

Determining the isotopic composition of elements from the electrospray ionization mass spectra of their chemical species

AUTHORS: E. Blanchard^{a b #}, E. Paredes^{a £}, A. Rincel^a, A. Nonell^a, F. Chartier^c, C. Bresson^{a*}

^a Université Paris-Saclay, CEA, Service d'Etudes Analytiques et de Réactivité des Surfaces F-91191, Gif-sur-Yvette, France

^b Sorbonne Université, F-75005 Paris, France

^c Université Paris-Saclay, CEA, Département de Physico-Chimie F-91191 Gif-sur-Yvette, France

Current address:

[#] Normandie Univ, UNIROUEN, Ecodiv, 76000 Rouen, France

[£] Departament de Dinàmica de la Terra i de l'Oceà, Facultat de Ciències de la Terra, Universitat de Barcelona, 08028 Barcelona, Spain

* CORRESPONDING AUTHOR:

Carole BRESSON

Tel: +33 (0)169088348

E-mail address: carole.bresson@cea.fr

KEYWORDS:

Isotopic composition, deconvolution, lanthanides, ESIMS, electrospray ionization mass spectrometry, chemical species, speciation

Supplementary information:

Table S1: ^{nat}Nd isotope ratios determined after deconvolution of ^{nat}Nd -EDTA mass spectra acquired using ESI-QqQ-MS and ESI-LIT-MS. The measured ratios were based on the average of ten measurements. Trueness after deconvolution was calculated in comparison with the reference ^{nat}Nd isotope ratios obtained by TIMS¹³. Repeatability was expressed at k=2 after deconvolution

^{nat}Nd isotope ratios		$^{142}\text{Nd}/^{144}\text{Nd}$	$^{143}\text{Nd}/^{144}\text{Nd}$	$^{145}\text{Nd}/^{144}\text{Nd}$	$^{146}\text{Nd}/^{144}\text{Nd}$	$^{148}\text{Nd}/^{144}\text{Nd}$	$^{150}\text{Nd}/^{144}\text{Nd}$
TIMS reference value ¹³		1.1397	0.5110	0.3487	0.7233	0.2430	0.2382
ESI-QqQ-MS	Average (n=10)	1.1745	0.5186	0.3524	0.7191	0.2422	0.2376
	Trueness (%)	3.1	1.5	1.1	-0.6	-0.4	-0.2
	Repeatability (%)	2.8	4.5	3.0	3.1	2.9	3.3
ESI-LIT-MS	Average (n=10)	1.1520	0.5110	0.3468	0.7339	0.2435	0.2367
	Trueness (%)	1.1	0.0	-0.6	1.5	0.2	-0.6
	Repeatability (%)	0.6	1.0	0.8	0.4	0.8	0.9

Table S2: ^{nat}Sm isotope ratios determined after deconvolution of ^{nat}Sm -DTPA mass spectra acquired using ESI-QqQ-MS and ESI-LIT-MS. The measured ratios were based on the average of ten measurements. Trueness after deconvolution was calculated in comparison with the reference ^{nat}Sm isotope ratios obtained by TIMS data as a reference¹³. Repeatability was expressed at k=2 after deconvolution

^{nat}Sm isotope ratios		$^{144}\text{Sm}/^{150}\text{Sm}$	$^{147}\text{Sm}/^{150}\text{Sm}$	$^{148}\text{Sm}/^{150}\text{Sm}$	$^{149}\text{Sm}/^{150}\text{Sm}$	$^{152}\text{Sm}/^{150}\text{Sm}$	$^{154}\text{Sm}/^{150}\text{Sm}$
TIMS reference value ¹³		0.4194	2.0365	1.5257	1.8739	3.6173	3.0733
ESI-QqQ-MS	Average (n=10)	0.4193	2.0222	1.5223	1.8501	3.5812	3.0147
	Trueness (%)	0.0	-0.7	-0.2	-1.3	-1.0	-1.9
	Repeatability (%)	1.0	0.6	0.8	1.0	0.8	0.8
ESI-LIT-MS	Average (n=10)	0.4094	2.0124	1.5152	1.8621	3.5750	3.0273
	Trueness (%)	-2.4	-1.2	-0.7	-0.6	-1.2	-1.5
	Repeatability (%)	0.6	0.5	0.3	0.2	0.3	0.4

Figure captions

Figure S1: Isotopic patterns of ^{nat}Nd -DPTA and ^{nat}Nd a) experimental mass spectrum of ^{nat}Nd -DPTA recorded by ESI-LIT-MS in full scan mode, b) reference ^{nat}Nd isotopic pattern obtained by TIMS¹³, c) ^{nat}Nd -DPTA isotopic pattern calculated with the Yergey convolution method¹⁷ d) ^{nat}Nd isotopic pattern obtained by deconvolution of the experimental ESI mass spectrum of ^{nat}Nd -DPTA

Figure S2: Isotopic patterns of ^{nat}Nd -EDTA and ^{nat}Nd a) experimental mass spectrum of ^{nat}Nd -EDTA recorded by ESI-LIT-MS in full scan mode, b) reference ^{nat}Nd isotopic pattern obtained by TIMS¹³, c) ^{nat}Nd -EDTA isotopic pattern calculated with the Yergey convolution method¹⁷ d) ^{nat}Nd isotopic pattern obtained by deconvolution of the experimental ESI mass spectrum of ^{nat}Nd -EDTA

Figure S3: Isotopic patterns of ^{nat}Sm -DPTA and ^{nat}Sm a) experimental mass spectrum of ^{nat}Sm -DPTA recorded by ESI-LIT-MS in full scan mode, b) reference ^{nat}Sm isotopic pattern obtained by TIMS¹³, c) ^{nat}Sm -DPTA isotopic pattern calculated with the Yergey convolution method¹⁷ d) ^{nat}Sm isotopic pattern obtained by deconvolution of the experimental ESI mass spectrum of ^{nat}Sm -DPTA

Figure S1

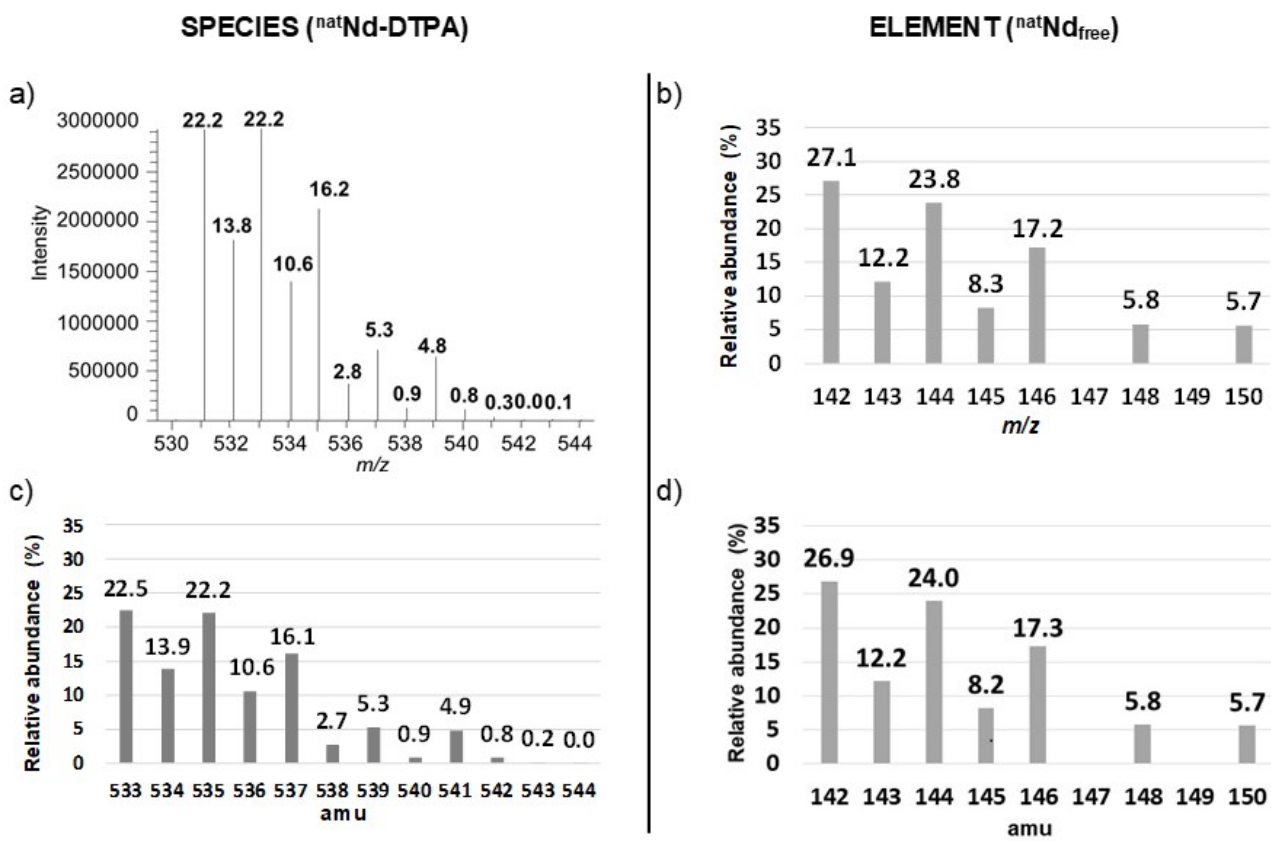


Figure S2

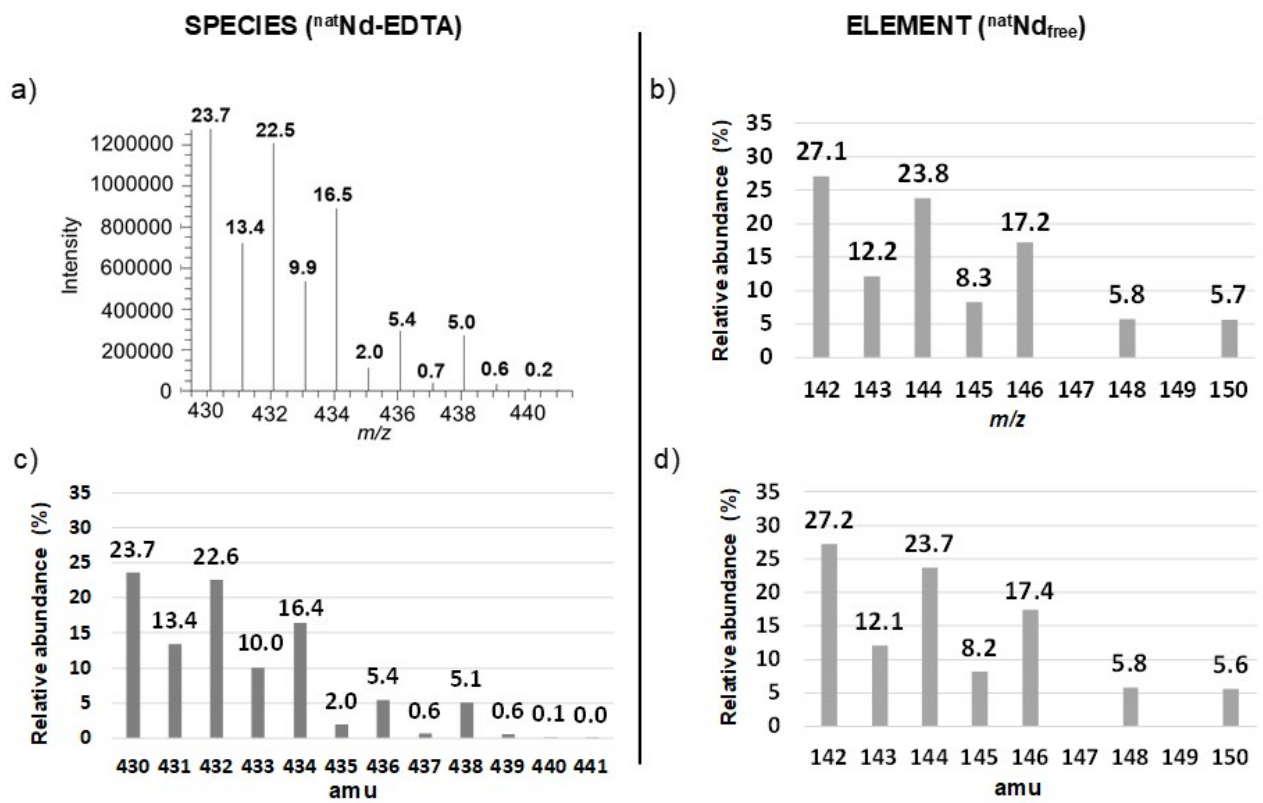


Figure S3

