

1. MS, FT-IR, ¹H NMR, ¹³C NMR Results of β-Caryophyllene alcohol

- (1) MS(m/z): 222.1, 207.0, 204.0, 189.0, 179.0, 161.1, 135.1, 111.1, 95.1, 81.0, 55.0
- (2) FTIR(cm⁻¹): 3387.0(s,OH), 2944.8(vs, cyclohexane),2926.0(vs, -(CH₂)_n-),2864.4(s,-CH₃), 1463.6(s, -(CH₂)_n-),1397.4、1376.2(m, isopropyl), 1355.6、1328.5(vw, -CH₃), 1206.5(m,C-O), 1154.3(w, isopropyl), 1096.4/1056.3/1015.8(w, cyclohexane), 956.6/925.6(v, cyclobutane).
- (3) ¹H NMR(500MHZ, DMSO, TMS,δppm): 3.915(1H,s,-OH, disappeared after the addition of D2O), 2.155~2.095(1H,q, -CH), 1.805~1.751(1H,m, -CH), 1.708~1.649(1H,q, -CH₂), 1.580~1.359(7H,m, -CH₂) 1.316~1.229(2H,m, -CH₂) ,1.190~1.131(1H,m, -CH₂), 1.046~1.009(1H,m,-CH₂), 1.001~0.956(7H,q,-CH₃, -CH₂),, 0.909~0.884(1H,d,-CH₂), 0.823(3H,s,-CH₃)
- (4) ¹³C NMR (500MHZ, CDCl₃, TMS, δppm) 70.6(C), 44.4(CH), 34.0(CH₂), 34.3(C), 39.1(CH), 21.5(CH₂), 37.1(CH₂), 34.6(C), 36.2(CH₂), 20.1(CH₂), 38.2(CH₂), 48.4(CH₂), 20.4(CH₃), 30.1(CH₃), 32.8(CH₃)

2. Physical properties of the two cation exchange resins

Table 1 Physical properties of the two cation exchange resins

Physical properties	NKC-9	D-72
Physical form	beads	beads
Resin structure	Styrene-DVB	Styrene-DVB
Functional group	-SO ₃ ⁻	-SO ₃ ⁻
Ionic form as shipped	Hydrogen	Hydrogen
Average size (mm)	0.400-1.250	0.400-1.250
Concentration of acid sites	4.7mol/kg	4.2mol/kg
Average pore diameter(nm)	12	20
Temperature stability (K)	473	473

3. Conditions of the direct hydration of β -Caryophyllene

Table 2 Conditions of the direct hydration of β -Caryophyllene

Temperature (K)	n(β -Caryophyllene): n (H ₂ O)	Resins' particle size (mm)	Catalyst loading (w/w %)	Conversion of β -Caryophyllene (%)	Selectivity of β -Caryophyllene alcohol (%)	composition of major products ^a (%)		
						β -Caryophyllene alcohol	Clovene	Dihydroclovene-9 β -ol
333.15	1:1	<0.6	20	8.03	35.93	3.14	1.07	1.15
338.15	1:1	<0.6	20	10.58	34.31	3.95	1.38	1.38
343.15	1:1	<0.6	20	18.10	32.14	6.33	2.29	2.01
348.15	1:1	<0.6	20	22.48	30.13	7.37	2.74	2.35
353.15	1:1	<0.6	20	50.16	29.90	16.32	6.17	5.74
358.15	1:1	<0.6	20	53.78	29.71	17.39	6.57	5.83
363.15	1:1	<0.6	20	83.89	29.15	26.43	8.78	6.42
363.15	1:1	<0.6	6	1.54	64.25	0.84	0.24	0.38
363.15	1:1	<0.6	10	3.58	40.56	1.58	0.37	0.83
363.15	1:1	<0.6	13	12.05	32.11	4.21	1.49	1.66
363.15	1:1	<0.6	17	38.78	29.38	12.40	4.57	4.26
363.15	1:1	<0.6	23	89.23	29.69	28.83	9.03	9.32
363.15	1:1	<0.6	27	91.11	29.02	28.77	9.36	9.24
363.15	1:0.4	<0.6	20	85.67	25.73	24.97	13.47	5.57
363.15	1:0.6	<0.6	20	88.39	26.09	26.12	11.91	5.83
363.15	1:0.8	<0.6	20	87.76	26.40	26.24	10.12	6.57
363.15	1:1.5	<0.6	20	23.67	30.94	7.97	2.91	2.57
363.15	1:2	<0.6	20	4.87	38.87	2.06	0.66	1.05
363.15	1:2.5	<0.6	20	1.45	62.11	0.98	0.25	0.43
363.15	1:3	<0.6	20	0.74	69.54	0.56	0.16	0.34
363.15	1:1	0.9-1.25	20	65.17	30.09	21.34	7.49	6.92
363.15	1:1	0.6-0.9	20	82.96	28.61	25.83	8.53	6.17
363.15	1:1	0.4-0.6	20	83.94	29.25	26.72	8.88	6.54
363.15	1:1	<0.4	20	84.09	29.35	26.86	9.01	6.73

catalyst: NKC-9; reaction time: 30 min; ^a the major products in the reaction system and the other impurities are not listed in the Table.

4. The value of k_c , k_1 , k_2 and k_3 at different temperatures are presented

Table 3 The values of k at different temperatures

T(K)	1/T(1/K)	$k_c(\text{mol} \cdot \text{Kg}^{-1} \cdot \text{h}^{-1})$	$k_1(\text{mol} \cdot \text{Kg}^{-1} \cdot \text{h}^{-1})$	$k_2(\text{mol} \cdot \text{Kg}^{-1} \cdot \text{h}^{-1})$	$k_3(\text{mol} \cdot \text{Kg}^{-1} \cdot \text{h}^{-1})$
333.15	0.00300	0.00084	7.027×10^{-5}	2.062×10^{-5}	1.167×10^{-4}
338.15	0.00296	0.00102	9.898×10^{-5}	3.137×10^{-5}	1.415×10^{-4}
343.15	0.00291	0.00219	2.390×10^{-4}	7.365×10^{-5}	2.953×10^{-4}
348.15	0.00287	0.00324	3.289×10^{-4}	1.104×10^{-4}	4.278×10^{-4}
353.15	0.00283	0.00813	9.636×10^{-4}	3.492×10^{-4}	1.042×10^{-3}
358.15	0.00279	0.01011	1.298×10^{-3}	4.225×10^{-4}	1.287×10^{-3}
363.15	0.00275	0.01446	2.002×10^{-3}	4.676×10^{-5}	1.843×10^{-3}

5. The value of E_{ac} , E_{an} , k_{0c} , k_{0n}

Table 4 Kinetic parameters of the pseudo-homogeneous model

E_{ac} (KJ/mol)	E_{a1} (KJ/mol)	E_{a2} (KJ/mol)	E_{a3} (KJ/mol)	k_{0c} (mol·g/h)	k_{01} (mol·g/h)	k_{02} (mol·g/h)	k_{03} (mol·g/h)
100.8	124.2	113.2	95.20	4.87×10^{12}	1.63×10^{14}	1.15×10^{13}	1.53×10^{11}