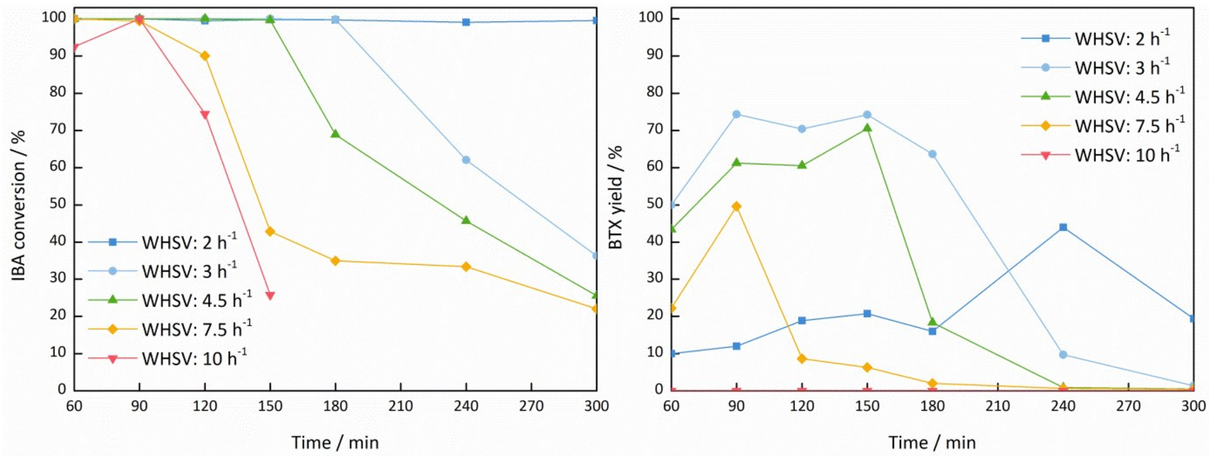

Fig. S4 The effect of WHSV on the aromatisation performance over HZSM-5(80) catalyst. Reaction conditions: IBA : N_2 = 10 : 1, WHSV = 2-10 h^{-1}, reaction pressure = 1 atm, reaction temperature = 400°C.

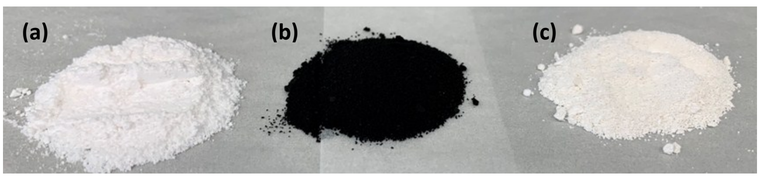

Fig. S5 H-ZSM-5(90) catalyst (a) before reaction, (b) after reaction (c) after regeneration.

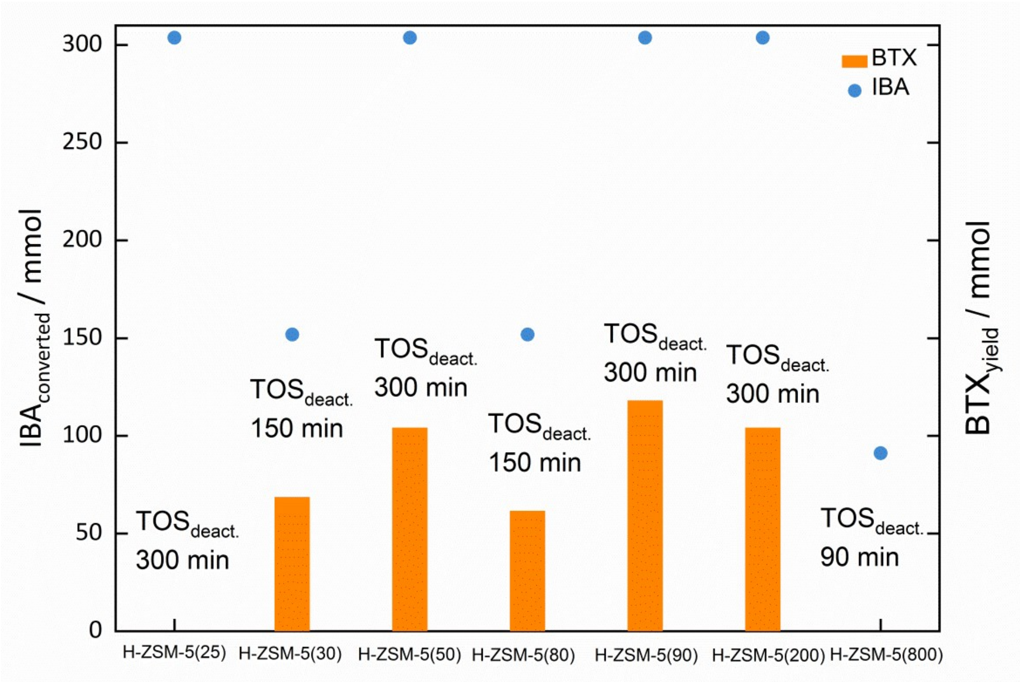

Fig. S6 IBA converted and BTX yielded until the start of catalyst deactivation for different HZSM-5. WHSV = 3 h^{-1}, reaction pressure = 1 atm, reaction temperature = 400°C. Deactivation defined as drop of conversion below 100%.

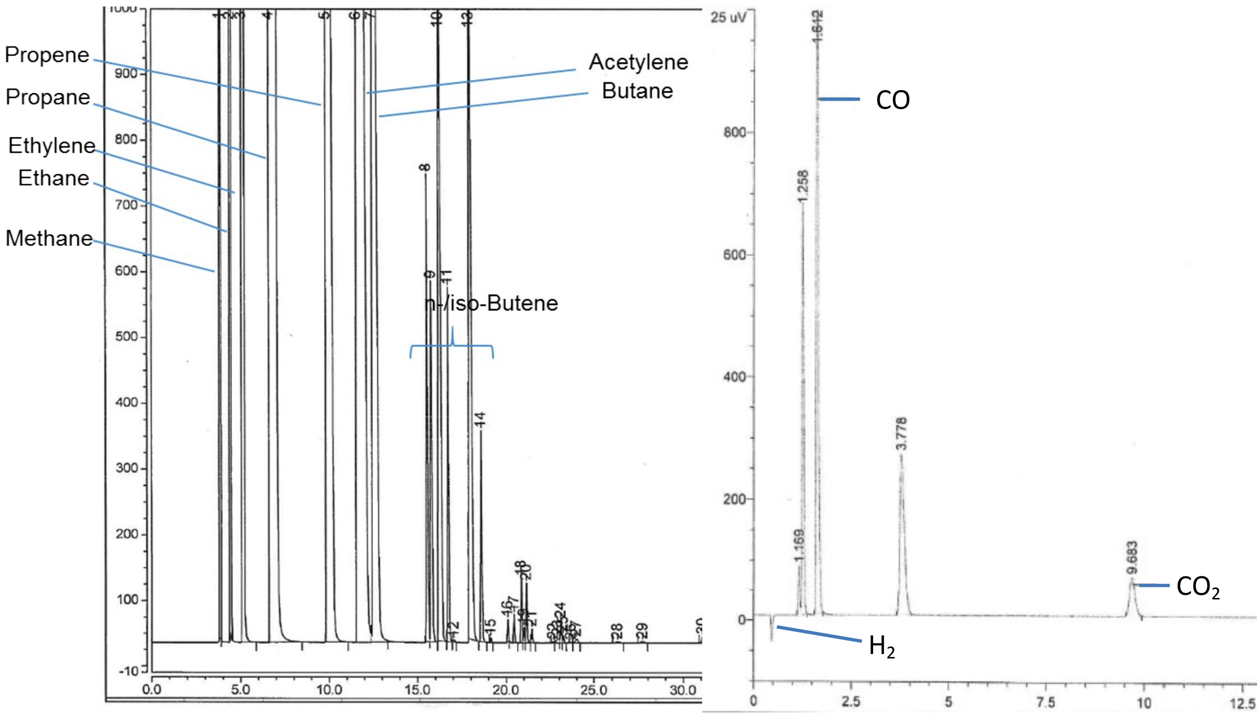

Fig. S7 Exemplary Gas-Phase GC-analysis of the aromatisation of IBA using a HZSM-5 80 zeolite. T = 400 °C, WHSV = 3h^{-1}.

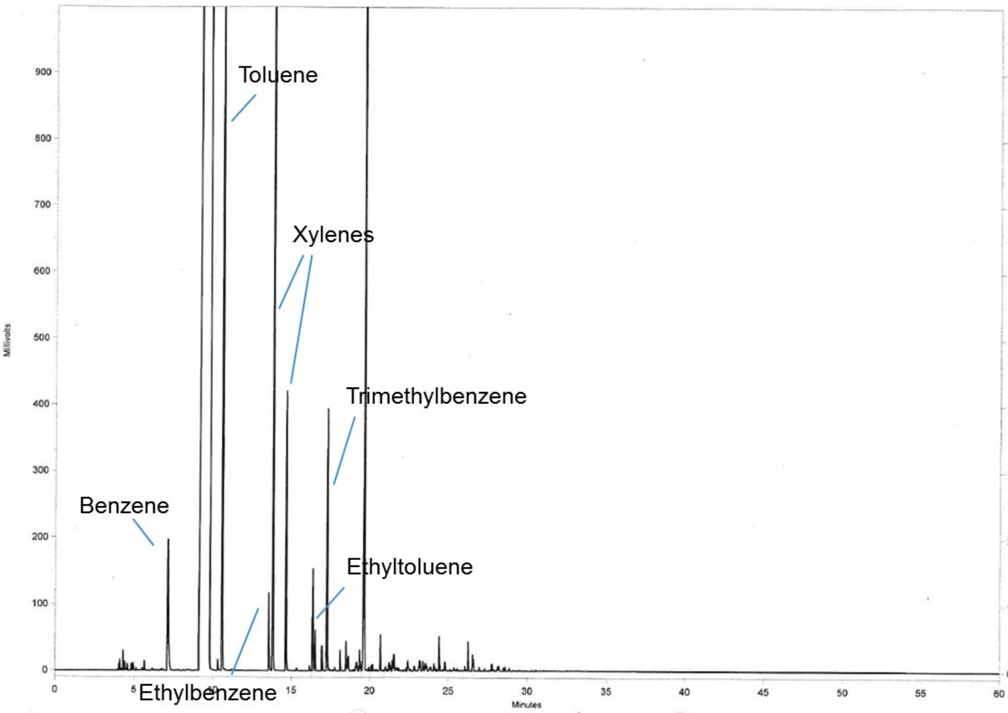

Fig. S8 Liquid phase GC-analysis of the aromatisation of IBA using a HZSM-5 80 zeolite. T = 400 °C, WHSV = $3h^{-1}$.

Table S1 Aromatic composition for the conversion of IBA over H-ZSM-5 (80). T = 400 °C, WHSV = $3h^{-1}$.

Aromatic hydrocarbons	Aromatics distribution [%]
Benzene	5.1
Toluene	28.9
p, *m*-Xylenes	33.8
o-Xylene	9.3
Ethylbenzene	4.6
p, *m*, *o*-Ethyltoluene	9.1
1,2,4-Trimethylbenzene	6
Naphthalenes	3.2

Table S2 Product composition over time for the conversion of IBA over HZSM-5(80) catalysts. T = 400 °C, WHSV = $3h^{-1}$.

		Product yield (%)							Aromatic yield (%)	BTX yield (%)
T (min)	Conversion (%)	C_1-C_4 gaseous	C_4-C_5	C_6	C_7	C_8	C_9	C_{10}+		
60	99.8	37.7	-	7.7	25.2	17.2	7.2	5.0	62.3	50.0-
90	100	10.2	-	10.2	33.8	30.4	10.1	5.3	89.8	74.4
120	100	15.4	-	8.9	31.2	30.3	10.1	4.1	84.6	70.4
150	100	9.9	-	8.2	31.4	34.6	11.8	4.1	90.1	74.2
180	99.8	20.4	0.3	5.7	25.3	32.6	12.1	3.5	79.3	63.6
240	62.1	86.7	0.4	0.5	3.3	5.9	2.6	0.6	12.9	9.7
300	36.3	98.0	0.4	0.26	0.4	0.7	0.3	0	1.6	1.3

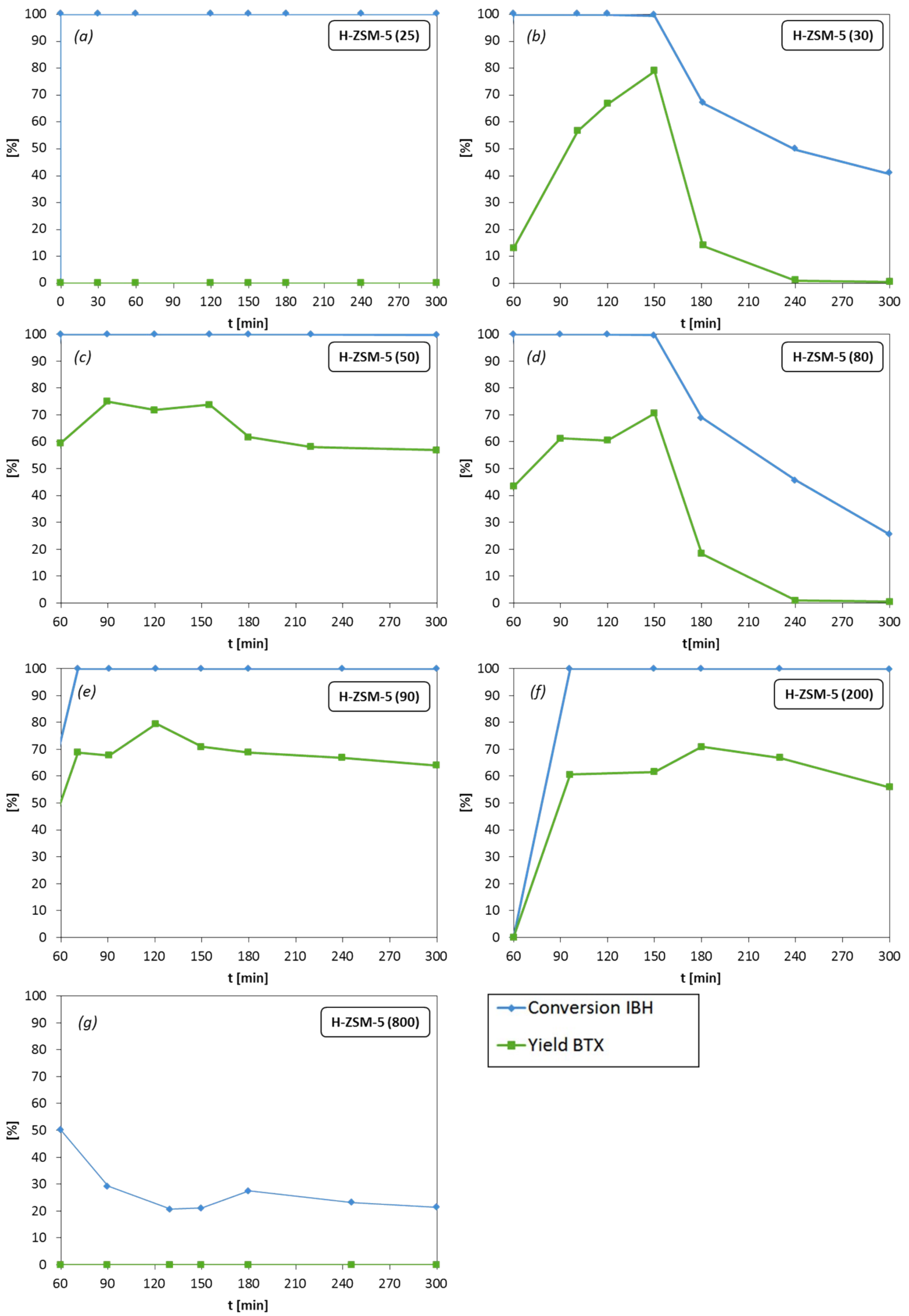

Fig. S9 BTX performance and IBA conversion for different HZSM-5 zeolites. T = 400 °C, WHSV = $3h^{-1}$.

Calculation to determine the yield (i = substance, $m_{i,GC}$ = mass of substance in GC sample, m_{Std} = mass of GC-standard medium, $Area_i$ = peak area of substance i, $k_{f,i}$ = calibration factor for substance i, $n_{i,GC}$ = amount of i in GC-sample, $n_{total,i}$ = amount of i in process, Y_i = yield of substance i):

$$m_{i,GC} = \frac{m_{Std} \cdot Area_i}{Area_{Std}} \cdot k_{f,i} \tag{1}$$

$$n_{i,GC} = \frac{m_{i,GC}}{M_i} \tag{2}$$

$$n_{total,i} = \frac{n_{i,GC} \cdot m_{total}}{m_{sample}} \tag{3}$$

$$Y_i = \frac{n_{total,i}}{n_{IBA,0}} \tag{4}$$

Calculation of IBA converted until the start of catalyst deactivation in Fig. S6 (n_{IBA} = amount of IBA in mmol, m = mass of IBA, X = conversion of IBA (in this case = 1)):

$$n(IBA_{converted}) = \frac{m_{IBA}}{M_{IBA}} \cdot X(IBA) \tag{5}$$

Calculation of BTX yielded until catalyst deactivation, under the assumption, that 1.75 mmol IBA (4 carbon) is needed to form 1 mmol of BTX (7 carbon) (Y(BTX) = yield of BTX):

$$n(BTX_{yielded}) = \frac{n(IBA_{converted}) \cdot Y(BTX)}{1.75} \tag{6}$$