

Supporting Information for:

One-step chromatographic purification of K, Ca, and Sr from geological samples for high precision stable and radiogenic isotope analysis by MC-ICP-MS

Xiaoqiang Li, Guilin Han*

Institute of Earth Sciences, China University of Geosciences (Beijing), Beijing 100083, China

*Corresponding author E-mail: hanguilin@cugb.edu.cn.

Xiaoqiang Li: xiaoqli@cugb.edu.cn.

Contents of this file

Figures S1

Tables S1–S3

Introduction

This supporting information provides the detailed description of methodology, figures, and tables to support the results presented in the main text.

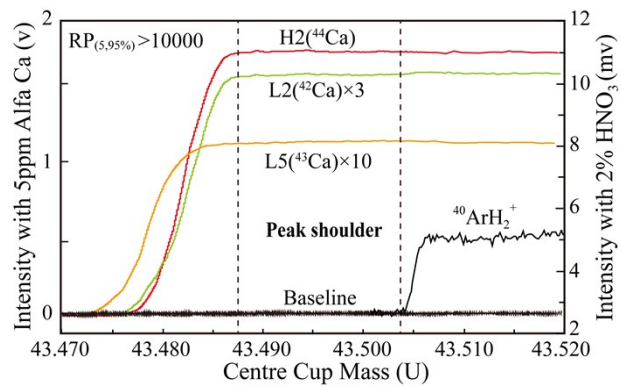


Fig. S1. A peak scan of the Alfa 5 ppm Ca solution left and 2 vol% HNO₃ right under high-resolution model on a Nu Plasma 3.

1 **Table S1.** Potential elemental and molecular isobaric interferences affecting K-Ca
 2 Isotopic Measurements.³¹

Isotope	Interference (required resolution)
³⁹ K ⁺	²³ Na ¹⁶ O ⁺ (1858); ³⁸ ArH ⁺ (5688)
⁴¹ K ⁺	²⁵ Mg ¹⁶ O ⁺ (2165); ²³ Na ¹⁸ O ⁺ (1511); ⁴⁰ ArH ⁺ (4888); ⁴⁰ CaH ⁺ (4768)
⁴² Ca ⁺	⁸⁴ Kr ⁺⁺ (14627); ⁸⁴ Sr ⁺⁺ (21993); ⁴¹ KH ⁺ (3805); ³⁰ Si ¹² C ⁺ (2770); ²⁶ Mg ¹⁶ O ⁺ (2221); ⁴⁰ ArH ₂ ⁺ (2161); ⁴⁰ CaH ₂ ⁺ (2139); ²⁸ Si ¹⁴ N ⁺ (1962); ²⁴ Mg ¹⁸ O ⁺ (1640); ²⁵ Mg ¹⁶ OH ⁺ (1401); ¹⁴ N ₃ ⁺ (829)
⁴³ Ca ⁺	⁸⁶ Sr ⁺⁺ (10392); ⁸⁶ Kr ⁺⁺ (12404); ⁴² CaH ⁺ (5596); ²⁷ Al ¹⁶ O ⁺ (2429); ³¹ P ¹² C ⁺ (2865); ²⁶ Mg ¹⁶ OH ⁺ (1617); ¹⁴ N ₃ H ⁺ (737)
⁴⁴ Ca ⁺	⁸⁸ Sr ⁺⁺ (16448); ⁴³ CaH ⁺ (3956); ²⁸ Si ¹⁶ O ⁺ (2687); ³² S ¹² C ⁺ (2650); ³⁰ Si ¹⁴ N ⁺ (2058); ²⁶ Mg ¹⁸ O ⁺ (1673); ²⁷ Al ¹⁶ OH ⁺ (1526); ¹² C ¹⁶ O ₂ ⁺ (1280); ¹⁴ N ₂ ¹⁶ O ⁺ (964)

Table S2. Testing the influences of double charge Sr on Ca isotopic analysis.

Ca/Sr	⁴⁴ Ca(V)	⁸⁸ Sr(mV)	^{43.5} Sr(mV)	$\delta^{44/42}\text{Ca}$	2SD	N	$\delta^{43/42}\text{Ca}$	2SD	N
100000	1.51	2.6	0.1	0.03	0.05	5	0.02	0.06	5
50000	1.51	3.6	0.2	0.07	0.04	5	0.13	0.07	5
20000	1.52	5.1	0.2	0.11	0.05	5	0.38	0.17	5
10000	1.52	11.6	0.2	0.21	0.06	5	0.58	0.18	5
7000	1.51	15.9	0.2	0.44	0.05	5	0.83	0.13	5
5000	1.52	22.1	0.3	0.53	0.07	5	1.05	0.17	5
3000	1.51	35.6	0.2	0.91	0.10	5	1.70	0.15	5
1000	1.51	103.1	0.3	2.89	0.27	5	5.27	0.47	5

Table S3. Ca isotopic composition of geological standards in this study and in the literature.

Sample	Reference	Method ^a	Ca (wt.%)	Ca/Sr after purification	$\delta^{44/42}\text{Ca}$	2SD ^b	N ^c
SRM 915b	This study		55.9	162000	0.34	0.05	20
	1	SSB, MC-ICP-MS			0.36	0.07	
	2	SSB, MC-ICP-MS			0.36	0.05	67
	3	SSB, MC-ICP-MS			0.36	0.01	3
	4	SSB, MC-ICP-MS			0.38	0.04	2
	5	SSB, MC-ICP-MS			0.35	0.02	2
	6	SSB, MC-ICP-MS			0.34	0.06	15
	7	DS-TIMS ^d			0.36	0.07	41
8	DS-TIMS			0.35	0.05	38	
Seawater, Atlantic	This study		0.04	94800	0.89	0.05	10
	9	SSB, MC-ICP-MS			0.86	0.08	6
	3	SSB, MC-ICP-MS			0.91	0.07	4
AGV-2, Andesite, USGS	This study		3.72	83100	0.34	0.04	12
	9	SSB, MC-ICP-MS			0.36	0.05	4
	2	SSB, MC-ICP-MS			0.33	0.04	6
	10	SSB, MC-ICP-MS			0.38	0.08	3
	7	DS-TIMS			0.35	0.04	3
	11	DS-TIMS			0.35	0.05	8
	8	DS-TIMS			0.38	0.04	9
	1	SSB, MC-ICP-MS			0.31	0.05	3
BCR-2, Basalt, USGS	This study		5.09	113500	0.39	0.04	9
	2	SSB, MC-ICP-MS			0.38	0.07	30
	5	SSB, MC-ICP-MS			0.40	0.02	4
	4	SSB, MC-ICP-MS			0.34	0.06	2
	10	SSB, MC-ICP-MS			0.42	0.15	3
	9	SSB, MC-ICP-MS			0.39	0.07	4
	3	SSB, MC-ICP-MS			0.41	0.05	4
	10	SSB, MC-ICP-MS			0.42	0.15	3
	7	DS-TIMS			0.38	0.06	4
	11	DS-TIMS			0.40	0.04	12
8	DS-TIMS			0.39	0.06	24	
BHVO-2, Basalt,	This study		8.17	89000	0.38	0.05	9

Hawaiian, USA	2	SSB, MC-ICP-MS			0.38	0.06	41
	3	SSB, MC-ICP-MS			0.41	0.05	5
	9	SSB, MC-ICP-MS			0.43	0.08	27
	4	SSB, MC-ICP-MS			0.38	0.06	2
	10	SSB, MC-ICP-MS			0.42	0.08	10
	12	DS-TIMS			0.44	0.05	5
	7	DS-TIMS			0.38	0.03	7
	11	DS-TIMS			0.39	0.05	16
	8	DS-TIMS			0.37	0.05	12
GSP-2, Granodiorite, USGS	This study		1.50	92800	0.35	0.05	12
	9	SSB, MC-ICP-MS			0.40	0.10	5
	2	SSB, MC-ICP-MS			0.33	0.03	5
	7	DS-TIMS			0.32	0.01	3
	1	SSB, MC-ICP-MS			0.27	0.02	6
JG-2, Granite, Japan	This study		0.51	108600	0.37	0.04	9
	11	DS-TIMS			0.31	0.06	3
RGM-2, Rhyolite, USGS	This study		0.88	98300	0.42	0.05	7
	11	DS-TIMS			0.38	0.05	6
	8	DS-TIMS			0.39	0.13	3
	9	SSB, MC-ICP-MS			0.44	0.04	4
W-2a, diabase, USGS	This study		7.76	113400	0.40	0.07	9
	11	DS-TIMS			0.41	0.09	9
	8	DS-TIMS			0.34	0.08	3
	13	DS-TIMS			0.46	0.24	
DNC-1a, dolerite, USGS	This study		8.22	124600	0.40	0.03	8
	2	SSB, MC-ICP-MS			0.41	0.03	4
	3	SSB, MC-ICP-MS			0.40	0.05	4
	4	SSB, MC-ICP-MS			0.38	0.04	2
	11	DS-TIMS			0.41	0.03	5
	8	DS-TIMS			0.40	0.04	9

^a Measurement method include double spike TIMS method (DS-TIMS) and standard-sample standard bracketing MC-ICP-MS method (SSB, MC-ICP-MS);

^b 2SD, 2 standard deviation;

^c replicate was measured from independent digestion of the given sample;

^d All the literature data were converted to the $\delta^{44/42}\text{Ca}$ from $\delta^{44/40}\text{Ca}$ by dividing 2.048, if only $\delta^{44/40}\text{Ca}$ has been reported and the corresponding uncertainty is also divided by 2.0

References

1. C. Chen, W. Dai, Z. Wang, Y. Liu, M. Li, H. Becker and S. F. Foley, *Geochimica et Cosmochimica Acta*, 2019, **249**, 121-137.
2. M. Li, Y. Lei, L. Feng, Z. Wang, N. S. Belshaw, Z. Hu, Y. Liu, L. Zhou, H. Chen and X. Chai, *Journal of Analytical Atomic Spectrometry*, 2018, **33**, 1707-1719.
3. L. Feng, L. Zhou, Y. Lu, W. Zhang, Q. Wang, S. Tong and Z. Hu, *Journal of Analytical Atomic Spectrometry*, 2018, **33**, 413-421.
4. M. Schiller, C. Paton and M. Bizzarro, *Journal of Analytical Atomic Spectrometry*, 2012, **27**, 38-49.
5. C. A. Colla, J. Wimpenny, Q.-Z. Yin, J. R. Rustad and W. H. Casey, *Geochimica Et Cosmochimica Acta*, 2013, **121**, 363-373.
6. K. Harouaka, M. Mansor, J. L. Macalady and M. S. Fantle, *Geochimica Et Cosmochimica Acta*, 2016, **184**, 114-131.
7. Y. He, Y. Wang, C. Zhu, S. Huang and S. Li, *Geostandards and Geoanalytical Research*, 2017, **41**, 283-302.
8. L.-p. Feng, L. Zhou, L. Yang, D. J. DePaolo, S.-Y. Tong, Y.-S. Liu, T. L. Owens and S. Gao, *Geostandards and Geoanalytical Research*, 2017, **41**, 93-106.
9. Z. Bao, C. Zong, K. Chen, N. Lv and H. Yuan, *International Journal of Mass Spectrometry*, 2020, **448**, 116268.
10. M. C. Valdes, M. Moreira, J. Foriel and F. Moynier, *Earth and Planetary Science Letters*, 2014, **394**, 135-145.
11. F. Liu, H. L. Zhu, X. Li, G. Q. Wang and Z. F. Zhang, *Geostandards and Geoanalytical Research*, 2017, **41**, 675-688.
12. T. Magna, N. Gussone and K. Mezger, *Earth and Planetary Science Letters*, 2015, **430**, 86-94.
13. M. Amini, A. Eisenhauer, F. Böhm, C. Holmden, K. Kreissig, F. Hauff and K. P. Jochum, *Geostandards and Geoanalytical Research*, 2009, **33**, 231-247.