Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

A Comparative Study on Coordination of Diglycolamide Isomers with Nd(III): Extraction, Third phase, Structure, and Computational Studies

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Characterization data of L^{II}: ^{1}H-NMR (400 MHz, $CDCl_3$, δ): 4.37 (s, 2H), 4.34 (s, 2H), 3.33 (t, 2H), 3.21 (t, 2H), 3.06 (s, 3H), 3.00 (s, 3H), 1.31 (m, 24H), 0.92(dt, 6H); ^{13}C-NMR (100 MHz, $CDCl_3$, δ): 168.97, 168.55, 168.43, 46.97, 45.84, 36.35, 35.47, 31.86, 31.80, 29.43, 29.01, 22.70, 19.16, 14.16. IR ν_{max} (cm^{-1}): 2926 (s, CH, aliphatic), 2856 (s, CH, aliphatic), 1649 (s, C=O), 1464 (s, C-N), 1116 (m, C-O).

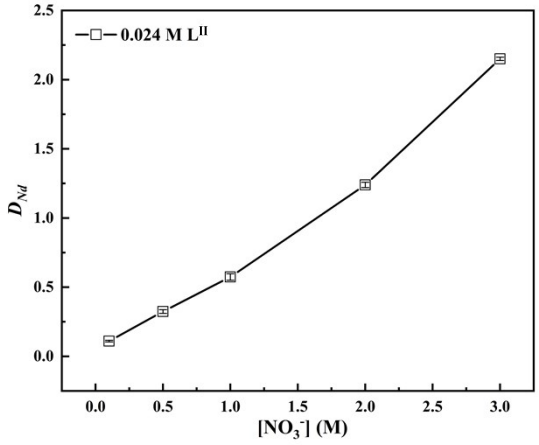

Fig. S1 Effect of NO_3^- on the extraction of Nd^{3+} by L^{II} in 40/60 (V/V)% n-octanol/kerosene([H^+]=0.1M, O:A = 1:1, $[Nd^{3+}]_{init}$ = 3 mM)

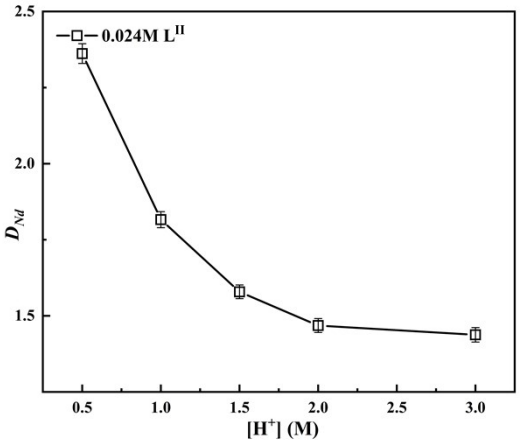

Fig. S2 Effect of H^+ on the extraction of Nd^{3+} by L^{II} in 40/60 (V/V)% n-octanol/kerosene([NO_3^-]=3 M, O:A = 1:1, $[Nd^{3+}]_{init}$ = 3 mM)

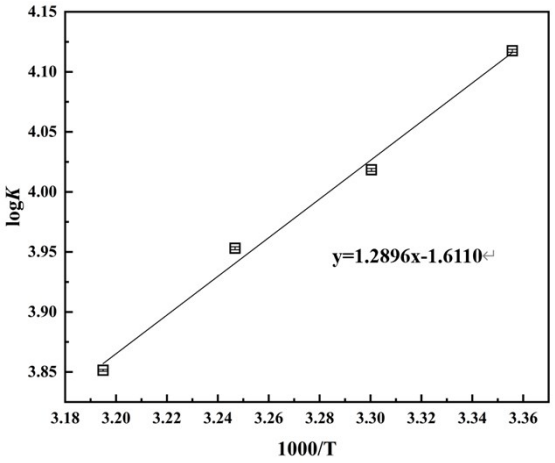

Fig. S3 Effect of temperature on the *K* ($[HNO_3]$=3 M, O:A = 1:1, $[Nd^{3+}]_{init}$ = 3 mM)

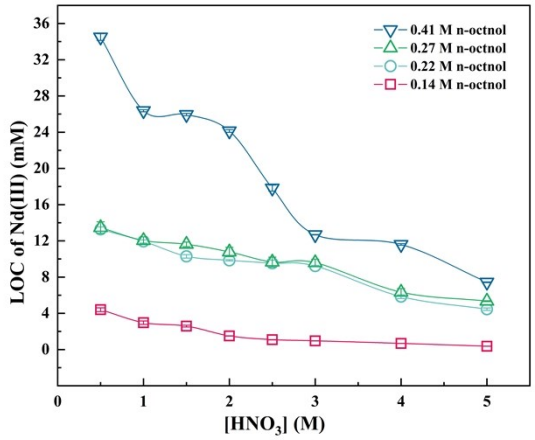

Fig. S4 LOC of Nd(III) as a function of aqueous phase acidity at different n-octanol concentrations, $[L^{II}]$=0.12 M

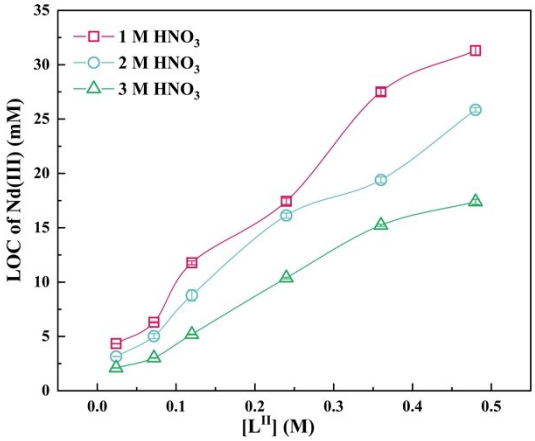

Fig. S5 LOC of Nd(III) as a function of L^{II} concentration, [n-octanol]=0.27 M

Table S1 Effect of nitric acid concentration on the stripping efficiencies of Nd(III) , O:A= 1:1

$[HNO_3]$ (M)	0.5	0.1	0.05	0.01	0.005	0.001	0
Stripping Efficiency	69.70%	70.77%	71.67%	76.91%	78.33%	81.10%	78.16%

Table S2 Mulliken charges (Q) on the O_{ether} and O_{amide} of the Four Ligands

Ligands	Q-O_{ether}	Q-O_{amid1}	Q-O_{amid2}
L^{I}	0.35	0.38	0.38
L^{II}	0.35	0.39	0.37

Table S3 Average Nd–O bond lengths (Å) of the $[NdL^{I}_3]^{3+}$ and $[NdL^{II}_3]^{3+}$ complexes at the B3LYB/6-311G(d)/RECP level of theory in the gas phase

□	L^{I}			L^{II}		
□	O_{ether}-Nd	O_{amide1}-Nd	O_{amide2}-Nd	O_{ether}-Nd	O_{amide1}-Nd	O_{amide2}-Nd
Bond Length	2.655	2.445	2.445	2.655	2.456	2.431
	2.650	2.446	2.445	2.648	2.456	2.432
	2.655	2.446	2.446	2.661	2.458	2.438