

Supplemental Material

Characterization of the ALSEP Process at Equilibrium: Speciation and Stoichiometry of the Extracted Complex

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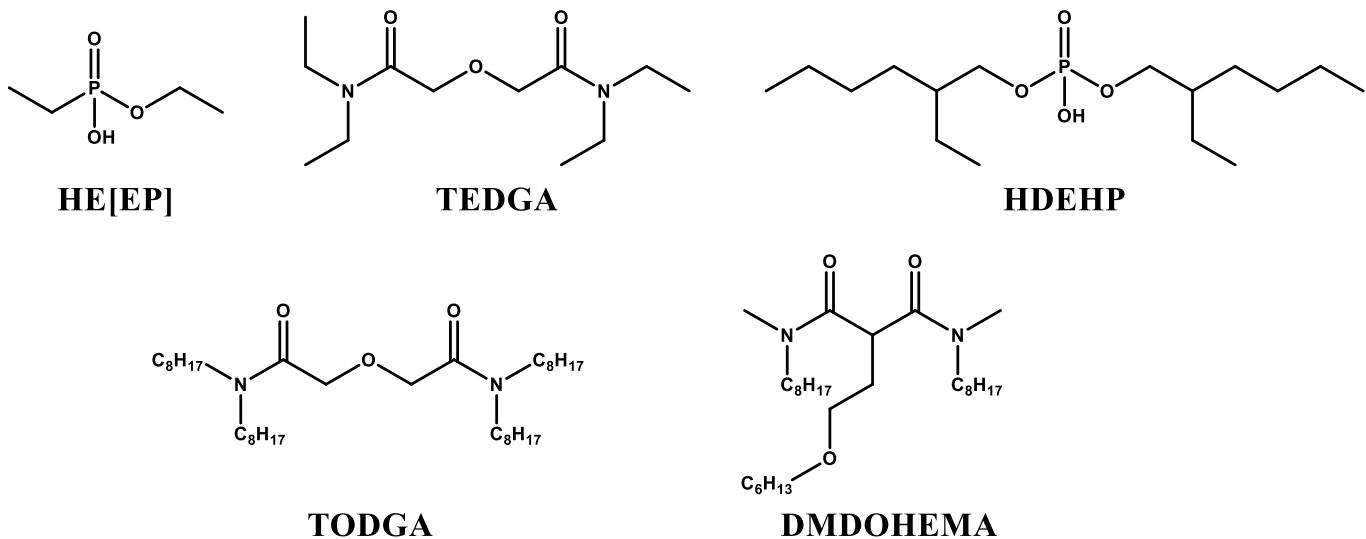


Figure S1. Chemical structures for ethyl phosphonic acid monoethyl ester (HE[EP]) and *N,N,N',N'*-tetraethyldiglycolamide (TEDGA), the extractants with truncated alkyl chains used in the computational analysis, as well as bis(2-ethylhexyl)phosphoric acid (HDEHP), *N,N,N',N'*-tetraoctyldiglycolamide (TODGA), and *N,N'-dimethyl-N,N'-dioctylhexylethoxymalonamide* (DMDOHEMA), extractants used in liquid-liquid extraction processes related to the ALSEP process.

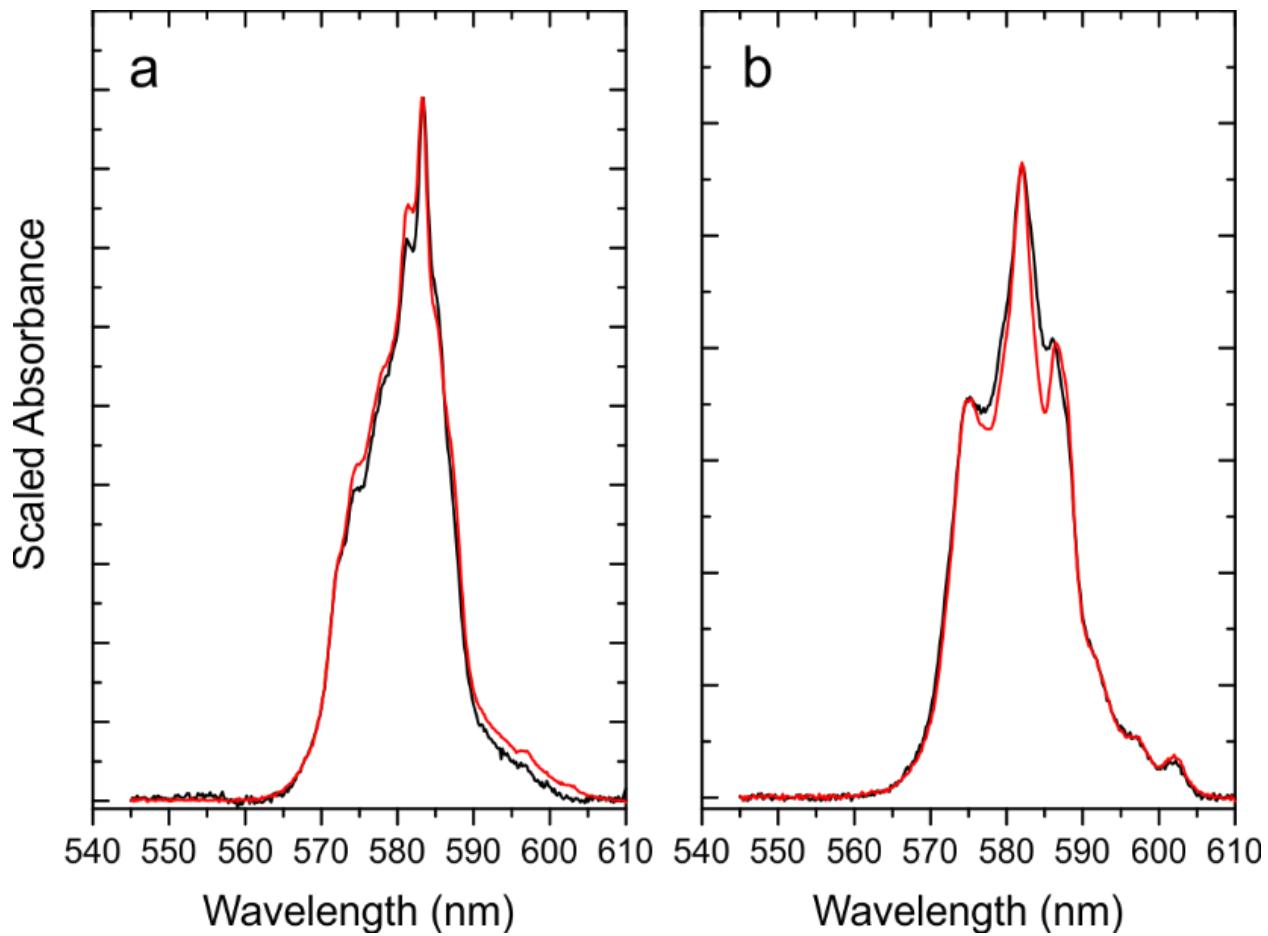


Figure S2. Comparison of the spectra of the Nd complexes created by extraction into specific organic phases with the spectra of the two Nd complexes present in the HEH[EHP] dependence experiments. (a) (—) Spectrum of $\text{Nd}(\text{NO}_3)_3(\text{TEHDGA})_3$ extracted from 2 M HNO_3 into 0.2 M TEHDGA/*n*-dodecane at 25 °C compared to (—) the spectrum of the initial Nd species observed in the HEH[EHP] dependence experiments at 35 °C. (b) (—) Spectrum of the Nd complex extracted from 4 M HNO_3 into 0.05 M TEHDGA/0.75 M HEH[EHP]/*n*-dodecane at 25 °C compared to (—) the spectrum of the final Nd species observed in the HEH[EHP] dependence experiments at 35 °C, 0.05 M TEHDGA/0.075 M HEH[EHP]/*n*-dodecane.

Measurement of Nitric Acid Extracted by HEH[EHP] and TEHDGA

The extraction of nitric acid by HEH[EHP] and TEHDGA in the ALSEP system were studied in order to calculate the concentrations of free extractant in the ALSEP process. Titration of the organic phases to determine the concentration of acid either directly or in a two-phase titration were not possible due to the presence of substantial amounts of titratable hydrogen associated with HEH[EHP]. Instead, the nitrate content of the organic phases was analyzed after stripping the organic phase.

Nitrate extraction by the extractants was quantified by spectrophotometric analysis using a modification of the method by Cataldo *et al.*¹ after stripping the nitrate into a fresh aqueous phase. Organic phase solutions of 0.75 M HEH[EHP]/0.05 M TEHDGA/*n*-dodecane or 0.75 M HEH[EHP]/*n*-dodecane were equilibrated with 2 volumes of fresh 0.3 - 4 M nitric acid twice. Once equilibration was completed, the extracted nitric acid was stripped from the acid-loaded organic phases with a solution of 0.004 M H₂SO₄/0.096 M Na₂SO₄ in a 1:3 organic to aqueous ratio by vortex mixing for two minutes followed by centrifugation. For higher concentrations of nitric acid uptake, a 1:6 organic:aqueous phase volume ratio was used. Aliquots of the strip solution were pipetted into individual 25 mL volumetric flasks and mixed with 0.8 mL concentrated H₂SO₄ / 5% (w/v) salicylic acid. After 20 minutes 15.0 mL 2.5 M NaOH were added and, after cooling, the solution was diluted to the mark with 18 MΩ water. The nitrate concentration was determined from the absorbance at 410 nm. Nitrate standards were made from standardized nitric acid solutions diluted in the H₂SO₄/Na₂SO₄ solution to match the matrix of the strip solution and analyzed as described above.

The experimentally determined nitric acid content of the 0.75M HEH[EHP]/*n*-dodecane and 0.05 M TEHDGA/0.75 M HEH[EHP]/*n*-dodecane was used to calculate equilibrium constants for the extraction of nitric acid as a function of the activity of undissociated nitric acid. Equilibria S1a, S4a, S5a, and S6a were used to analyze the system, as described below, and we considered the presence of 0.05 M TEHDGA

in the ALSEP solvent to be a perturbation of the extraction equilibrium found for the system containing only 0.75 M HEH[EHP]. Results are summarized in Figures S3 – S5.

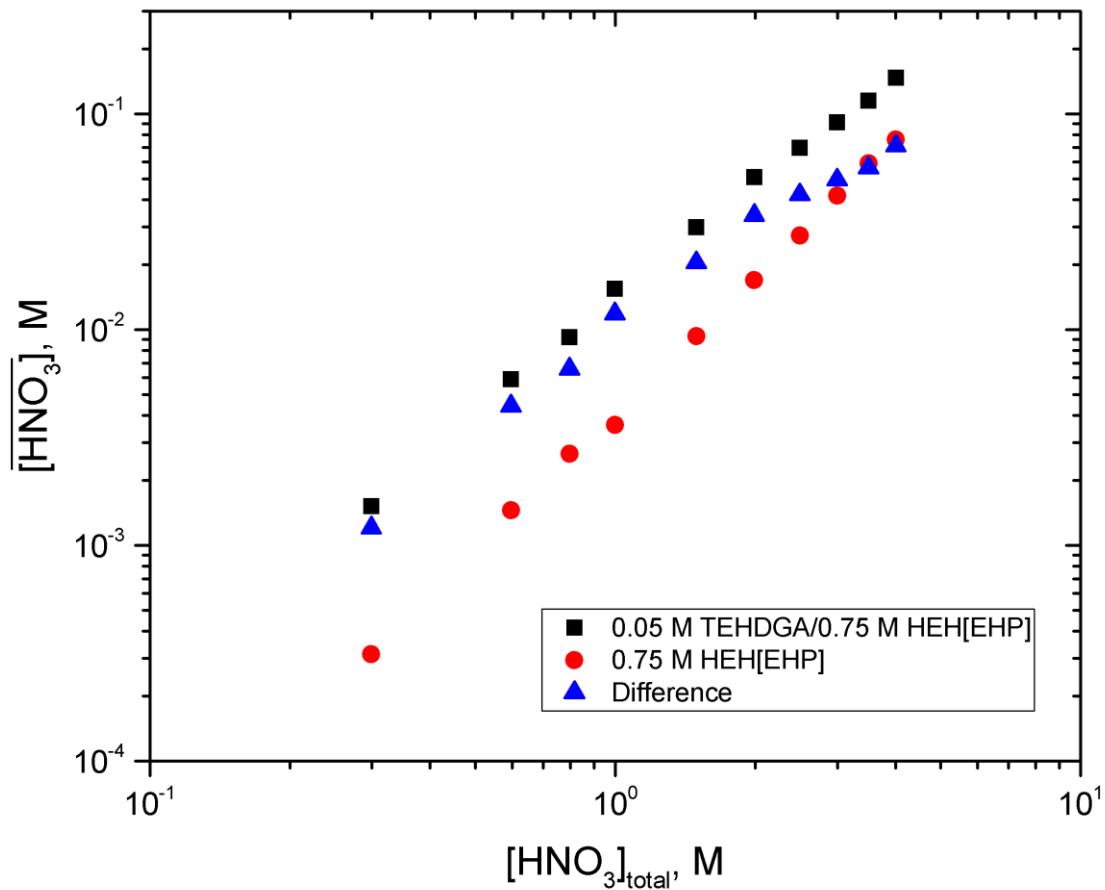


Figure S3. Equilibrium concentrations of nitric acid extracted into the organic phase of (■) the ALSEP process solvent 0.05 M TEHDGA/0.75 M HEH[EHP]/*n*-dodecane, (●) 0.75 M HEH[EHP]/*n*-dodecane, and (▲) by the 0.05 M TEHDGA in the ALSEP process solvent, which is calculated as the difference between the extraction in the ALSEP solvent and the extraction by 0.75 M HEH[EHP]/*n*-dodecane.

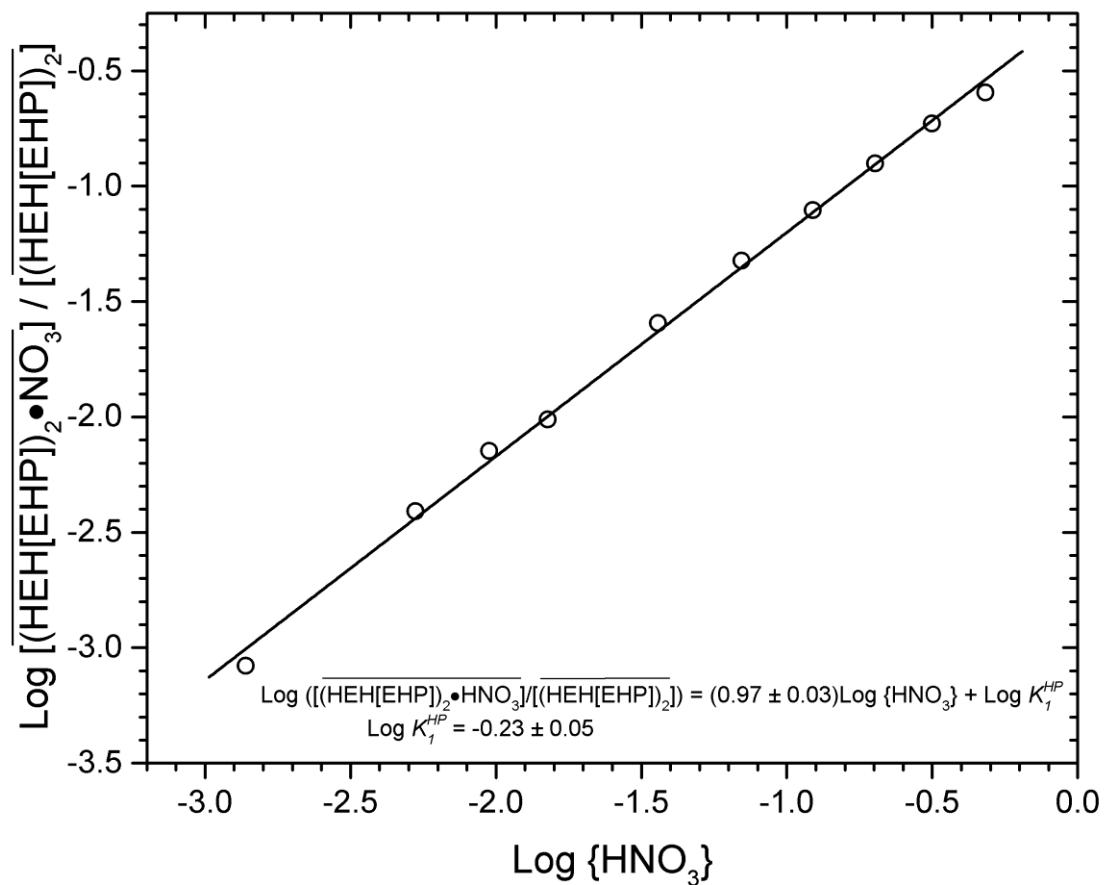


Figure S4. Determination of the equilibrium constant for nitric acid extraction by 0.75 M HEH[EHP] in *n*-dodecane from 0.3 – 4 M HNO₃ analyzed as a function of the activity of undissociated nitric acid in the aqueous phase according to Equilibrium S6a and Equation S6b.

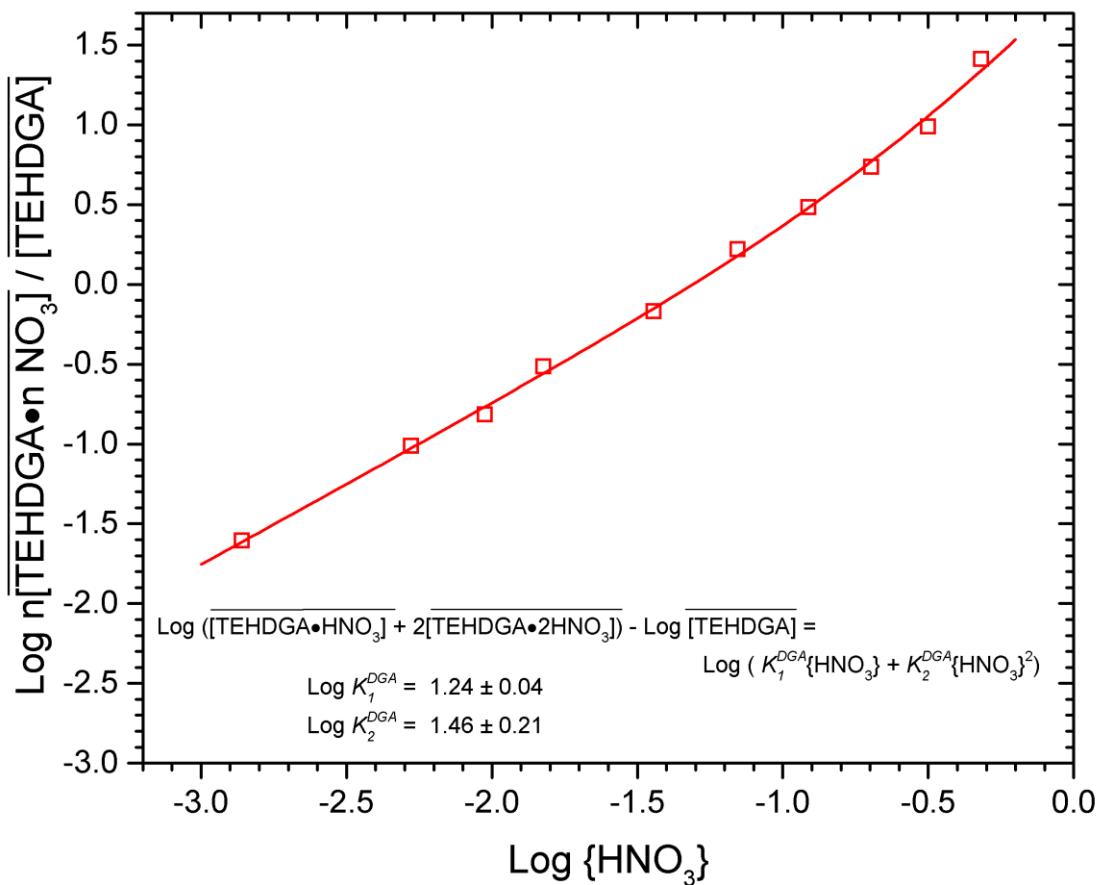


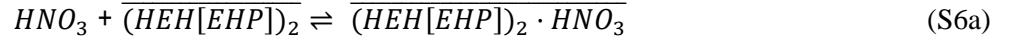
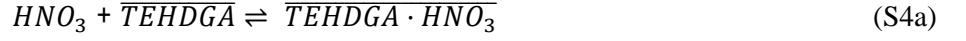
Figure S5. Nitric acid extraction by TEHDGA in the ALSEP process solvent, 0.05 M TEHDGA/0.75 M HEH[EHP]/*n*-dodecane, from 0.3 – 4 M HNO₃ as a function of the activity of undissociated nitric acid in the aqueous phase. The concentration of nitric acid associated with TEHDGA in the ALSEP organic phase was taken as the difference between the total amount of nitrate extracted by the ALSEP process solvent and the amount nitrate extracted by 0.75 M HEH[EHP] (Triangles in Figure S3).

Thermodynamic model for ALSEP extraction

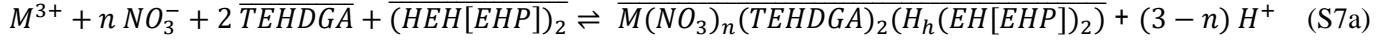
A model of trivalent f-element cation extraction by the ALSEP organic solvent under acidic conditions was developed to determine the effects of nitric acid on metal distribution. The model was based on models for actinide nitrate extraction by solvating extractants developed by Vandegrift and coworkers.²⁻³ It considered variations in the activity coefficients of aqueous solutes and the activity of water including the corresponding changes in the degree of metal-nitrate complex formation and the nitric acid extraction equilibria. The activity coefficients of organic phase species were considered to be independent of the aqueous phase composition and thus constant for our nitric acid dependence experiments.

The activity of a solvent is usually not considered in equilibrium constant expressions. However, the activity of water decreases by approximately 25% across the range of nitric acid concentrations studied, and extraction of actinide nitrates liberates a substantial number of water molecules from the inner coordination spheres of the metal cation and nitrate anions for each metal extracted. For this reason, the thermodynamic model proposed by Chaiko and Vandegrift for americium nitrate extraction in the TRUEX process explicitly considered the changes in water activity by including water liberated from the hydrated Am^{3+} cation as a product in the nitrate complexation reactions (Eq. S2a and S3a) and the extraction equilibrium (Eq. S7a) with a total inner sphere hydration number of 9 for Am^{3+} .² Each complexed nitrate was considered to liberate 1 inner sphere water molecule from the Am^{3+} cation, and extraction of Am^{3+} into the organic phase was considered to liberate all 9 inner sphere water molecules. A more recent version of this model extended for plutonium (IV) nitrate extraction by tributylphosphate considered nitrate complexation to liberate 2 water molecules per complexed nitrate when aqueous plutonium-nitrate complexes form.³ We adopted the approach from the plutonium-tributylphosphate extraction model to account for complexation-induced dehydration in the americium-nitrate stability constants (Eq. S2b and S3b) because the liberation of 2 water molecules per complexed nitrate aligns well with fluorescence studies of curium-nitrate complexation.⁴ We further extended this model to include dehydration of both the metal cation (9 inner sphere water molecules per americium)⁵⁻⁶ and the coextracted anions (3 inner sphere water molecules per nitrate).⁷⁻⁸

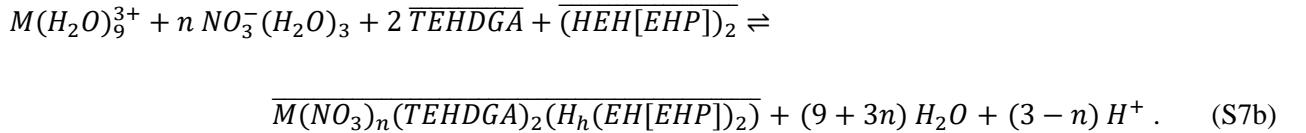
Omitting the waters of hydration for aqueous species and denoting organic phase species with an overbar, the equilibria considered in this model are



and



where $h = n - 1$ and $h = 0, 1$, or 2 . The full, general equilibrium for trivalent f-element extraction in ALSEP, including inner sphere waters of hydration is:



The corresponding equilibrium constant expressions including water molecules liberated from the inner hydration spheres of the metal cation and nitrate anions are

$$K_a = \frac{\{H^+\}\{NO_3^-\}}{\{HNO_3\}} \quad (\text{S1b})$$

$$\beta_1 = \frac{\{M(NO_3)^{2+}\}\{H_2O\}^2}{\{M^{3+}\}\{NO_3^-\}} \quad (\text{S2b})$$

$$\beta_2 = \frac{\{M(NO_3)_2^+\}\{H_2O\}^4}{\{M^{3+}\}\{NO_3^-\}^2} \quad (\text{S3b})$$

$$K_1^{DGA} = \frac{[TEHDGA \cdot HNO_3]}{[TEHDGA]\{HNO_3\}} \quad (\text{S4b})$$

$$K_2^{DGA} = \frac{[TEHDGA \cdot 2HNO_3]}{[TEHDGA]\{HNO_3\}^2} \quad (\text{S5b})$$

$$K_1^{HP} = \frac{[(HEH[EHP])_2 \cdot HNO_3]}{[(HEH[EHP])_2]\{HNO_3\}} \quad (\text{S6b})$$

$$K_{ex} = \frac{[\overline{M(NO_3)_n(TEHDGA)_2(H_h(EH[EHP])_2)}]\{H^+\}^{3-n}\{H_2O\}^{9+3n}}{\{M^{3+}\}\{NO_3^-\}^n[\overline{TEHDGA}]^2[(HEH[EHP])_2]} \quad (\text{S7c})$$

and

where the square brackets denote concentrations and curly braces denote activities, which are related by the activity coefficient, γ , of each species as $\{A\} = \gamma_A[A]$.

The mass balance of americium in the aqueous phase,

$$[Am]_{total} = [Am^{3+}] + [Am(NO_3)^{2+}] + [Am(NO_3)_2^+] , \quad (S8)$$

can be combined with the conditional stability constants for americium-nitrate complexation, β_1' and β_2' ,

$$\beta_1' = \beta_1 \frac{\gamma_{M^{3+}} \gamma_{NO_3^-}}{\gamma_{M(NO_3)^{2+}} \{H_2O\}^2} = \frac{[M(NO_3)^{2+}]}{[M^{3+}][NO_3^-]} \quad (S9)$$

and

$$\beta_2' = \beta_2 \frac{\gamma_{M^{3+}} (\gamma_{NO_3^-})^2}{\gamma_{M(NO_3)_2^+} \{H_2O\}^4} = \frac{[M(NO_3)_2^+]}{[M^{3+}][NO_3^-]^2} , \quad (S10)$$

to give

$$[Am]_{total} = [Am^{3+}] (1 + \beta_1' [NO_3^-] + \beta_2' [NO_3^-]^2) . \quad (S11)$$

Equation S11 can be rewritten in terms of the activity of Am^{3+} as

$$[Am]_{total} = \{Am^{3+}\} / \gamma_{Am^{3+}} (1 + \beta_1' [NO_3^-] + \beta_2' [NO_3^-]^2) \quad (S12)$$

and combined with the definition of the americium distribution ratio and the relevant equilibria to express K_{ex} as a function of D_{Am} ,

$$D_{Am} = \frac{[\overline{Am}]_{total}}{[Am]_{total}} = \frac{[\overline{Am(No_3)_n(TEHDGA)_2(H_h(EH[EHP])_2)}]}{\{Am^{3+}\}/\gamma_{Am^{3+}}(1 + \beta_1'[No_3^-] + \beta_2'[No_3^-]^2)}, \quad (S13)$$

which is substituted into Equation S7c to give

$$K_{ex} = \frac{D_{Am}(1 + \beta_1'[No_3^-] + \beta_2'[No_3^-]^2)\{H^+\}^{3-n}\{H_2O\}^{9+3n}}{\gamma_{Am^{3+}}\{No_3^-\}^n[TEHDGA]^2[(HEH[EHP])_2]}. \quad (S14)$$

Because nitric acid is a strong acid that is present in the aqueous phase at much higher concentrations than Am³⁺ and there are no other significant sources of hydronium cations or nitrate anions in our system at these acidities, [H⁺] ≈ [NO₃⁻]. In the absence of single ion activity coefficients, the average activity coefficient of the hydrogen ion and nitrate (γ_{\pm}) is used to represent the hydrogen ion and nitrate activity coefficients.⁹ Therefore, $\gamma_{\pm}[H^+] \approx \gamma_{\pm}[NO_3^-]$ and {H⁺} ≈ {NO₃⁻} in the aqueous phase. Substituting this equality into Equation S14 and rearranging gives

$$K_{ex}\{No_3^-\}^{2n-3} = \frac{D_{Am}(1 + \beta_1'[No_3^-] + \beta_2'[No_3^-]^2)\{H_2O\}^{9+3n}}{\gamma_{Am^{3+}}[TEHDGA]^2[(HEH[EHP])_2]}, \quad (S15)$$

which can be used to determine *n*, the number of nitrate anions extracted with americium in the ALSEP system under acidic conditions.

Equation S15 only applies when nitric acid is the sole significant source of hydronium cations or nitrate anions in the system. Because of the equivalence of {H⁺} and {NO₃⁻} in the aqueous phase, an unusual dependence of the distribution ratio on nitrate activity is observed for Equation S15 where the slope of the nitrate dependence does not necessarily reflect the number of nitrate anions present in the extracted complex. This arises because there

are two possible ways to balance the charge of the extracted metal cation in this system, extraction of nitrate anions and exchange of acidic hydrogens from $(\text{HEH}[\text{EHP}])_2$. Increasing the nitric acid concentration will increase the concentration of nitrate anions, promoting extraction if $n > 0$. But, increasing the nitric acid concentration also proportionately increases the concentration of hydronium cations, which reduces exchange of acidic hydrogens from $(\text{HEH}[\text{EHP}])_2$ and opposes metal extraction when $h < 2$ (i.e. $n < 3$). Consequently, increasing the nitrate (and hydronium) activity by increasing the nitric acid concentration will increase the metal distribution ratio as the n -th power of the nitrate activity, but it will also decrease the distribution ratio by the $(3 - n)$ -th power of the nitrate (hydronium) activity when $3 - n$ protons are liberated from $(\text{HEH}[\text{EHP}])_2$ by metal extraction. Together these effects create the $\{\text{NO}_3^-\}^{2n-3}$ dependence in Equation S15.

To model the extraction in Equilibrium S7b using Equation S15, values for K_a , β_1 , and K_2 ($K_2 = \beta_2/\beta_1$) were taken from the literature,^{2, 9-10} while K_1^{DGA} , K_2^{DGA} , and K_1^{HP} were derived by fitting experimental data for nitric acid extraction as a function of nitric acid activity (Figures S3 – S5). The equilibrium constants used as input for the calculations are summarized in Table S1.

The activity coefficients of the organic phase species were considered to be constant in these experiments since compositions of the organic phases undergo only modest changes compared to the aqueous phases in these experiments. Consequently, the extraction constant, K_{ex} , derived from this model is a conditional constant applicable for 0.05 M TEHDGA/0.075 M HEH[EHP]/*n*-dodecane.

The activity coefficient of HNO_3 and the average activity coefficient of H^+ and NO_3^- were calculated on the molar scale for each HNO_3 concentration following the empirical equation of Levanov.⁹ Molal scale activity coefficients for tracer Am^{3+} in nitric acid were calculated using the Bromley Equation with coefficients for $\text{Nd}(\text{NO}_3)_3$ in nitric acid¹¹ and converted to molar scale activity coefficients.¹² Water activities were calculated using the Pitzer and Simonson model with parameters for nitric acid solutions as described by Brimblecombe and Clegg.¹³ Lacking activity coefficients for $\text{Am}(\text{NO}_3)^{2+}$ and $\text{Am}(\text{NO}_3)_2^{+}$, molar scale conditional stability constants β_1' and β_2' (Eq. S9 and S10) were calculated from β_1 and β_2 for each aqueous solution composition by the SIT method using the ion

interaction coefficients for Am^{3+} , NO_3^- , and their complexes¹⁰ with $\Delta\epsilon = -0.06$ and -0.35 for the formation of $\text{Am}(\text{NO}_3)^{2+}$ and $\text{Am}(\text{NO}_3)_2^{+}$ on the molal scale, respectively.

Equation S15 was fit to the experimental americium distribution data between 1 and 5 M HNO_3 with n and K_{ex} as varied parameters using the Excel Solver, yielding $n = 3.05 \pm 0.06$ and $\log K_{ex} = 4.35 \pm 0.09$. The uncertainties in the fitted parameters were estimated at the 95% confidence level using the jackknife method.¹⁴

Table S1. Equilibrium constants used to model nitrate extraction dependence.

Equilibrium Constant	Log K	Reference
K_a	1.55	9
K_1^{DGA}	1.24 ± 0.04	Fig. S5
K_2^{DGA}	1.46 ± 0.21	Fig. S5
K_1^{HP}	-0.23 ± 0.05	Fig. S4
β_I	1.33	10
K_2	-0.13	2

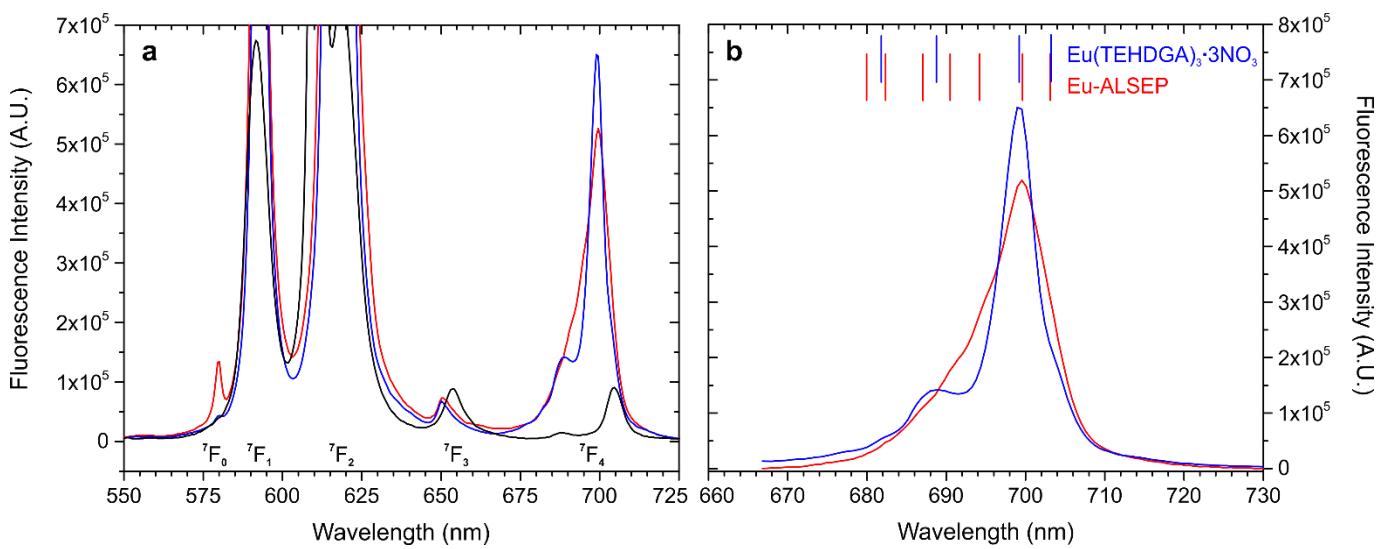


Figure S6. Fluorescence emission spectra of organic phase Eu complexes from Manuscript Figure 3. Extraction of Eu (—) from 0.001 M HNO₃/1 M NaNO₃ into 0.75 M HEH[EHP]/*n*-dodecane, (—) from 3.5 M HNO₃ into 0.2 M TEHDGA/*n*-dodecane, and (—) from 4 M HNO₃ into 0.05 M TEHDGA/0.75 M HEH[EHP]/*n*-dodecane (ALSEP). (a) Spectra with an expanded vertical scale highlight the weaker ⁵D₀ → ⁷F₀, ⁷F₃, and ⁷F₄ transitions. (b) Spectra with expanded vertical and horizontal scales illustrate the broadening of the ⁵D₀ → ⁷F₄ emission band when Eu is extracted into 0.05 M TEHDGA/0.75 M HEH[EHP]/*n*-dodecane. The positions of the 4 readily discernable ⁷F₄ sublevels of the 1:3 Eu:TEHDGA complex and the 7 readily discernable sublevels of the Eu-ALSEP complex are indicated as vertical lines color coded to match the spectra.

Table S2. Eu-O bond distances for optimized Eu(TEDGA)₂(H(E[EP])₂)·2NO₃ complexes with geometry A (eight coordinated) and B (nine coordinated).

Eu-O Bond	Geometry A Eu-O length (Å)	Geometry B Eu-O length (Å)
Eu-TEDGA-1a	2.436	2.403
Eu-TEDGA-1b	2.619	2.734
Eu-TEDGA-1c	2.433	2.480
Eu-TEDGA-2a	2.411	2.477
Eu-TEDGA-2b	2.632	2.613
Eu-TEDGA-2c	2.426	2.544
HE[EP]-a	2.285	2.351
HE[EP]-b	2.336	2.297
NO ₃ ⁻	--	2.459

Optimized coordinates for the five Eu-complexes under investigation

Table S3. Cartesian coordinates for Eu(TEDGA)₃·3NO₃.

Atom	Coordinates (Angstroms)		
	X	Y	Z
O	1.92314300	1.32400900	0.93117800
C	2.93899000	0.79259000	1.78187700
H	3.89557000	0.70896900	1.24215000
H	3.06257200	1.43536700	2.66408000
C	2.07004500	2.70529500	0.64043400
H	3.11160300	2.92645400	0.37533100
H	1.77655300	3.31178100	1.50751600
C	2.47483200	-0.59202600	2.20755500
C	1.13556300	3.01790100	-0.52622200
O	1.42143400	-1.06506800	1.72235700
O	0.37120700	2.11247600	-0.93995200
N	3.18444700	-1.26093700	3.12717300
N	1.16093100	4.22835900	-1.08504100
C	2.70722200	-2.59753700	3.52195700
H	2.40047400	-3.12601800	2.61536300
H	3.56472000	-3.12900600	3.94209300
C	4.53193700	-0.84365800	3.55133600
H	5.16184900	-1.73785100	3.51863500
H	4.95457700	-0.17837700	2.79693300
C	1.89753600	5.36999800	-0.50730100
H	1.14163600	6.03945000	-0.08209000
H	2.50903600	5.01153800	0.32091200
C	0.15912200	4.52792900	-2.13201500
H	-0.02393200	5.60268700	-2.09322100
H	-0.77390000	4.03738900	-1.84799500
C	1.55487200	-2.56118100	4.52810400
H	0.68971400	-2.04838900	4.10157000
H	1.25444900	-3.58197800	4.78742400
H	1.84549600	-2.04884500	5.45031800
C	4.56166100	-0.22261800	4.94918100
H	5.58747200	0.05543200	5.21113500
H	3.94309100	0.67940900	5.00091200
H	4.19888500	-0.92226000	5.70906700
C	0.59676100	4.07443800	-3.52519100
H	-0.18154800	4.32278800	-4.25441500
H	1.52329800	4.56431800	-3.83909500
H	0.75155100	2.99243200	-3.54740200
C	2.79314900	6.07853300	-1.52323000
H	3.54150600	5.39904700	-1.94398400
H	2.21486100	6.50584000	-2.34717000
H	3.31740000	6.90308600	-1.03022300
Eu	0.02432100	-0.05840000	-0.00242100

O	0.49658400	-2.49424300	-0.70852300
C	-0.39448200	-3.56141600	-0.42700100
H	-0.89945300	-3.88919400	-1.34495500
H	0.15128400	-4.40736900	0.01124500
C	1.71743300	-2.88466600	-1.31664100
H	1.52445300	-3.55494600	-2.16440300
H	2.36159900	-3.39732000	-0.58961700
C	-1.43478300	-3.02782800	0.55900800
C	2.40655400	-1.60394300	-1.78933100
O	-1.40231600	-1.81592500	0.86660500
O	1.90276700	-0.50333000	-1.47149500
N	-2.33636800	-3.86792700	1.07614900
N	3.50996100	-1.69105500	-2.53586400
C	-2.52235600	-5.25208600	0.60021100
H	-3.45697500	-5.26319800	0.02892000
H	-1.72116200	-5.49648800	-0.09762200
C	-3.40227200	-3.29559100	1.92830700
H	-3.69228000	-2.33518600	1.49755900
H	-4.26587000	-3.95656800	1.83857500
C	4.24596000	-2.95140800	-2.75315300
H	5.17677000	-2.86802700	-2.18112300
H	3.67836400	-3.77203600	-2.31342000
C	4.20072600	-0.43226900	-2.89388700
H	5.25275600	-0.68127900	-3.03918500
H	4.14905400	0.23221500	-2.02882700
C	-2.52909500	-6.27833100	1.73348200
H	-3.34843800	-6.10334800	2.43621100
H	-2.66658200	-7.27997900	1.31441700
H	-1.58853300	-6.26676300	2.29412100
C	-2.97389500	-3.11896200	3.38525000
H	-3.80401600	-2.70301800	3.96571800
H	-2.68525800	-4.07091100	3.84107500
H	-2.12920200	-2.42883500	3.45687100
C	3.60088400	0.24704000	-4.12519500
H	4.15411500	1.16580700	-4.34607300
H	3.65020000	-0.39830300	-5.00752100
H	2.55577600	0.51372500	-3.94752800
C	4.50206900	-3.24681100	-4.23109700
H	3.56680700	-3.33292400	-4.79425100
H	5.11330500	-2.47063400	-4.70019800
H	5.04675500	-4.19162800	-4.32344300
O	-2.29600500	0.87719300	-0.16018400
C	-2.85367400	1.74768900	0.82417600
H	-2.90237600	2.78117700	0.44608200
H	-3.85681800	1.40052200	1.10390600
C	-3.17927900	0.58454300	-1.23964700
H	-3.62370100	1.51214500	-1.62290800
H	-3.97152700	-0.10726500	-0.91527000
C	-1.92483200	1.70228900	2.02681600
C	-2.34806300	-0.09163000	-2.31889600
O	-0.85873200	1.04542600	1.95648600
O	-1.14750100	-0.37031000	-2.08610200

N	-2.28260100	2.33724700	3.15046900
N	-2.90659400	-0.34841100	-3.50811500
C	-3.42899900	3.26146100	3.20512500
H	-3.10053300	4.13511700	3.77575700
H	-3.62708100	3.64049200	2.20107400
C	-1.34752800	2.30052800	4.28801000
H	-0.33766200	2.44333900	3.89513900
H	-1.58301600	3.16076900	4.91941800
C	-4.35032400	-0.19630700	-3.75787600
H	-4.67076700	-1.08889000	-4.30372200
H	-4.88141800	-0.24330200	-2.80641000
C	-2.07949900	-1.02031600	-4.52594400
H	-2.76790200	-1.48663800	-5.23523800
H	-1.52336900	-1.81905200	-4.02871500
C	-4.67472200	2.64756700	3.84815600
H	-4.48277700	2.33513300	4.87967700
H	-5.48567100	3.38267200	3.86441300
H	-5.02426000	1.77209900	3.29157400
C	-1.42280800	1.00526100	5.09953700
H	-0.71260900	1.04596300	5.93239000
H	-2.42341600	0.85002500	5.51447400
H	-1.16759900	0.14649800	4.47420900
C	-1.11937300	-0.07591900	-5.25227600
H	-0.54619300	-0.63231400	-6.00156400
H	-1.65842300	0.72657600	-5.76473000
H	-0.41579200	0.37193400	-4.54671800
C	-4.70129300	1.06488300	-4.55021800
H	-4.39243900	1.97133300	-4.01986600
H	-4.21940800	1.06910700	-5.53300100
H	-5.78350100	1.11666300	-4.70635000
N	-4.56101400	-2.83743300	-1.12031500
O	-5.22563400	-1.77976000	-0.92261300
O	-3.41326900	-2.77190200	-1.65162600
O	-5.04079700	-3.94295300	-0.78105400
N	5.50039400	-1.11885000	0.05200600
O	4.49196900	-1.79204200	0.42184400
O	5.68782100	0.04301000	0.52114400
O	6.30918900	-1.59060000	-0.77875500
N	-1.51507400	5.11731100	0.65019100
O	-2.70193500	4.82051100	0.32174800
O	-0.82310800	4.29526700	1.32442200
O	-1.03121500	6.21815000	0.30045600

Table S4. Cartesian coordinates for Eu(TEDGA)₂(H(E[EP])₂)·2NO₃ complex A.

Atom	Coordinates (Angstroms)		
	X	Y	Z
O	0.18648900	-2.79873400	-0.10481700
C	1.49172200	-3.35974700	0.02949600
H	1.41635100	-4.42515700	0.28302600
H	2.06936600	-3.23069600	-0.89215200
C	-0.60578300	-3.37335200	-1.12806500
H	-0.77438900	-4.43586400	-0.92138500
H	-0.11041100	-3.27400600	-2.10555100
C	2.16199100	-2.56555700	1.15392600
C	-1.90696500	-2.56149400	-1.15690300
O	1.63039600	-1.48980300	1.51067200
O	-1.87766100	-1.40189600	-0.70439300
N	3.24820700	-3.05026200	1.76192800
N	-3.01348700	-3.09560700	-1.70106500
C	4.09118400	-4.10032400	1.17031600
H	3.63399100	-4.44345700	0.24276300
H	5.02384000	-3.60987300	0.87470900
C	3.84906900	-2.23080100	2.83589300
H	4.89500700	-2.53269200	2.91345300
H	3.84315200	-1.19214700	2.50425800
C	-3.04794800	-4.45982700	-2.25180700
H	-3.81154500	-4.45734000	-3.03489000
H	-2.10075700	-4.67060400	-2.75897400
C	-4.23315900	-2.25730400	-1.81761600
H	-4.54988800	-2.30826500	-2.86667900
H	-3.95041400	-1.23128300	-1.58641200
C	4.32839300	-5.27935300	2.11328900
H	3.38805200	-5.77192300	2.38220200
H	4.97549100	-6.01680300	1.62781000
H	4.82206600	-4.96650100	3.03836900
C	3.12888100	-2.39592200	4.17434600
H	3.62030400	-1.78233500	4.93698600
H	2.08856500	-2.07008900	4.09594800
H	3.14337600	-3.43618700	4.51548400
C	-5.37503800	-2.65938000	-0.88605800
H	-6.19529300	-1.95243600	-1.03216900
H	-5.74743500	-3.67038300	-1.08227300
H	-5.07442900	-2.56386700	0.15941100
C	-3.36214900	-5.55794800	-1.22880600
H	-2.61163700	-5.60030500	-0.43348000
H	-4.33419500	-5.39521700	-0.75919300
H	-3.37999500	-6.53249100	-1.72767600
Eu	0.04211700	-0.20090900	0.19402900
O	0.06573900	1.49258700	2.20836700
C	-1.22997800	1.65349900	2.78598800
H	-1.14557400	2.13289500	3.76877500

H	-1.87968200	2.24704500	2.13126000
C	0.75033000	2.71106100	1.95675200
H	1.04443500	3.17429700	2.90528400
H	0.11433400	3.40641500	1.38998000
C	-1.80243800	0.23913600	2.89410900
C	1.95697100	2.35369400	1.08100900
O	-1.31548600	-0.64688500	2.15394800
O	1.92463000	1.28572500	0.43921900
N	-2.75998000	-0.03850300	3.78307100
N	2.98707900	3.21120500	0.98749100
C	-3.58752500	0.99619600	4.42181900
H	-3.27963900	1.97499100	4.05595500
H	-4.60253800	0.85321200	4.03949800
C	-3.25245100	-1.43100000	3.84367000
H	-4.24736800	-1.39296600	4.29105800
H	-3.37758900	-1.78332400	2.81945100
C	3.03833600	4.47073500	1.74643200
H	3.63219600	5.16850300	1.14914400
H	2.03334300	4.90108000	1.79906900
C	4.09646000	2.90020100	0.04965100
H	4.29939500	3.82257900	-0.50686100
H	3.73320300	2.14750100	-0.64873100
C	-3.53373500	0.94792500	5.94840700
H	-2.51759500	1.12096800	6.31816200
H	-4.18686000	1.72032800	6.36684700
H	-3.87360200	-0.01747900	6.33590100
C	-2.32622900	-2.34842400	4.64261900
H	-2.74235900	-3.36120000	4.66991500
H	-1.33863000	-2.39958300	4.17739800
H	-2.20739600	-2.00301800	5.67462200
C	5.36658000	2.37342600	0.71551900
H	6.09268200	2.14470400	-0.06810100
H	5.81208100	3.09707100	1.40632000
H	5.17497600	1.42986200	1.23064200
C	3.64086800	4.35180500	3.15151000
H	3.07078900	3.66078200	3.78005600
H	4.67139700	3.99343000	3.11265400
H	3.63686100	5.33264200	3.63834600
P	-1.34077100	2.89093500	-1.41221300
O	-0.96095800	1.74569000	-0.45726400
O	-0.82191000	2.77671800	-2.84544800
H	0.39684900	2.08872000	-3.15525100
O	-0.73837900	4.26965100	-0.72919500
P	1.17583500	-0.01311100	-3.36268600
O	1.26281500	1.55390900	-3.41757000
O	0.15800600	-0.52643900	-4.51867200
O	0.72298400	-0.57011200	-2.01005700
C	-1.24373300	-0.16170100	-4.47515700
H	-1.33362400	0.92862800	-4.45924400
H	-1.68223500	-0.54689500	-3.54751400
C	0.21566400	5.09382800	-1.42648700
H	1.22704100	4.71624800	-1.22474300

H	0.04789700	5.01997000	-2.50439000
C	-1.91695000	-0.75840400	-5.69704600
H	-1.47197300	-0.36380400	-6.61488600
H	-1.81463100	-1.84809700	-5.70803200
H	-2.98297600	-0.50886900	-5.69481000
C	0.06782500	6.52490000	-0.93692900
H	0.22363900	6.59122400	0.14491300
H	0.80289700	7.16989400	-1.43011100
H	-0.93239700	6.90834700	-1.15847400
C	2.77234600	-0.61352700	-3.93700000
H	3.01173200	-0.01794900	-4.82451000
H	3.49584300	-0.36603800	-3.14893400
C	2.81582900	-2.11486300	-4.24494700
H	3.80574000	-2.37935900	-4.62799100
H	2.66012500	-2.69477300	-3.33275200
H	2.06949500	-2.40113500	-4.99165500
C	-3.13151300	3.14443400	-1.37264300
H	-3.59026200	2.19105000	-1.65278300
H	-3.42601200	3.27583900	-0.32744600
C	-3.61279800	4.29569200	-2.26216700
H	-4.70362800	4.37329800	-2.22219900
H	-3.19711900	5.25369300	-1.93257600
H	-3.31877500	4.14197900	-3.30453000
N	-4.66666000	0.60179700	0.88756200
O	-4.06639300	1.59736700	1.38614900
O	-5.03810600	-0.33785300	1.63767900
O	-4.90070800	0.55877600	-0.34430200
N	4.65563500	-0.97185700	-0.71104300
O	5.25033700	-1.05518600	0.39409700
O	4.80874400	0.03893300	-1.44234500
O	3.90409600	-1.91818900	-1.09444200

Table S5. Cartesian coordinates for Eu(TEDGA)₂(H(E[EP])₂)·2NO₃ complex B.

Atom	Coordinates (Angstroms)		
	X	Y	Z
O	0.13263600	-0.80772200	-2.30382900
C	0.89596200	0.20358600	-2.96287100
H	1.18680100	-0.14574400	-3.96031500
H	0.32916500	1.13828300	-3.04370900
C	-1.09600700	-1.09074000	-2.94595400
H	-0.91578700	-1.61169100	-3.89524500
H	-1.65392100	-0.16424000	-3.14403800
C	2.10038000	0.44382900	-2.06075600
C	-1.91043100	-1.92857700	-1.96470900
O	1.95027400	0.27194900	-0.83178100
O	-1.66302300	-1.82729500	-0.74686300
N	3.29253100	0.76269400	-2.58542700
N	-2.89363700	-2.73594100	-2.40459700
C	3.45526700	1.32635700	-3.93574100
H	2.47457200	1.43778400	-4.39478700
H	3.81656900	2.34881900	-3.79222700
C	4.42132600	0.93183700	-1.65133600
H	5.17624800	1.52602600	-2.16890700
H	4.07594900	1.53054500	-0.80734600
C	-3.68729300	-3.46624100	-1.38595800
H	-4.01298800	-4.39974300	-1.85565000
H	-3.01691700	-3.71036700	-0.56019600
C	-3.24343700	-2.89372600	-3.82429200
H	-3.73211600	-3.86738000	-3.91669500
H	-2.32518300	-2.95753200	-4.41596400
C	4.38404600	0.49454000	-4.81940100
H	3.99034800	-0.51558700	-4.97643500
H	4.49529400	0.97425800	-5.79728300
H	5.38389400	0.40129900	-4.38300200
C	5.00508400	-0.40478000	-1.18917800
H	5.84284000	-0.23013300	-0.50403100
H	4.24615900	-0.99289800	-0.66710400
H	5.37814700	-0.99459000	-2.03277700
C	-4.15416900	-1.79792900	-4.38701800
H	-4.35500300	-1.99085500	-5.44607900
H	-5.11046000	-1.76800200	-3.85881000
H	-3.69194800	-0.81088900	-4.30233500
C	-4.88469300	-2.67656400	-0.85289100
H	-4.56053300	-1.75635400	-0.36037800
H	-5.59798900	-2.42384700	-1.64388800
H	-5.41042600	-3.28443300	-0.10946800
Eu	-0.10250200	-0.39500900	0.38883600
O	2.01565300	-0.90102600	1.83304800
C	2.45640300	-2.23888700	2.00303200
H	3.54270700	-2.25687800	2.15857300

H	1.94518200	-2.70918100	2.85059400
C	2.68826900	0.06996800	2.60613100
H	3.77066600	-0.01078600	2.45362800
H	2.48151400	-0.06640100	3.67986000
C	2.07741100	-2.98896500	0.72267900
C	2.14844900	1.43203100	2.15009800
O	1.31705200	-2.44931700	-0.09606700
O	1.05951000	1.45837100	1.55131200
N	2.60472700	-4.21032700	0.49894000
N	2.86366900	2.53447700	2.43847100
C	3.34316500	-4.97146500	1.51211600
H	3.34270400	-4.41804200	2.45149800
H	2.78353600	-5.89283200	1.71152000
C	2.11616900	-4.94598700	-0.68278800
H	2.33200200	-6.00365300	-0.50789400
H	1.02925800	-4.83032500	-0.71888900
C	4.05953400	2.48873500	3.29494100
H	4.07543600	3.42442400	3.86113400
H	3.94292300	1.69512700	4.04002200
C	2.33267800	3.86568700	2.04661700
H	1.85203300	4.30147100	2.93371300
H	1.56950800	3.69641000	1.28960600
C	4.77925600	-5.29360900	1.09266000
H	5.35527800	-4.37823500	0.92413400
H	5.27769600	-5.87650000	1.87382900
H	4.80471100	-5.88188600	0.17038100
C	2.74671900	-4.48233300	-1.99686300
H	2.36166900	-5.08619700	-2.82560900
H	2.49790300	-3.43674100	-2.18876500
H	3.83601100	-4.58763000	-1.97715700
C	3.37880300	4.81855900	1.47346500
H	2.87469500	5.75817900	1.23545300
H	4.18812700	5.03986000	2.17807900
H	3.77622700	4.43984300	0.52848700
C	5.38234200	2.31837800	2.53907200
H	5.41032300	1.37940200	1.97762400
H	5.53849300	3.13245200	1.82963600
H	6.21589900	2.31212300	3.24950200
P	-3.03080200	0.25008300	2.49306600
O	-1.59094000	0.40864400	2.02214800
O	-4.08776000	0.31748700	1.32666800
H	-3.89696200	1.08186700	0.62169300
O	-3.37735400	1.39051300	3.58982600
P	-2.35796900	2.19458400	-1.13494600
O	-3.60127700	2.17197000	-0.24314700
O	-2.79195500	1.86645000	-2.69598100
O	-1.27643600	1.14228200	-0.85060300
C	-3.89301300	2.57286900	-3.30230800
H	-3.66861700	2.59882800	-4.37398300
H	-3.91639500	3.61130900	-2.95139500
C	-3.10921800	2.78174700	3.28793100
H	-2.03029100	2.90879700	3.15228400

H	-3.60470100	3.04647200	2.34783500
C	-5.23380100	1.90073900	-3.03877900
H	-5.23339000	0.87101600	-3.40791600
H	-5.44406200	1.88835200	-1.96773000
H	-6.03182600	2.44791700	-3.55371100
C	-3.62939500	3.61640700	4.44318000
H	-3.13667800	3.33494100	5.37877300
H	-3.43437100	4.67711400	4.25437000
H	-4.70754200	3.47942700	4.56673300
N	-0.87049100	-3.46853000	1.90802700
O	0.04749600	-4.28228000	2.13289300
O	-0.60202800	-2.20398200	1.97773000
O	-2.02913800	-3.83234400	1.65820500
N	2.08936400	3.88948600	-1.83256700
O	1.52409400	4.66244000	-1.02311900
O	3.34327400	3.72956500	-1.79186000
O	1.40600700	3.26774800	-2.69978100
C	-1.62897800	3.85632300	-1.17809000
H	-2.29160600	4.50911900	-1.75854300
H	-0.67386300	3.78851700	-1.71065600
C	-1.40893100	4.44368200	0.22159400
H	-2.35907200	4.61922100	0.73484100
H	-0.80339100	3.76996200	0.83440400
H	-0.86485700	5.38732100	0.13805200
C	-3.40090700	-1.26675100	3.39931000
H	-4.47406900	-1.24594700	3.61706400
H	-3.20939700	-2.09055900	2.70401100
C	-2.56999900	-1.44097500	4.67725100
H	-2.74150500	-0.62199100	5.38122100
H	-2.83785100	-2.38033500	5.17058200
H	-1.50531100	-1.47963500	4.43414500

Table S6. Cartesian coordinates for Eu(TEDGA)₂(HE[EP])₂·3NO₃ complex C.

Atom	Coordinates (Angstroms)		
	X	Y	Z
O	-1.10021600	-2.23024200	1.02252300
C	-1.05209300	-2.58020600	2.40563300
H	-2.05675100	-2.84301900	2.74845900
H	-0.37193500	-3.43454600	2.53892200
C	-1.78904900	-3.19524300	0.23206600
H	-2.85596600	-3.16888800	0.47108900
H	-1.39340800	-4.19842400	0.44535100
C	-0.47274100	-1.38019900	3.12765200
C	-1.46960000	-2.87234000	-1.21643000
O	0.21997000	-0.57006200	2.46812900
O	-0.55124300	-2.06039000	-1.47444500
N	-0.66593400	-1.26764100	4.45244300
N	-2.13837000	-3.52001100	-2.17992600
C	-0.04597000	-0.14573400	5.17489200
H	0.48847200	0.45211400	4.43769100
H	-0.85164500	0.47243700	5.58980400
C	-1.67253200	-2.07388700	5.18192100
H	-1.91624300	-1.50016300	6.08018500
H	-2.58568800	-2.10276100	4.58039000
C	-3.28843900	-4.39808200	-1.88556900
H	-3.32201800	-5.14498400	-2.68347400
H	-3.08738000	-4.95150700	-0.96427600
C	-1.71167900	-3.31937000	-3.58028400
H	-2.03817500	-4.20222100	-4.13645700
H	-0.61938700	-3.31090100	-3.58702900
C	0.90577800	-0.59740800	6.28416400
H	1.71864700	-1.20640900	5.87745400
H	1.34567000	0.27898200	6.77068700
H	0.39278100	-1.17986500	7.05544800
C	-1.20186900	-3.47283400	5.58621300
H	-1.98469100	-3.96115000	6.17514200
H	-1.00396600	-4.10908200	4.71923600
H	-0.29195500	-3.43481800	6.19219000
C	-2.25270700	-2.04053200	-4.22097600
H	-1.86527800	-1.94951300	-5.24128900
H	-3.34527400	-2.04778300	-4.27705800
H	-1.93575500	-1.16435300	-3.65156000
C	-4.62895700	-3.66123600	-1.78235200
H	-4.63318800	-2.92248800	-0.97417800
H	-4.87088900	-3.15346700	-2.72069000
H	-5.42402100	-4.38605000	-1.57872100
Eu	0.06342700	-0.20979100	0.01333800
O	-1.23121000	1.61572100	1.14382700
C	-0.60418000	2.61957200	1.93718300

H	-1.07889900	3.58645800	1.74462900
H	-0.68852100	2.36473900	3.00273800
C	-2.65000000	1.76403200	0.95794900
H	-2.89638700	2.82870000	0.93923100
H	-3.18561400	1.21886200	1.74691300
C	0.86498500	2.62272900	1.53519700
C	-2.94535500	1.11308100	-0.38154400
O	1.31820500	1.60664900	0.95316700
O	-2.08238600	0.33306300	-0.87119100
N	1.63969800	3.66607600	1.86041600
N	-4.08629600	1.38099400	-1.00987000
C	1.08058700	4.94077500	2.36037400
H	1.82234300	5.70651000	2.11953400
H	0.19432600	5.18323400	1.76773000
C	3.04823100	3.67271000	1.41972300
H	3.23107500	2.74387300	0.88052800
H	3.16180500	4.49758000	0.70631600
C	-5.15858400	2.19122900	-0.40797400
H	-6.08946800	1.63056400	-0.54763400
H	-4.99872200	2.23138900	0.67002900
C	-4.31352900	0.79717600	-2.34211100
H	-5.39299500	0.82067600	-2.51618600
H	-4.00626900	-0.25042700	-2.30165600
C	0.80151800	4.96240500	3.86502500
H	1.69993100	4.72923900	4.44463400
H	0.45580900	5.95931900	4.15663200
H	0.02037000	4.25210800	4.15088900
C	4.03513300	3.82618900	2.57725000
H	5.05754900	3.82440000	2.18655300
H	3.89207800	4.76399300	3.12372100
H	3.94185000	2.99849700	3.28733500
C	-3.56546800	1.53413400	-3.45657600
H	-3.76328800	1.04704600	-4.41777900
H	-3.87784300	2.57858900	-3.52413500
H	-2.48948000	1.52200900	-3.27122500
C	-5.26704900	3.60067300	-0.99355900
H	-4.32108200	4.13884400	-0.89329300
H	-5.53599900	3.56843100	-2.05401000
H	-6.05443700	4.15129400	-0.46769300
N	-1.39543800	4.46529100	-0.62960300
O	-0.13747300	4.48532100	-0.50481800
O	-2.11645100	4.81645900	0.35839000
O	-1.92577400	4.08722400	-1.69678000
N	-4.02678200	-1.47514000	2.01120500
O	-3.50441600	-0.68107900	2.84846300
O	-4.08728300	-2.70941900	2.28200400
O	-4.45293300	-1.04862800	0.91047600
N	1.50768400	-4.32147600	-1.40967200
O	2.23416200	-3.21947800	-1.74324000
O	1.11857700	-4.41225500	-0.25108100
O	1.32068000	-5.10912900	-2.31510600
P	3.61740200	-0.85413800	0.38972500

O	4.11789800	0.38139200	-0.33599100
O	2.17256300	-1.32525800	0.00135200
O	4.60815800	-2.11985800	0.14032900
P	1.85446100	1.06192100	-3.01119900
O	0.86772500	0.70150800	-1.90844400
O	1.37538700	2.27703100	-3.92157600
O	3.28437600	1.44051100	-2.46595600
H	3.58656300	1.00817400	-1.57794500
C	5.39976300	-2.24642000	-1.06452500
H	4.79178400	-2.75097800	-1.82349100
H	5.65988800	-1.24755600	-1.42793700
C	1.18067300	3.62164200	-3.36176800
H	2.17423700	4.05674300	-3.21565400
H	0.66544800	3.55586600	-2.40159100
C	0.35303000	4.41675900	-4.34851800
H	0.22355300	5.43317400	-3.96493500
H	0.83687700	4.46843800	-5.32914400
H	-0.64001000	3.97442900	-4.45653500
C	6.63969600	-3.05870700	-0.73633500
H	7.24188500	-3.20076300	-1.63981900
H	7.25347800	-2.54727700	0.01098400
H	6.36739400	-4.04346800	-0.34576000
H	2.18124900	-2.56734900	-0.95487900
C	1.98913500	-0.29100000	-4.20849900
H	2.22140000	-1.19106500	-3.62746000
H	0.98463700	-0.43754900	-4.62041700
C	3.01925400	-0.05838300	-5.32133900
H	3.06022300	-0.92524400	-5.98774100
H	2.75974300	0.82038600	-5.91736200
H	4.01753200	0.09926700	-4.90413700
C	3.69557400	-0.69182800	2.19599900
H	2.90872100	0.01767700	2.46865900
H	3.41079900	-1.66303200	2.61482800
C	5.06843900	-0.24353600	2.71151800
H	5.35769400	0.71367700	2.26957100
H	5.05367700	-0.12915400	3.80021600
H	5.83890400	-0.97765400	2.45965900

Table S7. Cartesian coordinates for Eu(TEDGA)₂(HE[EP])₂·3NO₃ complex D.

Atom	Coordinates (Angstroms)		
	X	Y	Z
O	0.36880800	-1.61579300	-1.10436300
C	0.53655300	-1.27260400	-2.48200500
H	1.51391400	-1.62952000	-2.84364400
H	-0.28151900	-1.70514600	-3.07223100
C	0.39279200	-3.02051800	-0.88074700
H	1.28884100	-3.46281000	-1.33862900
H	-0.50822900	-3.47418900	-1.30859000
C	0.49699200	0.24135000	-2.55800900
C	0.41401200	-3.22050700	0.63241500
O	0.35605500	0.90571700	-1.50300400
O	0.57780500	-2.21871000	1.36891900
N	0.58393100	0.84300700	-3.75243400
N	0.24438900	-4.44048200	1.15050300
C	0.59849000	2.31678300	-3.77061600
H	1.22653100	2.65007900	-2.94028600
H	1.08930100	2.61764200	-4.69958300
C	0.96013400	0.12112000	-4.98090900
H	1.74160900	0.71369800	-5.46591200
H	1.44694200	-0.81645300	-4.70999800
C	-0.02508400	-5.64870800	0.35130500
H	-1.06029600	-5.94368600	0.54716800
H	0.02017800	-5.39126300	-0.70556100
C	0.09178300	-4.54603600	2.61768800
H	-0.45771200	-5.47142000	2.80525700
H	-0.54564500	-3.71996100	2.93858300
C	-0.79186200	2.94704300	-3.66838900
H	-1.30775400	2.60804100	-2.76682100
H	-0.70262000	4.03819800	-3.62482800
H	-1.40732200	2.69843900	-4.53846100
C	-0.21196600	-0.10273300	-5.93768300
H	0.13603000	-0.62501900	-6.83462500
H	-0.99594100	-0.71116600	-5.47571300
H	-0.65976800	0.84475900	-6.25474400
C	1.41879100	-4.52722700	3.37733400
H	1.22716600	-4.62173200	4.45129800
H	2.07068200	-5.35248300	3.07567900
H	1.94505100	-3.58492400	3.20940100
C	0.95822700	-6.78387100	0.63980200
H	1.98813900	-6.48385300	0.42241000
H	0.91066600	-7.11516200	1.68106100
H	0.71199800	-7.64371900	0.00916400
Eu	0.67744900	0.08485100	0.74108300
O	2.48011000	1.90485200	0.30678700
C	2.25125900	3.28759500	0.49628900

H	2.86679700	3.66039800	1.32603800
H	2.49676000	3.84878700	-0.41671900
C	3.82285000	1.57531100	-0.03413000
H	4.50784100	2.02442900	0.69326100
H	4.04715900	1.91449900	-1.05308600
C	0.76813100	3.43934100	0.84229500
C	3.92526600	0.05405300	0.00099300
O	0.06293600	2.42039000	0.95548300
O	2.88799800	-0.62343500	0.19411700
N	0.24663300	4.66536400	1.01047100
N	5.11160800	-0.52429800	-0.18895200
C	1.03288600	5.90265700	0.94449000
H	0.81688400	6.47899200	1.85135500
H	2.09443800	5.65431500	0.99128200
C	-1.18874900	4.76089600	1.36322300
H	-1.39694700	4.00301100	2.12198700
H	-1.32970300	5.74583600	1.81836000
C	6.33895400	0.21747100	-0.52148000
H	6.64139500	-0.10758400	-1.52086800
H	6.10011700	1.27747500	-0.60798100
C	5.16159400	-1.99943000	-0.27744200
H	6.07133500	-2.24621200	-0.82839500
H	4.32025400	-2.32333100	-0.89435600
C	0.74498100	6.74938900	-0.29844400
H	-0.30063700	7.06700200	-0.33150600
H	1.36898700	7.64862300	-0.28892900
H	0.95938800	6.19145700	-1.21515200
C	-2.13941200	4.56685200	0.17974100
H	-3.17144100	4.67871000	0.52619800
H	-1.96296800	5.30330200	-0.61042000
H	-2.04138700	3.56401300	-0.24061400
C	5.13008800	-2.68918300	1.08713800
H	5.16955900	-3.77519600	0.94975800
H	5.98055100	-2.39521200	1.70911100
H	4.21094500	-2.44233900	1.62329800
C	7.44976700	0.02562700	0.51221700
H	7.13192300	0.36003300	1.50457600
H	7.75677500	-1.02163200	0.58638900
H	8.32940100	0.60605000	0.21592800
N	2.45769300	1.44736300	3.13785900
O	1.60562900	0.50023100	2.84485700
O	3.66660500	1.21745200	3.01697800
O	2.00923000	2.53958900	3.52396100
N	4.06323600	-0.79243500	-3.26207300
O	3.45679200	0.26476600	-2.90846000
O	3.39332300	-1.82108500	-3.57892400
O	5.31074700	-0.82785200	-3.29524600
N	-2.98382500	-3.57357800	0.24069500
O	-3.43837200	-2.37371800	0.08085000
O	-2.55673900	-4.19092200	-0.75879800
O	-2.98235900	-4.06238800	1.38112500
P	-4.00148100	0.04231500	-2.19062300

O	-3.55735400	1.09692200	-1.19282300
O	-3.16606900	-1.29818500	-2.17481100
O	-5.57386900	-0.31455100	-2.05547100
P	-2.73495000	0.44215900	2.24666200
O	-1.44661100	-0.00809600	1.57607400
O	-2.48851300	1.63739300	3.30707800
O	-3.81081600	1.06697800	1.29309600
H	-3.64048900	1.06326900	0.26821300
C	-6.18156000	-0.59736900	-0.76664900
H	-5.69897400	-1.47950900	-0.33370200
H	-6.00993600	0.25370000	-0.10006100
C	-1.42877100	1.54294200	4.29996700
H	-0.45915300	1.59081400	3.80006400
H	-1.50311100	0.58161800	4.82389400
C	-1.60279800	2.69215400	5.27431300
H	-0.80934600	2.65597700	6.02705800
H	-1.53451200	3.65293300	4.75585900
H	-2.57128600	2.64055000	5.78055400
C	-7.66197800	-0.83201800	-0.99891600
H	-8.15684400	-1.04925000	-0.04680000
H	-8.13242900	0.05215600	-1.43928700
H	-7.81978000	-1.68010700	-1.67122800
H	-3.22384300	-1.83489100	-1.28179200
C	-3.91077500	0.60653400	-3.90774600
H	-2.84646800	0.71221400	-4.13983700
H	-4.29747100	-0.20616900	-4.53091700
C	-4.66732800	1.91622800	-4.16147100
H	-4.56129700	2.22365000	-5.20641000
H	-5.73282200	1.79621700	-3.94849600
H	-4.28347000	2.71841000	-3.52541200
C	-3.48752200	-0.93372300	3.15227000
H	-3.57168100	-1.75728800	2.43484400
H	-2.75643300	-1.25145500	3.90543500
C	-4.83681800	-0.59759700	3.80059400
H	-5.57143900	-0.30818300	3.04471100
H	-5.22426800	-1.47037600	4.33434500
H	-4.74730000	0.22728000	4.51376000

References

1. Cataldo, D.; Haroon, M.; Schrader, L.; Youngs, V. L., Rapid Colorimetric Determination of Nitrate in Plant Tissue by Nitration of Salicylic Acid. *Comm. Soil Sci. Plant Anal.* **1975**, *6*, 71-80.
2. Chaiko, D. J.; Fredrickson, D. R.; Reichley-yinger, L.; Vandegrift, G. F., Thermodynamic Modeling of Chemical Equilibria in Metal Extraction. *Sep. Sci. Technol.* **1988**, *23*, 1435-1451.
3. Tkac, P.; Paulenova, A.; Vandegrift, G. F.; Krebs, J. F., Modeling of Pu(IV) Extraction from Acidic Nitrate Media by Tri-n-butyl Phosphate. *J. Chem. Eng. Data* **2009**, *54*, 1967-1974.
4. Skerencak, A.; Panak Petra, J.; Hauser, W.; Neck, V.; Klenze, R.; Lindqvist-Reis, P.; Fanghänel, T., TRLFS Study on the Complexation of Cm(III) with Nitrate in the Temperature Range from 5 to 200 °C. *Radiochim. Acta* **2009**, *97*, 385-393.
5. Kimura, T.; Kato, Y., Luminescence Study on Determination of the Inner-sphere Hydration Number of Am(III) and Nd(III). *J. Alloys Compd.* **1998**, *271-273*, 867-871.
6. Lindqvist-Reis, P.; Apostolidis, C.; Rebizant, J.; Morgenstern, A.; Klenze, R.; Walter, O.; Fanghänel, T.; Haire, R. G., The Structures and Optical Spectra of Hydrated Transplutonium Ions in the Solid State and in Solution. *Angew. Chem. Int. Ed. Engl.* **2007**, *46* (6), 919-922.
7. Wang, X.-B.; Yang, X.; Wang, L.-S.; Nicholas, J. B., Photodetachment and theoretical study of free and water-solvated nitrate anions, $\text{NO}_3^-(\text{H}_2\text{O})_n$ ($n=0-6$). *J. Chem. Phys.* **2002**, *116*, 561-570.
8. Goebbert, D. J.; Garand, E.; Wende, T.; Bergmann, R.; Meijer, G.; Asmis, K. R.; Neumark, D. M., Infrared Spectroscopy of the Microhydrated Nitrate Ions $\text{NO}_3^-(\text{H}_2\text{O})_{1-6}$. *J. Phys. Chem. A* **2009**, *113*, 7584-7592.
9. Levanov, A. V.; Isaikina, O. Y.; Lunin, V. V., Dissociation constant of nitric acid. *Russ. J. Phys. Chem. A* **2017**, *91*, 1221-1228.
10. Silva, R. J.; Bidoglio, G.; Rand, M. H.; Robouch, P. B.; Wanner, H.; Puigdomenech, I., *Chemical Thermodynamics of Americium*. Elsevier: New York, 1995; Vol. 2.
11. Lalleman, S.; Bertrand, M.; Plasari, E.; Sorel, C.; Moisy, P., Determination of the Bromley contributions to estimate the activity coefficient of neodymium electrolytes. *Chem. Eng. Sci.* **2012**, *77*, 189-195.
12. Borge, G.; Castaño, R.; Carril, M. P.; Corbillón, M. S.; Madariaga, J. M., Development of a Modified Bronley's Methodology (MBM) for the Estimation of Ionic Media Effects of Solution Equilibria. Part 1. Calculation of the Interaction Parameters in the Molar and Molal Scales at 25 °C. *Fluid Phase Equil.* **1996**, *121*, 85-98.
13. Clegg, S. L.; Brimblecombe, P., Equilibrium Partial Pressure and Mean Activity and Osmotic Coefficients of 0-100 % Nitric Acid as a Function of Temperature. *J. Phys. Chem.* **1990**, *94*, 5369-5380.
14. Caceci, M. S., Estimating Error Limits in Parametric Curve Fitting. *Anal. Chem.* **1989**, *61*, 2324-2327.