Supporting information

Xylene isomerization over Beta zeolites in liquid phase.

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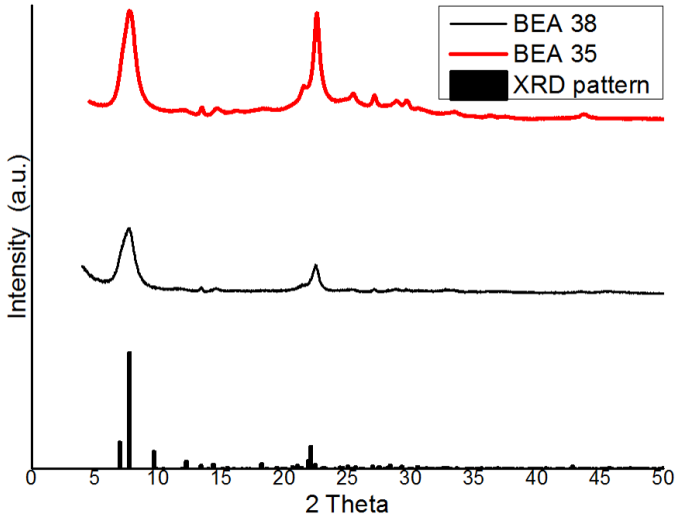

Figure S1 X-ray diffraction (XRD) of BEA35 and BEA38 compared to reported powder pattern by International Zeolite Association (www.iza-structure.org)

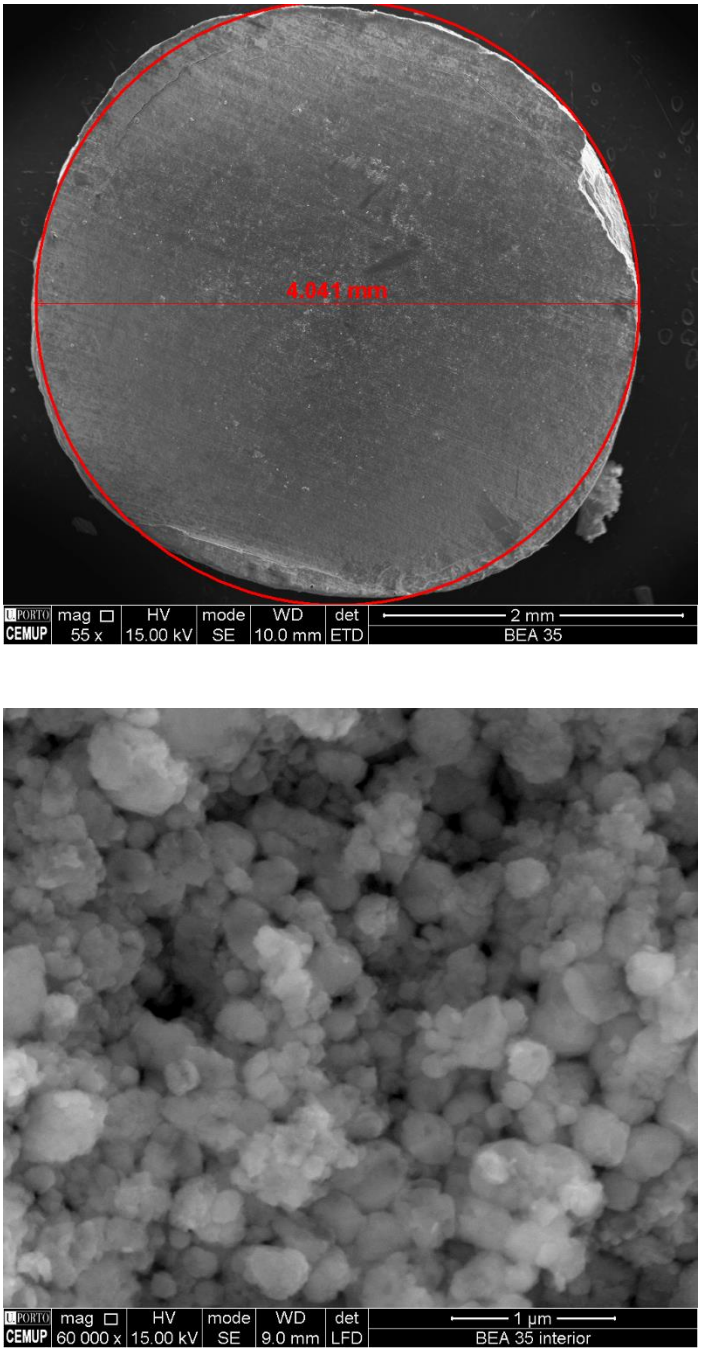

Figure S2 Scanning electron microscopy (SEM) images of BEA35

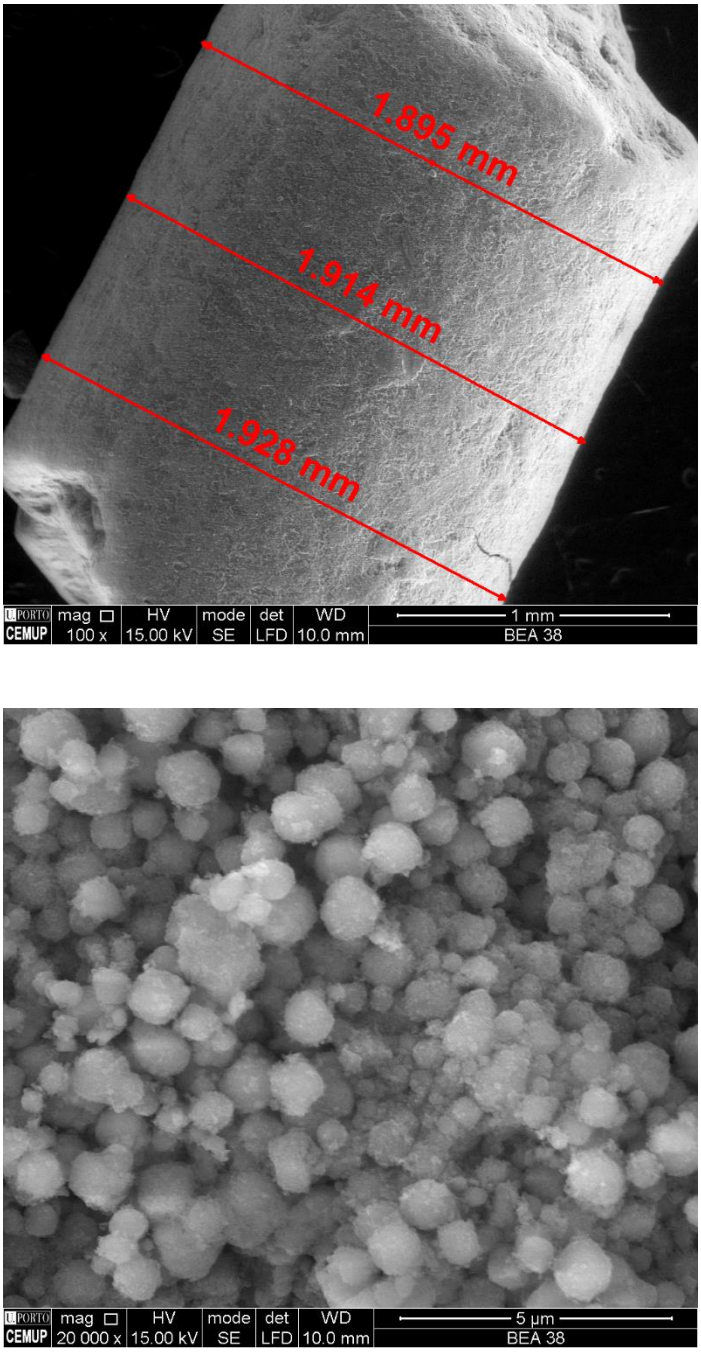

Figure S3 Scanning electron microscopy (SEM) images of BEA38

Table S1 Crushing strength data in Newton (N) obtained by application of the tablet tester.

			BEA35	BEA38
Number of particles (n)		n	50	50
Average		N	54.8	8.3
Standard deviation (s)		N	28.8	3.0
Relative standard deviation (RSD)		%	52.6	36.5
95 % Confidence interval		N	8.0	0.8
Range	Minimum (x)	N	5	3
	Maximum (x)	N	114	17

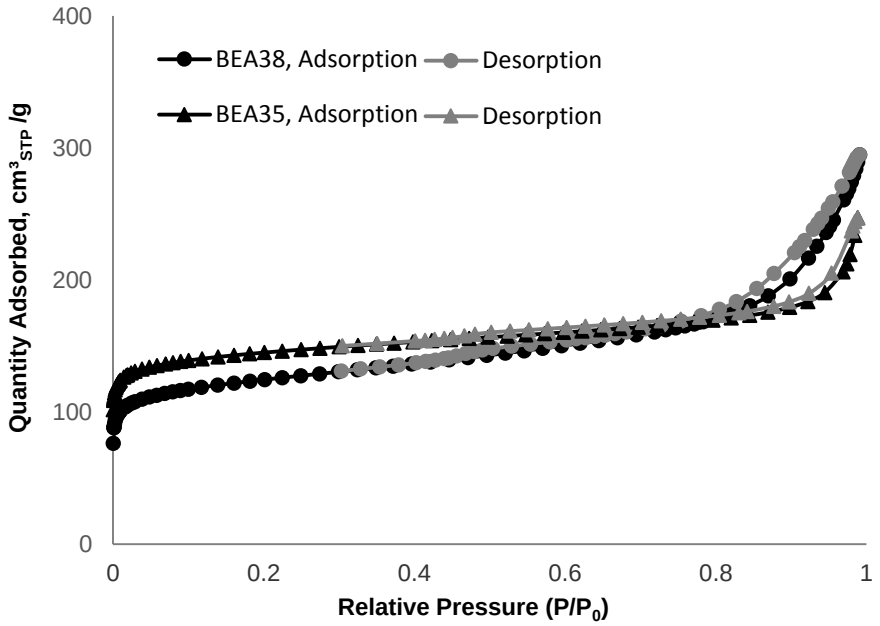

Figure S4 Nitrogen adsorption equilibrium isotherms on BEA35 and BEA38 pellets at 77 K.

Table S2 Estimated concentration of acid sites of BEA35 and BEA38

	BEA35	BEA38
Total amount of NH_3 desorbed (mmol/g)	0.91	0.65
Ammonia desorbed from weak adsorption sites (peak l) (mmol/g)	0.32	0.18
Ammonia desorbed from acid sites (peak h1) (mmol/g)	0.53	0.40
Ammonia desorbed from acid sites (peak h2) (mmol/g)	0.06	0.07

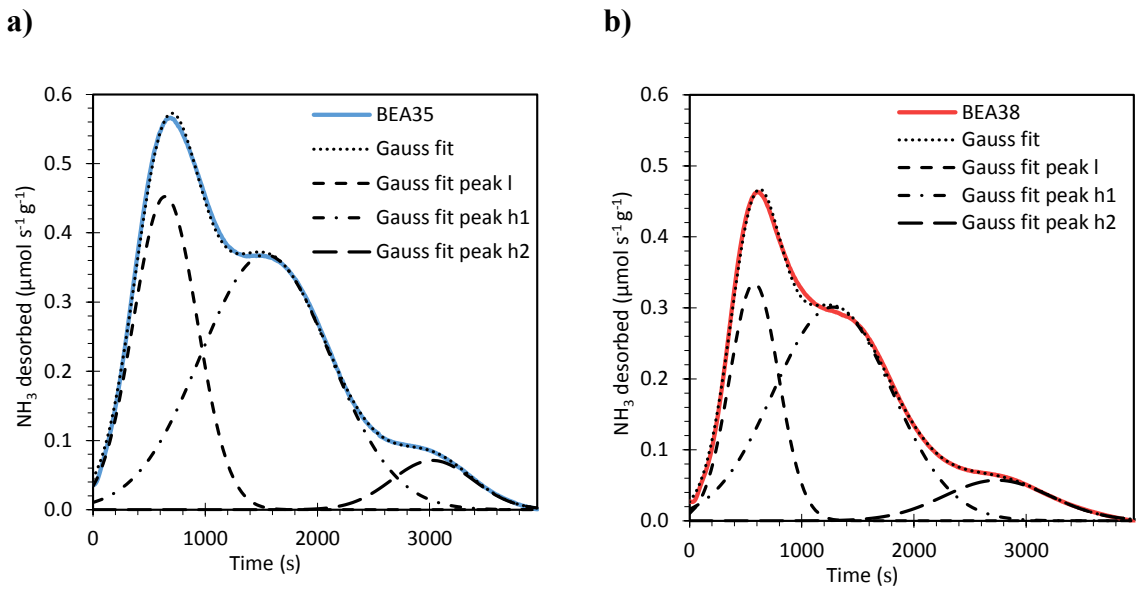

Figure S5 Deconvolution of Ammonia TPD spectra of BEA35 (a) and BEA38 (b) into three Gaussian peaks

Table S3 External mass-transfer of xylene isomerization experiments on BEA38 at 513 K and BEA35 at 493 K

Catalyst	Feed	Flow (mL/min)	R_{obs} (mol/(g_{cat} s))	Re	D_m (cm^2/s)	k_f (cm/s)	Ca
	OX	1.92	5.68×10^{-7}	14	4.59×10^{-5}	2.45×10^{-3}	0.0012
BEA38	MX	1.87	7.67×10^{-7}	14	6.10×10^{-5}	2.94×10^{-3}	0.0014
	PX	1.94	8.63×10^{-7}	15	6.46×10^{-5}	3.07×10^{-3}	0.0015
	OX	4.00	1.53×10^{-6}	28	1.29×10^{-4}	1.29×10^{-4}	0.0028
BEA35	MX	4.00	1.57×10^{-6}	35	1.28×10^{-4}	1.28×10^{-4}	0.0025
	PX	4.00	1.59×10^{-6}	56	1.27×10^{-4}	1.27×10^{-4}	0.0021

Table S4 The internal mass-transfer of xylenes isomerization on BEA38 at 513 K and BEA35 at 493 K

Catalyst	Feed	Flow (mL/min)	D_e (cm^2/s)	$\eta\phi^2$	Sphere/cylinder	
					ϕ	η
	OX	1.92	1.34×10^{-5}	7.10×10^{-3}	0.08	1.00
BEA38	MX	1.87	1.47×10^{-5}	9.31×10^{-3}	0.10	0.99
	PX	1.94	1.49×10^{-5}	1.06×10^{-2}	0.10	1.00
	OX	4.00	1.06×10^{-5}	5.71×10^{-2}	0.24	0.97
BEA35	MX	4.00	1.06×10^{-5}	5.63×10^{-2}	0.24	0.97
	PX	4.00	1.05×10^{-5}	5.35×10^{-2}	0.23	0.97

Table S5 Products distribution of pure xylene feedstock on BEA38 at 513 K

Run	Feed	Flow (mL/min)	Conversion	Effluent concentration (mol/L)		
				OX	MX	PX
1	OX	1.92	16.9%	6.856	1.258	0.092
2	OX	2.95	8.9%	7.444	0.745	0.039
3	OX	4.83	5.2%	7.821	0.395	0.026
4	OX	7.92	3.2%	7.982	0.240	0.023
5	OX	12.09	2.4%	8.048	0.175	0.023
6	MX	1.87	19.9%	0.664	6.493	0.923
7	MX	2.87	13.8%	0.454	6.982	0.649
8	MX	4.83	7.2%	0.245	7.515	0.334
9	MX	7.79	4.6%	0.159	7.731	0.214
10	MX	11.84	3.5%	0.128	7.817	0.158
11	PX	1.94	21.2%	0.065	1.572	6.360
12	PX	2.91	15.4%	0.040	1.154	6.829
13	PX	4.95	7.9%	0.013	0.604	7.432
14	PX	7.90	4.3%	0.009	0.331	7.721
15	PX	12.09	2.9%	0.008	0.226	7.836

Table S6 Products distribution of pure xylene feedstock on BEA38 at 493 K

Run	Feed	Flow (mL/min)	Conversion	Effluent concentration (mol/L)		
				OX	MX	PX
1	OX	1.68	8.1%	7.579	0.609	0.033
2	OX	1.90	6.9%	7.681	0.511	0.025
3	OX	3.00	3.6%	7.950	0.270	0.024
4	OX	4.90	2.5%	8.041	0.180	0.016
5	OX	8.00	1.2%	8.150	0.083	0.016
6	MX	1.46	11.5%	0.358	7.174	0.553
7	MX	2.16	7.9%	0.256	7.458	0.383
8	MX	3.00	4.7%	0.158	7.718	0.224
9	MX	4.82	2.4%	0.084	7.904	0.112
10	MX	8.07	1.8%	0.062	7.954	0.078
11	PX	1.47	17.9%	0.043	1.329	6.622
12	PX	2.00	12.6%	0.027	0.948	7.056
13	PX	3.00	7.2%	0.011	0.544	7.485
14	PX	5.14	3.4%	0.005	0.253	7.795
15	PX	7.90	2.4%	0.008	0.158	7.880

Table S7 Products distribution of pure xylene feedstock on BEA38 at 473 K

Run	Feed	Flow (mL/min)	Conversion	Effluent concentration (mol/L)		
				OX	MX	PX
1	OX	0.95	6.5%	7.712	0.480	0.024
2	OX	1.53	4.5%	7.882	0.324	0.015
3	OX	1.90	3.2%	7.990	0.226	0.013
4	OX	3.13	1.9%	8.091	0.139	0.010
5	OX	5.17	1.2%	8.154	0.085	0.009
6	MX	0.96	4.8%	0.151	7.710	0.233
7	MX	1.47	4.2%	0.134	7.764	0.194
8	MX	2.00	2.9%	0.093	7.869	0.137
9	MX	3.13	1.8%	0.059	7.955	0.081
10	MX	5.12	1.2%	0.040	8.003	0.049
11	PX	0.88	6.9%	0.014	0.516	7.515
12	PX	1.41	5.9%	0.010	0.445	7.595
13	PX	2.10	4.2%	0.007	0.312	7.732
14	PX	3.06	2.4%	0.008	0.178	7.875
15	PX	5.16	1.2%	0.006	0.092	7.972

Table S8 The kinetic parameters of xylene isomerization on BEA38 with the corresponding 95% confidence limit

	Linear – Equilibrium from Literature	Linear	Triangular - Equilibrium from Literature	Triangular
$E_{a,1}$ (kJ/mol)	91 ± 9	89 ± 9	88 ± 10	89 ± 10
$E_{a,2}$ (kJ/mol)	-	116 ± 24	-	100 ± 20
$E_{a,3}$ (kJ/mol)	90 ± 8	87 ± 14	89 ± 6	106 ± 14
$E_{a,4}$ (kJ/mol)	-	85 ± 6	-	87 ± 6
$E_{a,5}$ (kJ/mol)	-	-	-	60 ± 200
$E_{a,6}$ (kJ/mol)	-	-	65 ± 1200	60 ± 400
$k_{01}\times10^{8}$ (m^3/kg_{cat} s)	3.5 ± 0.3	3.3 ± 0.2	3.5 ± 0.3	3.3 ± 0.3
$k_{02}\times10^{8}$ (m^3/kg_{cat} s)	-	1.5 ± 0.3	-	1.7 ± 0.3
$k_{03}\times10^{8}$ (m^3/kg_{cat} s)	2.35 ± 0.12	2.6 ± 0.3	2.36 ± 0.12	2.3 ± 0.3
$k_{04}\times10^{8}$ (m^3/kg_{cat} s)	-	5.3 ± 0.2	-	5.1 ± 0.3
$k_{05}\times10^{8}$ (m^3/kg_{cat} s)	-	-	-	0.1 ± 0.2
$k_{06}\times10^{8}$ (m^3/kg_{cat} s)	-	-	0.02 ± 0.19	0.07 ± 0.2

Table S9 The kinetic parameters of xylene isomerization on BEA38 at 513 K with the corresponding 95% confidence limit

Parameter	Linear - Equilibrium from Literature	Linear	Triangular - Equilibrium from Literature	Triangular
k_1×10^8 (m^3/kg_{cat} s)	8.4 ± 0.7	7.9 ± 0.6	8.3 ± 0.8	7.7 ± 0.6
k_2×10^8 (m^3/kg_{cat} s)	-	4.4 ± 0.6	-	4.3 ± 0.6
k_3×10^8 (m^3/kg_{cat} s)	5.3 ± 0.4	6.1 ± 0.7	5.2 ± 0.4	6.1 ± 0.6
k_4×10^8 (m^3/kg_{cat} s)	-	10 ± 2	-	10.00 ± 1.4
k_5×10^8 (m^3/kg_{cat} s)	-	-	-	0.2± 0.6
k_6×10^8 (m^3/kg_{cat} s)	-	-	0.1 ± 0.6	0.7 ± 0.9
Keq1	0.383 [a]	0.557	0.38 3 [a]	0.558
Keq2	2.243 [a]	1.639	2.243 [a]	1.639
Keq3	-	-	1.162 [a]	3.500

[b] k2=k1*Keq1; k4=k3*Keq2; k5=k6*Keq3. Linear with equilibrium and triangular with equilibrium mean the models combined with the thermodynamic equilibrium equations proposed by Gonçalves and Rodrigues[20].

Table S10 The kinetic parameters of xylene isomerization on BEA38 at 493 K with the corresponding 95% confidence limit

Parameter	Linear - Equilibrium from Literature	Linear	Triangular - Equilibrium from Literature	Triangular
$k_1 \times 10^8$ (m^3/kg_{cat} s)	3.2 ± 0.3	3.1 ± 0.3	3.2 ± 0.3	3 ± 0.4
$k_2 \times 10^8$ (m^3/kg_{cat} s)	-	1.7 ± 0.3	-	1.7 ± 0.3
$k_3 \times 10^8$ (m^3/kg_{cat} s)	2.79 ± 0.15	2.6 ± 0.4	2.79 ± 0.14	2.6 ± 0.3
$k_4 \times 10^8$ (m^3/kg_{cat} s)	-	6.4 ± 0.3	-	6.3 ± 0.4
$k_5 \times 10^8$ (m^3/kg_{cat} s)	-	-	-	0.18 ± 0.3
$k_6 \times 10^8$ (m^3/kg_{cat} s)	-	-	0.10 ± 0.22	0.18 ± 0.3
Keq1	0.377 [a]	0.548	0.377 [a]	0.567
Keq2	2.268 [a]	2.461	2.268 [a]	2.423
Keq3	-	-	1.169 [a]	1.000

[a] k2=k1*Keq1; k4=k3*Keq2; k5=k6*Keq3. Linear with equilibrium and triangular with equilibrium mean the models combined the thermodynamic equilibrium equations proposed by Gonçalves and Rodrigues[20].

Table S11 The kinetic parameters of xylene isomerization on BEA38 at 473 K with the corresponding 95% confidence limit

Parameter	Linear - Equilibrium from Literature	Linear	Triangular - Equilibrium from Literature	Triangular
$k_1 \times 10^8$ (m^3/kg_{cat} s)	1.80 ± 0.40	1.57± 0.38	1.4 ± 0.3	1.40 ± 0.13
$k_2 \times 10^8$ (m^3/kg_{cat} s)	-	0.5 ± 0.4	-	0.48 ± 0.14
$k_3 \times 10^8$ (m^3/kg_{cat} s)	0.72 ± 0.15	0.8 ± 0.4	0.7 ± 0.1	0.81 ± 0.14
$k_4 \times 10^8$ (m^3/kg_{cat} s)	-	1.61 ± 0.37	-	1.68 ± 0.13
$k_5 \times 10^8$ (m^3/kg_{cat} s)	-	-	-	0.05 ± 0.14
$k_6 \times 10^8$ (m^3/kg_{cat} s)	-	-	0.10 ± 0.2	0.6 ± 0.13
Keq1	0.370 [a]	0.318	0.370 [a]	0.343
Keq2	2.296 [a]	2.012	2.296 [a]	2.074
Keq3	-	-	1.177 [a]	12.00

[a] k2=k1*Keq1; k4=k3*Keq2; k5=k6*Keq3. Linear with equilibrium and triangular with equilibrium mean the models combined the thermodynamic equilibrium equations proposed by Gonçalves and Rodrigues[20].

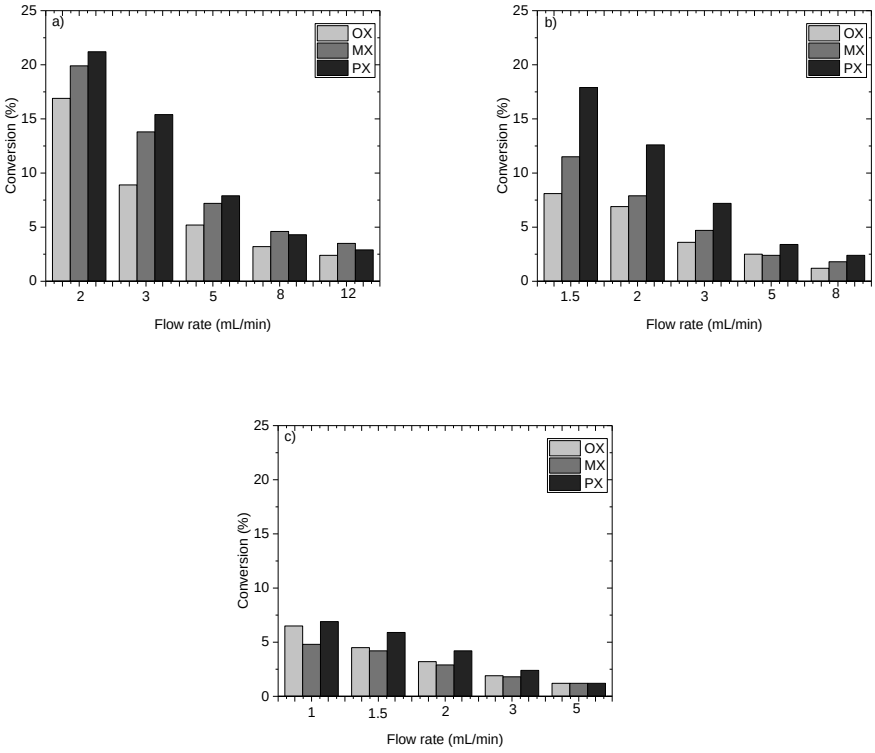

Figure S6 Comparison of the conversions of pure xylenes over BEA38 at different flow rates at a) 513 K, b) 493 K, and c) 473 K

Table S12 Products distribution of pure xylene feedstock on BEA35 at 493 K

Run	Feed	Flow (mL/min)	Conversion	Concentration (mol/L)		
				OX	MX	PX
1	OX	4.00	19.66%	6.628	1.432	0.142
2	OX	5.05	15.99%	6.931	1.181	0.106
3	OX	8.06	10.11%	7.416	0.767	0.058
4	OX	12.30	6.94%	7.678	0.539	0.038
5	OX	16.30	5.43%	7.802	0.423	0.032
6	MX	4.00	18.76%	0.607	6.582	0.868
7	MX	5.05	14.08%	0.456	6.961	0.649
8	MX	8.06	7.31%	0.235	7.509	0.331
9	MX	12.30	3.84%	0.125	7.791	0.167
10	MX	16.30	2.13%	0.069	7.929	0.086
11	PX	4.00	19.89%	0.068	1.494	6.465
12	PX	5.05	16.23%	0.049	1.234	6.760
13	PX	8.06	10.28%	0.028	0.803	7.241
14	PX	12.30	7.35%	0.021	0.581	7.477
15	PX	16.30	6.11%	0.021	0.486	7.577

Table S13 Products distribution of pure xylene feedstock on BEA35 at 473 K

Run	Feed	Flow (mL/min)	Conversion	Concentration (mol/L)		
				OX	MX	PX
1	OX	1.50	27.01%	6.022	1.903	0.220
2	OX	2.00	20.34%	6.572	1.468	0.139
3	OX	3.00	11.17%	7.328	0.841	0.055
4	OX	5.00	4.79%	7.855	0.379	0.020
5	OX	8.00	1.89%	8.094	0.144	0.010
6	MX	1.50	18.10%	0.569	6.635	0.844
7	MX	2.00	13.95%	0.444	6.972	0.644
8	MX	3.00	8.48%	0.270	7.415	0.389
9	MX	5.00	4.00%	0.134	7.778	0.183
10	MX	8.00	2.03%	0.070	7.938	0.089
11	PX	1.50	28.51%	0.184	1.898	5.769
12	PX	2.00	25.07%	0.105	1.765	6.047
13	PX	3.00	14.84%	0.035	1.085	6.872
14	PX	5.00	5.04%	0.009	0.380	7.663
15	PX	8.00	1.47%	0.006	0.127	7.951

Table S14 Products distribution of pure xylene feedstock on BEA35 at 453 K

Run	Feed	Flow (mL/min)	Conversion	Concentration (mol/L)		
				OX	MX	PX
1	OX	1.00	11.40%	7.310	0.850	0.052
2	OX	1.50	7.28%	7.650	0.562	0.030
3	OX	2.00	4.93%	7.843	0.384	0.021
4	OX	3.00	2.74%	8.024	0.219	0.014
5	OX	5.00	1.34%	8.139	0.110	0.011
6	MX	1.00	8.86%	0.285	7.384	0.418
7	MX	1.50	5.53%	0.177	7.654	0.257
8	MX	2.00	3.62%	0.117	7.809	0.159
9	MX	3.00	2.85%	0.094	7.871	0.118
10	MX	5.00	1.05%	0.031	8.017	0.033
11	PX	1.00	16.82%	0.054	1.225	6.713
12	PX	1.50	10.82%	0.018	0.831	7.197
13	PX	2.00	5.95%	0.008	0.475	7.590
14	PX	3.00	2.66%	0.003	0.222	7.855
15	PX	5.00	0.96%	0.000	0.095	7.992

Table S15 The kinetic parameters of xylene isomerization on BEA35 with the corresponding 95% confidence limit

	Linear – Equilibrium from Literature	Linear	Triangular - Equilibrium from Literature	Triangular
$E_{a,1}$ (kJ/mol)	91 ± 7	90 ± 7	93 ± 8	91 ± 9
$E_{a,2}$ (kJ/mol)	-	100 ± 25	-	96 ± 26
$E_{a,3}$ (kJ/mol)	84 ± 6	99 ± 18	83 ± 7	100 ± 18
$E_{a,4}$ (kJ/mol)	-	80 ± 6	-	80 ± 8
$E_{a,5}$ (kJ/mol)	-	-	-	95 ± 124
$E_{a,6}$ (kJ/mol)	-	-	68 ± 90	72 ± 145
$k_{01}\times10^{8}$ (m^3/kg_{cat} s)	8.7 ± 0.5	8.8 ± 0.5	8.3 ± 0.6	8.4 ± 0.6
$k_{02}\times10^{8}$ (m^3/kg_{cat} s)	-	2.9 ± 0.6	-	2.8 ± 0.6
$k_{03}\times10^{8}$ (m^3/kg_{cat} s)	4.4 ± 0.2	4.1 ± 0.6	4.4 ± 0.2	4.2 ± 0.6
$k_{04}\times10^{8}$ (m^3/kg_{cat} s)	-	10.4 ± 0.5	-	10.1 ± 0.6
$k_{05}\times10^{8}$ (m^3/kg_{cat} s)	-	-	-	0.6 ± 0.6
$k_{06}\times10^{8}$ (m^3/kg_{cat} s)	-	-	0.5 ± 0.4	0.5 ± 0.6

Table S16 The kinetic parameters of xylene isomerization on BEA35 at 493 K with the corresponding 95% confidence limit

Parameter	Linear - Equilibrium from Literature	Linear	Triangular - Equilibrium from Literature	Triangular
k_1×10^8 (m^3/kg_{cat} s)	20.8 ± 1.3	20.7 ± 1.3	20.6 ± 1.4	20.1 ± 1.5
k_2×10^8 (m^3/kg_{cat} s)	-	7.8 ± 1.4	-	7.8 ± 1.5
k_3×10^8 (m^3/kg_{cat} s)	9.9 ± 0.6	11.1 ± 1.5	9.7 ± 0.6	11.0 ± 1.5
k_4×10^8 (m^3/kg_{cat} s)	-	21.9 ± 1.4	-	21.7 ± 1.6
k_5×10^8 (m^3/kg_{cat} s)	-	-	-	1.1 ± 1.5
k_6×10^8 (m^3/kg_{cat} s)	-	-	0.5 ± 0.9	0.3 ± 1.5
Keq1	0.377 [a]	0.377	0.377 [a]	0.388
Keq2	2.268 [a]	1.973	2.268 [a]	1.973
Keq3	-	-	1.169 [a]	0.273

[a] k2=k1*Keq1; k4=k3*Keq2; k5=k6*Keq3. Linear with equilibrium and triangular with equilibrium mean the models combined with the thermodynamic equilibrium equations proposed by Gonçalves and Rodrigues[20].

Table S17 The kinetic parameters of xylene isomerization on BEA35 at 473 K with the corresponding 95% confidence limit

Parameter	Linear - Equilibrium from Literature	Linear	Triangular - Equilibrium from Literature	Triangular
k_1×10^8 (m^3/kg_{cat} s)	9.7 ± 0.9	10.0 ± 0.8	9.1 ± 1.0	9.5 ± 1.0
k_2×10^8 (m^3/kg_{cat} s)	-	3.0 ± 0.9	-	3.0 ± 1.0
k_3×10^8 (m^3/kg_{cat} s)	4.9 ± 0.4	4.5 ± 0.9	4.7 ± 0.4	4.4 ± 1.0
k_4×10^8 (m^3/kg_{cat} s)	-	11.5 ± 0.9	-	11.2 ± 1.1
k_5×10^8 (m^3/kg_{cat} s)	-	-	-	0.7 ± 1.0
k_6×10^8 (m^3/kg_{cat} s)	-	-	0.8 ± 0.7	0.8 ± 1.0
Keq1	0.370 [a]	0.300	0.370 [a]	0.316
Keq2	2.296 [a]	2.556	2.296 [a]	2.545
Keq3	-	-	1.176 [a]	1.143

[a] k2=k1*Keq1; k4=k3*Keq2; k5=k6*Keq3. Linear with equilibrium and triangular with equilibrium mean the models combined with the thermodynamic equilibrium equations proposed by Gonçalves and Rodrigues[20].

Table S18 The kinetic parameters of xylene isomerization on BEA35 at 453 K with the corresponding 95% confidence limit

Parameter	Linear - Equilibrium from Literature	Linear	Triangular - Equilibrium from Literature	Triangular
k_1×10^8 (m^3/kg_{cat} s)	2.6 ± 0.3	2.6 ± 0.3	2.4 ± 0.3	2.6 ± 0.3
k_2×10^8 (m^3/kg_{cat} s)	-	0.9 ± 0.3	-	0.9 ± 0.3
k_3×10^8 (m^3/kg_{cat} s)	1.59 ± 0.13	1.25 ± 0.31	1.52 ± 0.12	1.23 ± 0.30
k_4×10^8 (m^3/kg_{cat} s)	-	3.7 ± 0.3	-	3.7 ± 0.3
k_5×10^8 (m^3/kg_{cat} s)	-	-	-	0.10 ± 0.30
k_6×10^8 (m^3/kg_{cat} s)	-	-	0.2 ± 0.2	0.11 ± 0.31
Keq1 [b]	0.363 [a]	0.346	0.363 [a]	0.346
Keq2 [b]	2.325 [a]	2.960	2.325 [a]	3.008
Keq3 [b]	-	-	1.184 [a]	1.100

[a] k2=k1*Keq1; k4=k3*Keq2; k5=k6*Keq3. Linear with equilibrium and triangular with equilibrium mean the models combined with the thermodynamic equilibrium equations proposed by Gonçalves and Rodrigues[20].

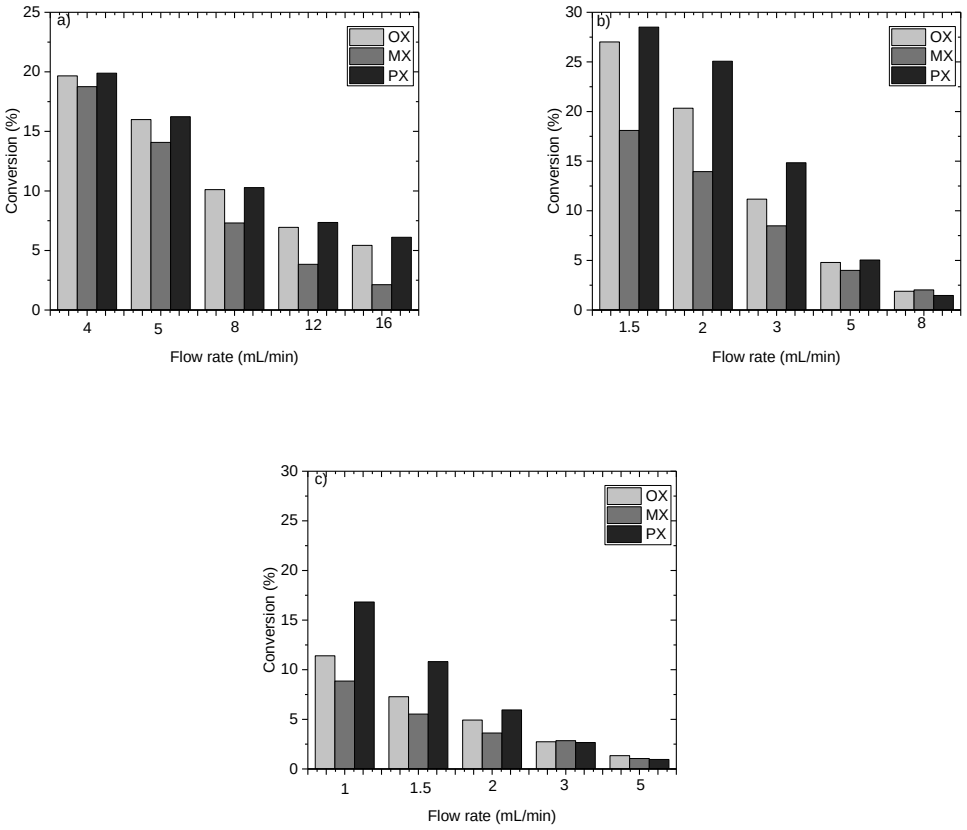

Figure S7 Comparison of the conversions of pure xylenes over BEA35 at different flow rates and temperature a) 493 K, b) 473 K, c) 453 K