

Selective extraction of lithium isotopes using B15C5 derivatives modified with different groups: Experimental and theoretical perspectives

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Table S1. Analytical values of total organic carbon for B15C5 derivatives

CE	c(TC) (mg L ⁻¹)	Nc	Mr (g mol ⁻¹)
4-tBu-B15C5	0.3348	18	324.41
4-NO ₂ -B15C5	0.4474	14	268.31
4-Br-B15C5	0.3504	14	347.20
B15C5	0.4943	14	313.31
4-Ac-B15C5	1.3500	16	310.35
4-NH ₂ -B15C5	1.4700	14	283.32
4-CH ₂ OH-B15C5	4.1300	15	298.33

Table S2. Energies as well as ionisation and affinity energies of different crown ether molecules in the N, N+1 and N-1 states (Hartree)

CE	E _N	E _{N+1}	E _{N-1}	EA	IP
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4-tBu-B15C5	-1078.7999	-1078.7507	-1078.5405	-0.0493	0.2594
4-Br-B15C5	-3495.1640	-3495.1282	-3494.8933	-0.0358	0.2707
4-Ac-B15C5	-1074.2163	-1074.2144	-1073.9404	-0.0019	0.2759
4-CH ₂ OH-B15C5	-1036.0965	-1036.0587	-1035.8367	-0.0378	0.2597
4-NH ₂ -B15C5	-976.9231	-976.8702	-976.6853	-0.0529	0.2378
4-NO ₂ -B15C5	-1126.0865	-1126.1140	-1125.7954	0.0275	0.2911
B15C5	-921.5660	-921.5124	-921.2991	-0.0536	0.2669

Table S3. Energies of B15C5 derivatives under SMD solvents of cyclohexanone or water

CE	E _{CYC} (Hartree)	E _{Wat} (Hartree)
4-tBu-B15C5	-1078.8254	-1078.8245
4-NO ₂ -B15C5	-1126.1134	-1126.1132
4-Br-B15C5	-3495.1897	-3495.1901
B15C5	-921.5902	-921.5920
4-Ac-B15C5	-1074.2452	-1074.2468
4-NH ₂ -B15C5	-976.9520	-976.9561
4-CH ₂ OH-B15C5	-1036.1252	-1036.1306

$$U(\%) = \frac{C_{Org}}{C_{CE}} \times 100\% \quad (\text{Eq. S1.})$$

Where U represents the utilization of B15C5 derivatives; C_{Org} represents the Li⁺ concentration of the organic phase; C_{CE} represents the concentration of the crown ether.

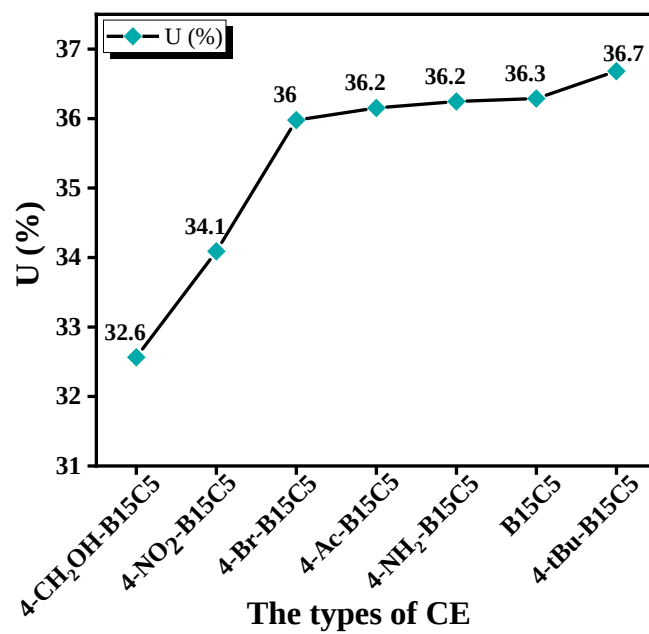


Figure S1. The utilization of B15C5 derivatives

($c_{\text{CE}}=0.5 \text{ mol L}^{-1}$, $c_{\text{Ca(NTf}_2)_2}=0.1 \text{ mol L}^{-1}$, $c_{\text{LiCl}}=1 \text{ mol L}^{-1}$, $V_{\text{Org}}: V_{\text{Aq}} = 1:1$, $c_{\text{HCl}}=1 \text{ mol L}^{-1}$, $V_{\text{HCl}}: V_{\text{Org}} = 3:1$)