Supporting information for

Mechanism analysis for separation of cyclohexane and tert-butanol system via ionic liquids as extractant and process optimization

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The SI includes of 7 pages, 6 Tables (from Table S1 to Table S6)

Table S1. Sources, CAS number, molar mass, purification, water contents by mass, w_w, and analysis method of the chemicals used in this work.
[a]Analysis by supplied

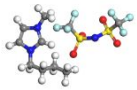
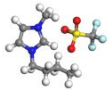
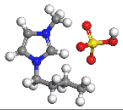
Chemical	Source	CAS number	Structure	Molar mass/(g·mol^{-1})	Mass purity stated by supplier	w_w /10^{-6}	Analysis method
cyclohexane	Tianjin Kermel Chemical Reagent Co., Ltd.	110-82-7		32.04	0.995[a]		GC
TBA	Tianjin Kermel Chemical Reagent Co., Ltd.	75-65-0		74.12	0.995[a]		GC
[BMIM][NTF$_2$]	Lanzhou Institute of Chemical Physics, Chinese Academy of Sciences.	174899-83-3		419.37	0.980[a]	<500[a]	
[BMIM][OTF]	Lanzhou Institute of Chemical Physics, Chinese Academy of Sciences.	174899-66-2		288.29	0.980[a]	<500[a]	
[BMIM][HSO$_4$]	Lanzhou Institute of Chemical Physics, Chinese Academy of Sciences.	262297-13-2		236.29	0.980[a]	<500[a]	

Table S2. Interaction energies between ILs and TBA.

System	E（hartree[a]）	E_{BSSE}	ΔE ($kJ \cdot mol^{-1}$)
TBA	-233.736502		
[BMIM]NTF_2	-2251.239308		
[BMIM]OTF	-1375.750388		
[BMIM]HSO_4	-1123.359296		
[BMIM]NTF_2 + TBA	-2484.972248	-0.000531	-65.357617
[BMIM]OTF + TBA	-1619.004155	-0.000574	-32.832415
[BMIM]HSO_4 + TBA	-1357.097050	-0.000628	-18.464295

[a]1 hartree = 27.211 eV = 627.509 $kcal \cdot mol^{-1}$ = 2625.753 $kJ \cdot mol$

Table S3. Experimental LLE data on mole fraction *x*, distribution coefficient *D* and separation factor *S* for ternary systems of cyclohexane (1) + TBA (2) + ILs (3) at T = 298.15 K and P= 101.325 kPa [a].

Upper phase		Lower phase		*D*	*S*
x_1	x_2	x_1	x_2		
cyclohexane (1) + TBA (2) + [BMIM][NTF_2] (3) 298.15 K					
0.9081	0.0919	0.1718	0.2065	2.2470	11.8772
0.8554	0.1446	0.1758	0.2717	1.8790	9.1426
0.8171	0.1826	0.1779	0.2769	1.5164	6.9650
0.7100	0.2897	0.1876	0.3525	1.2168	4.6051
0.5298	0.4697	0.1932	0.4535	0.9655	2.6477
0.4274	0.5710	0.1955	0.5308	0.9296	2.0323
cyclohexane (1) + TBA (2) + [BMIM][OTF] (3) 298.15 K					
0.9369	0.0626	0.0790	0.1843	2.9441	34.9154
0.8610	0.1381	0.0868	0.2291	1.6589	16.4556
0.7059	0.2927	0.1030	0.3269	1.1168	7.6542
0.6014	0.3946	0.1159	0.4101	1.0393	5.3928
0.5239	0.4719	0.1244	0.4581	0.9708	4.0883
0.4576	0.5380	0.1249	0.4922	0.9149	3.3518
0.3745	0.6209	0.1329	0.5386	0.8675	2.4444
cyclohexane (1) + TBA (2) + [BMIM][HSO_4] (3) 298.15 K					
0.8208	0.1788	0.0330	0.1417	0.7925	19.7118
0.7179	0.2809	0.0335	0.1985	0.7067	15.1436
0.6129	0.3858	0.0418	0.2496	0.6470	9.4863
0.4838	0.5144	0.0520	0.3523	0.6849	6.3720
0.3825	0.6147	0.0828	0.4877	0.7934	3.6651
0.3306	0.6650	0.0833	0.5267	0.7920	3.1434

[a] Standard uncertainties *u* are $u(x_i) = 0.0119$, $u(T) = 0.05$ K, $u(p) = 1.5$ kPa, $u(m_i) = 0.0006$g

$$u(m) = \frac{MAE}{\sqrt{3}}$$

Table S4. Binary interaction parameters Δg_{ij}, Δg_{ji} and nonrandomness factor α for NRTL model, binary interaction parameters Δu_{ij} and Δu_{ji} for UNIQUAC model and root-mean-square deviations, obtained from the experimental LLE data of studied ternary systems by NRTL and UNIQUAC models at T = 298.15 K and P = 101.325 kPa [a].

i-j	Δg_{ij} (kJ·mol^{-1})	Δg_{ji} (kJ·mol^{-1})	*rmsd*	α
	NRTL parameters			
	cyclohexane (1) + TBA (2) + [BMIM][NTF$_2$] (3) 298.15 K			
1-2	4.5087	2.1454	0.0156	0.30
1-3	9.9455	3.3221		
2-3	5.3949	2.2364		
	cyclohexane (1) + TBA (2) + [BMIM][OTF] (3) 298.15 K			
1-2	1.4888	0.0795	0.0184	0.30
1-3	16.1107	9.2316		
2-3	12.0814	-3.0355		
	cyclohexane (1) + TBA (2) + [BMIM][HSO$_4$] (3) 298.15 K			
1-2	4.0405	5.8748	0.0179	0.30
1-3	29.4979	12.171		
2-3	9.1468	18.0458		
i-j	Δu_{ij} (kJ·mol^{-1})	Δu_{ji} (kJ·mol^{-1})	*rmsd*	
	UNIQUAC parameters			
	cyclohexane (1) + TBA (2) + [BMIM][NTF$_2$] (3) 298.15 K			
1-2	1.0557	0.0968	0.0137	
1-3	3.4245	-0.185		
2-3	1.012	-0.081		
	cyclohexane (1) + TBA (2) + [BMIM][OTF] (3) 298.15 K			
1-2	-0.1912	1.7086	0.0187	
1-3	1.0867	0.9867		
2-3	2.4941	-1.6517		
	cyclohexane (1) + TBA (2) + [BMIM][HSO$_4$] (3) 298.15 K			
1-2	7.688	-2.6726	0.0184	
1-3	6.3258	1.3363		
2-3	4.9488	-1.9926		

[a] Standard uncertainties u were $u(T)$ = 0.05 K

Table S5. Volume (r_i) and surface area (q_i, q_i') of UNIQUAC equation.

Component	r_i	q_i	q_i'
cyclohexane[a]	4.0464	3.2400	3.2400
TBA[b]	3.4500	3.0500	3.0500
[BMIM][NTF_2][c]	11.9640	9.7530	9.7530
[BMIM][OTF][d]	12.4600	7.5180	7.5180
[BMIM][HSO_4][e]	8.2203	6.628	6.628

[a]From reference [33]
[b]From reference [34]
[c]From reference [35]
[d]From reference [36]
[e]From reference [37]

Table S6. Basis of economics and equipment sizing.

Items	Formulas and values
column vessel	column diameter (D) = Aspen tray sizing
	column length (L) = N_T trays with 2 ft spacing plus 20% extra length
	investment cost=$17640D^{1.066}L^{0.802}$ where D and L are in m
Reboilers	heat-transfer coefficient (K_R)=0.568kW/(K·m^2) differential temperature (ΔT_R)=steam temperature – base temperature
	$A_R = \frac{Q_R}{K_R \times \Delta T_R}$
	capital cost=$7296\ (A_R)^{0.65}$
Extraction column	length:NT trays with 4 ft HETP plus additional 3 ft at the top and 3 ft at the bottom capital cost = $17640(D)^{1.066}\ (L)^{0.802}$ (D and L are in meters)
Utilities cost	low pressure steam (160 ℃) = \$7.78/GJ
	medium pressure steam (184 ℃) = \$8.22/GJ
	high pressure steam (254 ℃) = \$9.88/GJ
	cooling water = \$0.354/GJ
	Electricity = \$0.094/kW·h
TAC = (investment cost/ plant life time) + operating cost plant life time = 3 years	