Understanding Am³⁺/Cm³⁺ separation with H₄TPAEN and its hydrophilic derivatives:　A quantum chemical study

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Electronic Supplementary Information

Table S1 Changes of Gibbs free energies (kcal/mol) for back extraction Am³⁺ and Cm³⁺ complexes with three TPAEN type ligands from *n*-dodecane to aqueous solution at the M06-L/6-311+G(2df,p)/RECP level of theory.

Back reactions	$\Delta G_{\text{back-ext.}}$	$\Delta\Delta G_{\text{back-ext.}}$[b]
An(TMDGA)$_3$(NO$_3$)$_{3,\text{org}}$+H$_2$L$_a^{2-}$$_{\text{aq}}$→[AnL$_a$]$^-$$_{\text{aq}}$+3NO$_3^-$$_{\text{aq}}$+2H$^+$$_{\text{aq}}$+3TMDGA$_{\text{org}}$	-37.864/-41.065	-3.201
An(TMDGA)$_3$(NO$_3$)$_{3,\text{org}}$+H$_2$L$_b^{2-}$$_{\text{aq}}$→[AnL$_b$]$^-$$_{\text{aq}}$+3NO$_3^-$$_{\text{aq}}$+2H$^+$$_{\text{aq}}$+3TMDGA$_{\text{org}}$	-28.452/-30.522	-2.071
An(TMDGA)$_3$(NO$_3$)$_{3,\text{org}}$+H$_2$L$_c^{2-}$$_{\text{aq}}$→[AnL$_c$]$^-$$_{\text{aq}}$+3NO$_3^-$$_{\text{aq}}$+2H$^+$$_{\text{aq}}$+3TMDGA$_{\text{org}}$	-32.907/-33.095	-0.188
An(TMDGA)$_3$(NO$_3$)$_{3,\text{org}}$+H$_3$L$_a^-$$_{\text{aq}}$→[AnL$_a$]$^-$$_{\text{aq}}$+3NO$_3^-$$_{\text{aq}}$+3H$^+$$_{\text{aq}}$+3TMDGA$_{\text{org}}$	-23.055/-26.255	-3.201
An(TMDGA)$_3$(NO$_3$)$_{3,\text{org}}$+H$_3$L$_b^-$$_{\text{aq}}$→[AnL$_b$]$^-$$_{\text{aq}}$+3NO$_3^-$$_{\text{aq}}$+3H$^+$$_{\text{aq}}$+3TMDGA$_{\text{org}}$	-23.620/-25.691	-2.071
An(TMDGA)$_3$(NO$_3$)$_{3,\text{org}}$+H$_3$L$_c^-$$_{\text{aq}}$→[AnL$_c$]$^-$$_{\text{aq}}$+3NO$_3^-$$_{\text{aq}}$+3H$^+$$_{\text{aq}}$+3TMDGA$_{\text{org}}$	-24.561/-24.749	-0.188
An(TMDGA)$_3$(NO$_3$)$_{3,\text{org}}$+H$_4$L$_{a,\text{aq}}$→[AnL$_a$]$^-$$_{\text{aq}}$+3NO$_3^-$$_{\text{aq}}$+4H$^+$$_{\text{aq}}$+3TMDGA$_{\text{org}}$	-6.991/-10.191	-3.201
An(TMDGA)$_3$(NO$_3$)$_{3,\text{org}}$+H$_4$L$_{b,\text{aq}}$→[AnL$_b$]$^-$$_{\text{aq}}$+3NO$_3^-$$_{\text{aq}}$+4H$^+$$_{\text{aq}}$+3TMDGA$_{\text{org}}$	-10.254/-12.325	-2.071
An(TMDGA)$_3$(NO$_3$)$_{3,\text{org}}$+H$_4$L$_{c,\text{aq}}$→[AnL$_c$]$^-$$_{\text{aq}}$+3NO$_3^-$$_{\text{aq}}$+4H$^+$$_{\text{aq}}$+3TMDGA$_{\text{org}}$	-10.128/-10.317	-0.188

[a]…/… represents results with An=Cm and Am, respectively.

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