Supporting information for:

Study on the Alkoxylation of Dihydromyrcene over Cation Exchange Resins

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SUPPORTING INFORMATION

Table S1 Properties of five different resin catalysts

Physical properties	Lewatit2620	Amberlyst 15	Amberlyst 35	CT151	CT275
Physical form	Beads	Beads	Beads	Beads	Beads
Ionic form as shipped	Hydrogen	Hydrogen	Hydrogen	Hydrogen	Hydrogen
Average size (mm)	0.5-0.62	0.3-0.425	0.3-1.18	0.425-1.2	0.425-1.2
Concentration of acid sites (eq/kg)	⩾5.2	⩾4.7	⩾5.0	⩾5.1	⩾5.0
BET surface area (m^2/g)	42	42	34	25	27
Average pore diameter (nm)	41	30	30	25	65
Temperature stability (K)	413	393	423	418	403

Table S2 Comparison of physical properties between unused and eight-time used Lewatit2620

Physical properties	Lewatit2620-new	Lewatit2620-old
Physical form	Beads	Beads
Ionic form as shipped	Hydrogen	Hydrogen
Average size (mm)	0.50-0.62	0.48-0.61
Concentration of acid sites (eq/kg)	⩾5.2	⩾5.3
BET surface area (m^2/g)	42	42
Average pore diameter (nm)	41	42
Temperature stability (K)	413	\

Table S3 Analysis results of the reaction (5h) at different initial molar ratios

Initial molar ratio	1:0.3	1:0.4	1:0.5	1:0.8	1:1	1:1.5	1:2
Conversion (%)	19.007	24.079	27.760	28.424	31.529	32.370	32.727
Yield (%)	9.854	15.589	19.648	21.588	24.277	24.964	25.313
Selectivity (%)	51.84	64.74	70.78	75.95	77.00	77.12	77.34

Table S4 Analysis results of the reaction (10h) at different temperatures

T/K	343.15	348.15	353.15	358.15	363.15
Conversion (%)	27.274	32.281	33.277	30.400	27.411
Yield (%)	21.069	24.914	25.603	22.611	19.488
Selectivity (%)	77.24	77.18	76.94	74.378	71.10

Table S5 Volume and area parameters of the functional groups

	Classification of functional groups			$V_k^{(i)}$	Volume parameter	Area parameter
	Group name	Main-group	Sub-group		R_k	Q_k
DHM	CH_3	1	1	3	0.9011	0.848
	CH_2	1	2	2	0.6744	0.540
	CH	1	3	1	0.4469	0.228
	CH_2=CH	2	5	1	1.3454	1.176
	CH=C	2	7	1	1.1173	0.988
MPO	CH_3	1	1	1	0.9011	0.848
	CH_2	1	2	2	0.6744	0.54
	CH	1	3	1	0.4469	0.228
	OH	5	15	2	1.000	1.200
DHMPO	CH_3	1	1	4	0.9011	0.848
	CH_2	1	2	4	0.6744	0.540
	CH	1	3	2	0.4469	0.228
	C	1	4	1	0.2195	0.000
	CH_2=CH	2	5	1	1.3454	1.176
	OH	5	15	1	1.000	1.200
	CH_2O	13	26	1	0.9183	0.780

Table S6 Interaction parameters of the functional groups (a_{mn}/K)

n \ m	1 CH_3	2 CH_2	3 CH	4 C	5 CH_2=CH	7 CH=C	15 OH	26 CH_2O
1 CH_3	0	0	0	0	86.02	86.02	986.5	251.5
2 CH_2	0	0	0	0	86.02	86.02	986.5	251.5
3 CH	0	0	0	0	86.02	86.02	986.5	251.5
4 C	0	0	0	0	86.02	86.02	986.5	251.5
5 CH_2=CH	-35.36	-35.36	-35.36	-35.36	0	0	524.1	214.5
7 CH=C	-35.36	-35.36	-35.36	-35.36	0	0	524.1	214.5
15 OH	156.4	156.4	156.4	156.4	457.0	457.0	0	28.06
26 CH_2O	83.36	83.36	83.36	83.36	26.51	26.51	237.7	0

Table S7 Calculated equilibrium constants for the reaction

T/K	K_x	K_γ	K_e
343.15	1.4567	0.1390	0.2025
348.15	1.0883	0.1384	0.1506
353.15	0.8361	0.1403	0.1173
358.15	0.6521	0.1422	0.09274
363.15	0.5432	0.1443	0.07836