

# Extraction mechanism of lithium from the alkali solution with diketonate-based ionic liquid extractants

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**Table S1. Purities of ILs and their separation factor ( $\beta_{\text{Li}/\text{Na}}$ ) by IL+TRPO with different initial pH of aqueous solution at: IL = 0.5 mol·L<sup>-1</sup>, A/O = 1:1, and T=298.15 K.**

ILs	Purity (%)	Separation factors ( $\beta_{\text{Li}/\text{Na}}$ )			
		pH=1.26	pH=6.56	pH=10.17	pH=13.1
[A336]BTA	95.12	15.07	47.54	125.09	275.95
[A336]TTA	97.65	35.37	76.45	160.53	284.04
[A336]TFBA	96.83	7.90	30.86	97.90	212.38
[A336]TTBA	97.26	3.84	16.48	60.37	190.80

**Table S2. Standard-state chemical potentials and enthalpies of formation of species.**

Species	$-\Delta\mu_i^0 / (\text{kJ}\cdot\text{mol}^{-1})$	$-\Delta_f H_i^0 / (\text{kJ}\cdot\text{mol}^{-1})$	Ref.
Li <sup>+</sup> (aq)	293.80	278.50	[37,38]
CO <sub>3</sub> <sup>2-</sup> (aq)	528.10	676.20	[37,38]
Li <sub>2</sub> CO <sub>3</sub> (s)	1133.00	1216.00	[37,38]

**Table S3. Effect of HCl concentration on stripping of Li loaded in organic phase at: A/O = 1:1, T = 298.15 K.**

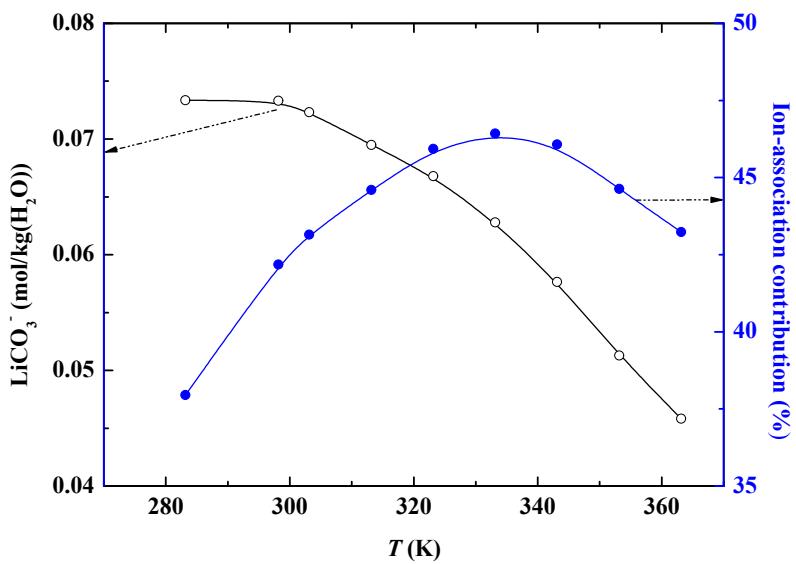
HCl concentration (mol·L <sup>-1</sup> )	Stripping percentage (%)	
	Li	Na
0.00	24.62	43.17
0.10	49.03	61.46
0.20	73.64	62.20
0.30	88.21	62.44
0.40	93.95	63.41
0.50	95.59	66.10

**Table S4. Thermodynamic parameters of extracting Li by [A336]TTA.**

Temperature (K)	$\Delta H$ (kJ/mol)	$\Delta G$ (kJ/mol)
298.15		-7.97
303.15		-6.83
313.15	-10.63	-6.55
323.15		-6.52
333.15		-6.38
343.15		-6.19

**Table S5. Compositions of the mother solution used in section 3.6.**

Components	Content/(g·L <sup>-1</sup> )
Li	1.41
Ca	3.29×10 <sup>-3</sup>
Mg	1.94×10 <sup>-7</sup>
Na	63.23
Cl	73.79
SO <sub>4</sub>	7.83
CO <sub>3</sub>	16.76
B <sub>2</sub> O <sub>3</sub>	0.00



**Figure S1.** Relationships of  $\text{LiCO}_3^-$  concentration and ion-association contribution with temperatures.