# Supporting Information

# Study on the extraction of lanthanides by isomeric diglycolamide extractants: An experimental and theoretical study

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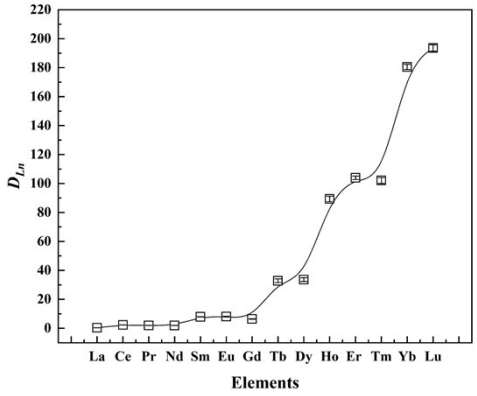


**Fig. S1** The distribution ratios of Ln(III) with different atomic numbers

O:A =1:1, $[HNO_3]$= 0.001 M, $[Ln^{3+}]_{init}$=3 mM

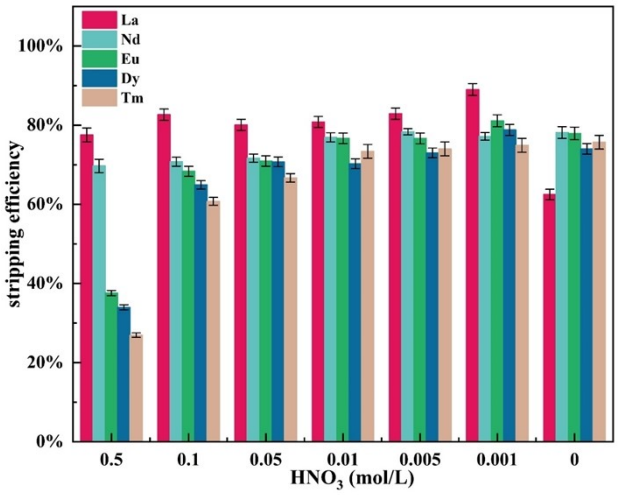


**Fig. S2** Effect of nitric acid concentration on the stripping efficiencies

of La(III), Nd(III), Eu(III), Dy(III), Tm(III), O:A= 1:1

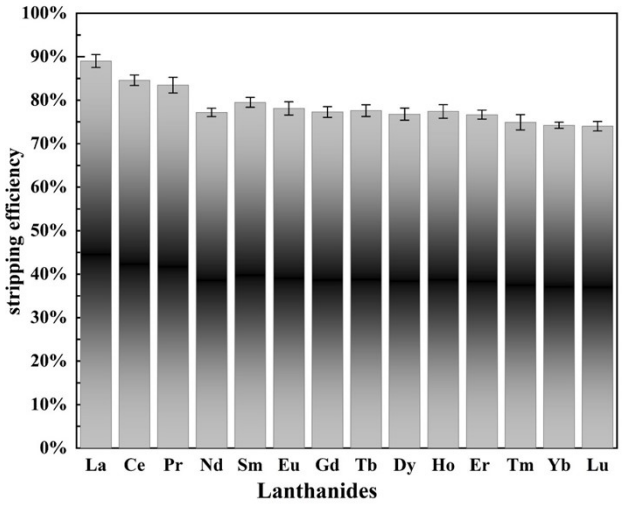


**Fig. S3** Effect of lanthanides atom number on the stripping efficiency by nitric acid, O:A =1:1, [$HNO_3$]= 0.001 M

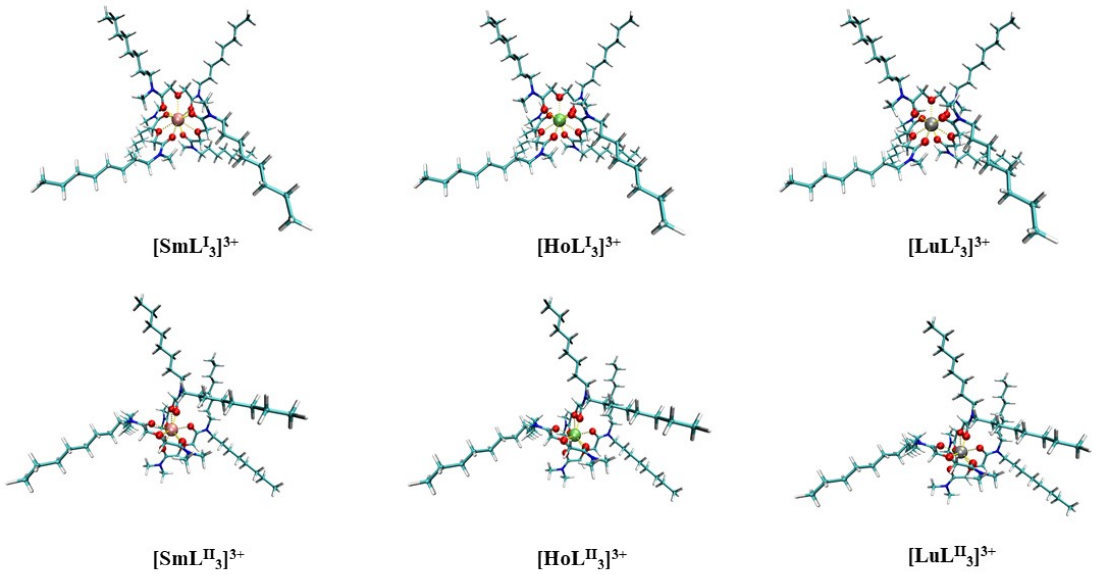


**Fig. S4** The optimized complex structure of Ln-$L^{I}$/$L^{II}$, pink-Sm, green-Ho, gray-Lu, cyan-carbon, white-hydrogen, red-oxygen, blue-nitrogen

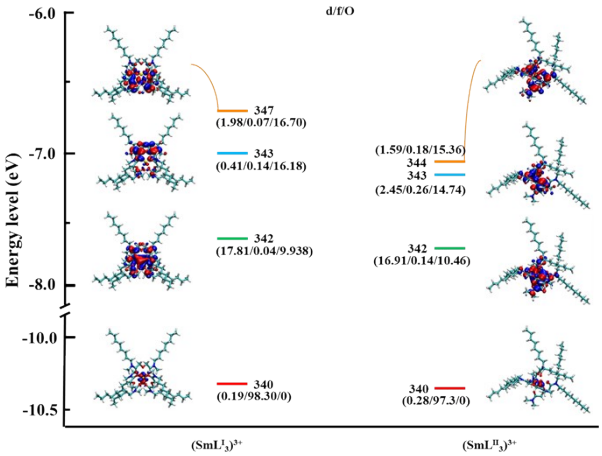


**Fig. S5** The energy levels (eV) of the α-spin valence MOs and the corresponding diagrams in the [SmL3]3+ complexes (isosurface value: 0.02 au).

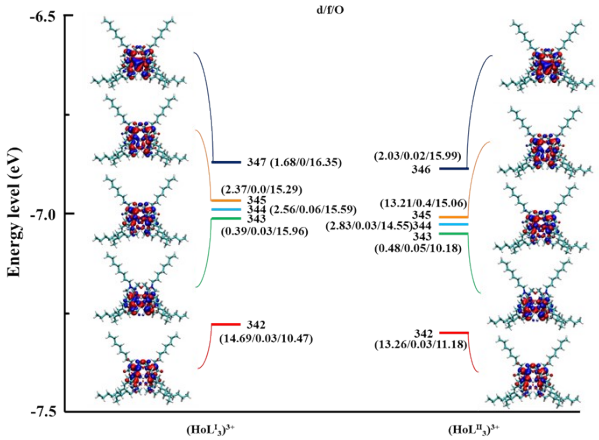


**Fig. S6** The energy levels (eV) of the α-spin valence MOs and the corresponding diagrams in the $[HoL_3]^{3+}$ complexes (isosurface value: 0.02 au).

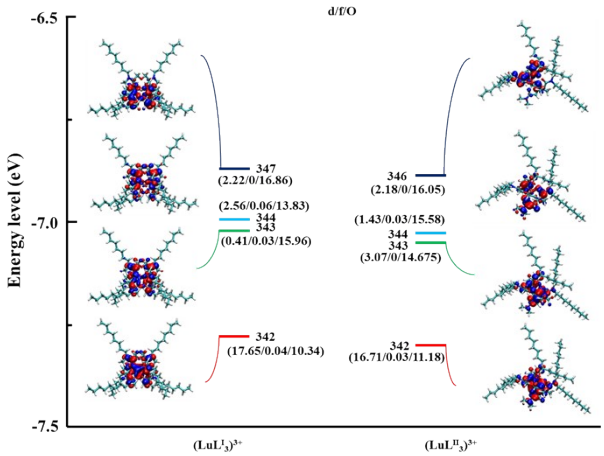


**Fig. S7** The energy levels (eV) of the α-spin valence MOs and the corresponding diagrams in the $[LuL_3]^{3+}$ complexes (isosurface value: 0.02 au).

**Table S1** The calculated average MBOs of the M-L complexes (M=La, Sm, Eu, Ho, Lu)

| Species | $M\text{-}L^{I}$ | | | $M\text{-}L^{II}$ | | |
|---|---|---|---|---|---|---|
| | $M\text{-}O_{ether}$ | $M\text{-}O_{amide1}$ | $M\text{-}O_{amide2}$ | $M\text{-}O_{ether}$ | $M\text{-}O_{amide1}$ | $M\text{-}O_{amide2}$ |
| La | 0.113 | 0.325 | 0.325 | 0.112 | 0.312 | 0.335 |
| | 0.2543 | | | 0.2530 | | |
| Sm | 0.105 | 0.318 | 0.318 | 0.105 | 0.314 | 0.320 |
| | 0.2472 | | | 0.2466 | | |
| Eu | 0.103 | 0.315 | 0.315 | 0.102 | 0.327 | 0.299 |
| | 0.2442 | | | 0.2430 | | |
| Ho | 0.094 | 0.321 | 0.321 | 0.093 | 0.307 | 0.331 |
| | 0.2457 | | | 0.2435 | | |
| Lu | 0.101 | 0.316 | 0.316 | 0.100 | 0.303 | 0.322 |
| | 0.2443 | | | 0.2418 | | |