

Supplementary Information

Trace element analysis in lithium matrices using Micro-Discharge Optical Emission Spectroscopy

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The following supplementary information provides additional raw data to support the presented results of the corresponding paper. The tables list the intensities of the emission lines used at the respective time and/or concentration level.

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Table A1 Intensities in a.u. of Li 670.7 nm and Li 812.6 nm at different integration settings (n=3).

Li in mg/L	Single pulse			Pulse series		
	Li 670.7 nm	Li 812.6 nm	H 486.1 nm	Li 670.7 nm	Li 812.6 nm	H 486.1 nm
0	0.21	0.07	77.01	0	9.20	3721.94
0.05	32.38	0.69	78.98	1452.95	16.70	3681.78
0.10	86.98	0.88	84.94	4177.26	44.96	4083.04
0.25	249.38	2.36	87.26	11774.45	126.45	4177.04
0.50	459.25	5.28	89.63	17525.73*	263.66	4401.03
0.75	672.98	8.06	95.55	20895.38	412.50	4731.98
1.0	853.28	10.94	95.80	22678.47	562.17	4529.98
1.25	981.98	13.48	88.73	24164.93	726.54	4241.60
2.0	1207.43*	20.00	83.20	26686.96	1046.07	3969.43
2.5	1368.11	24.31	82.11	28274.34	1289.25	3791.57
3.0	1482.69	28.91	80.06	29654.30	1515.92	3790.98
5.0	1925.02	46.09	81.10	34075.35	2377.08*	3935.69
10	3325.13	110.93	93.50	44276.69	4891.86	4494.34

*linear model no longer accepted according to Mandel's linearity test ($\alpha=0.99$)

Table A2 Intensities in a.u. of Li 670.7 nm and Li 812.6 nm of the blank measurements (n=20), which were used to calculate the detection limits.

No	Single pulse			Pulse series		
	Li 670.7 nm	Li 812.6 nm	H 486.1 nm	Li 670.7 nm	Li 812.6 nm	H 486.1 nm
1	0.12	0.17	46.35	0*	1.32	3721.94
2	0.23	0.58	75.91	0	5.63	3610.46
3	0.70	0.22	80.43	20.94	6.77	3768.39
4	0.14	0.10	77.00	70.30	8.45	3728.54
5	1.25	0.78	79.91	100.70	12.17	3835.45
6	1.26	0.40	75.48	137.12	9.68	3698.89
7	0.82	0.36	78.48	133.23	11.53	3804.26
8	0.93	0.26	78.14	0	9.58	3851.39
9	0.49	0.02	77.74	69.88	10.24	3723.37
10	1.22	0.04	80.05	131.76	9.09	3948.18
11	1.59	0.67	79.06	191.08	8.28	3769.71
12	0.77	0.51	78.39	198.21	11.15	3837.30
13	2.47	0.26	77.10	334.22	10.97	3651.31
14	4.65	0.23	76.11	496.84	14.91	3754.19
15	4.53	0.17	71.16	504.61	15.05	3590.59
16	1.57	0.34	71.55	37.88	11.38	3487.08
17	1.40	0.24	74.82	0	9.74	3454.30
18	0.97	0.21	75.49	0	8.30	3692.85
19	0.26	0.79	74.81	0	10.43	3792.57
20	0.04	0.26	75.81	0	9.42	3519.14

*negative intensity values were set to zero

Table A3 Intensities in a.u. of the lithium and sodium calibration series, which were used for the multi-linear regression model.

Li in mg/L	Na in µg/L	Parameter setting C		
		Li 812.6 nm	Na 589.5 nm	H 486.1 nm
0	0	31.95	19.17	5513.13
0	0	30.24	17.80	5498.74
0	0	30.31	15.14	5226.02
0	0	31.80	15.63	5311.85
0	0	31.95	19.17	5513.13
0.3	0	121.01	16.96	4497.36
0.3	0	171.97	19.80	5735.83
0.3	0	133.46	16.94	4866.81
0.3	0	135.54	17.55	4917.01
0.3	0	153.29	19.42	5678.53
0.3	9	147.18	75.56	5492.92
0.3	9	175.80	87.72	6081.90
0.3	9	147.34	77.56	5079.33
0.3	9	129.48	73.51	4889.01
0.3	9	148.57	78.05	5371.25
0.3	18	160.96	145.08	5571.51
0.3	18	143.54	131.10	5205.34
0.3	18	160.13	143.54	5704.73
0.3	18	145.24	130.01	5152.02

Li in mg/L	Na in µg/L	Parameter setting C		
		Li 812.6 nm	Na 589.5 nm	H 486.1 nm
0.3	18	134.00	122.59	4873.24
0.3	27	165.94	212.57	5671.71
0.3	27	175.23	226.83	5816.24
0.3	27	164.49	212.81	5646.74
0.3	27	149.22	195.00	5274.35
0.3	27	144.89	184.29	5254.30
0.3	36	149.36	252.30	5084.08
0.3	36	153.23	261.12	6471.27
0.3	36	161.39	264.86	5454.74
0.3	36	168.47	277.75	6181.78
0.3	36	171.92	273.16	6206.94
0.3	44	159.75	320.00	5418.20
0.3	44	135.49	278.34	4926.80
0.3	44	158.21	316.16	5504.59
0.3	44	164.12	331.00	5815.90
0.3	44	153.55	304.49	5656.14
0.6	0	303.09	20.16	5491.79
0.6	0	307.48	18.07	5492.35
0.6	0	341.77	19.67	5814.50
0.6	0	320.75	19.65	5740.92
0.6	0	354.53	20.43	5844.05
0.6	9	342.34	84.10	5955.23
0.6	9	262.15	69.00	5003.98
0.6	9	344.78	89.22	5961.93
0.6	9	337.30	87.69	6105.47
0.6	9	305.09	81.11	5476.45
0.6	18	306.50	142.29	5602.66
0.6	18	327.82	149.57	5924.28
0.6	18	315.93	144.88	5407.83
0.6	18	285.21	133.03	5401.59
0.6	18	325.20	151.28	5870.98
0.6	27	339.88	225.31	6111.97
0.6	27	323.97	211.80	5634.19
0.6	27	308.47	202.26	5561.49
0.6	27	348.10	225.20	5815.77
0.6	27	350.82	232.52	5828.55
0.6	36	322.81	271.88	5667.80
0.6	36	323.18	273.90	5996.75
0.6	36	319.62	272.68	5655.83
0.6	36	319.41	277.24	5691.92
0.6	36	325.56	272.69	6010.36
0.6	44	318.96	348.23	5697.90
0.6	44	282.53	294.96	5413.81
0.6	44	298.17	318.44	5460.31
0.6	44	301.63	303.22	5467.86
0.6	44	296.45	312.07	5536.93
0.9	0	611.17	25.28	5772.72
0.9	0	547.72	20.45	5490.40
0.9	0	531.62	25.73	6857.30
0.9	0	533.02	19.00	5385.13

Li in mg/L	Na in µg/L	Parameter setting C		
		Li 812.6 nm	Na 589.5 nm	H 486.1 nm
0.9	0	469.22	20.75	4965.01
0.9	9	532.55	86.56	5526.88
0.9	9	582.50	99.40	6402.02
0.9	9	539.90	92.72	5614.92
0.9	9	518.97	86.87	5482.81
0.9	9	510.85	87.77	5526.04
0.9	18	494.74	148.06	5460.81
0.9	18	562.11	169.57	5869.33
0.9	18	455.44	136.37	5164.16
0.9	18	558.56	164.72	5864.12
0.9	18	469.43	141.46	5187.79
0.9	27	478.32	207.74	5535.40
0.9	27	492.48	210.49	5368.05
0.9	27	539.24	234.61	5730.12
0.9	27	443.27	194.11	5194.09
0.9	27	537.13	226.04	5679.35
0.9	36	541.29	300.33	6175.64
0.9	36	553.64	306.50	5762.29
0.9	36	592.35	327.50	6185.11
0.9	36	508.63	279.99	5765.77
0.9	36	538.46	299.63	6979.42
0.9	44	453.85	320.77	5157.15
0.9	44	524.37	355.60	5672.68
0.9	44	534.93	357.54	5816.74
0.9	44	464.49	314.64	5342.94
0.9	44	498.84	335.99	5683.25
1.2	0	674.56	27.41	5405.29
1.2	0	784.12	26.74	6386.23
1.2	0	757.80	21.26	5806.78
1.2	0	638.99	18.44	5255.19
1.2	0	813.40	21.74	5794.53
1.2	9	762.07	92.77	5698.49
1.2	9	785.46	97.59	5954.89
1.2	9	701.84	90.58	5465.10
1.2	9	640.18	82.17	5301.19
1.2	9	651.27	82.56	5315.21
1.2	18	559.69	130.03	7751.24
1.2	18	559.74	128.02	4939.98
1.2	18	599.12	132.79	4951.71
1.2	18	564.99	131.36	4868.09
1.2	18	584.44	129.77	4938.94
1.2	27	650.34	209.33	5420.03
1.2	27	781.74	250.46	5832.81
1.2	27	788.04	255.17	5786.66
1.2	27	643.80	206.55	5241.63
1.2	27	618.97	210.12	5236.69
1.2	36	724.80	300.68	5885.98
1.2	36	726.30	301.41	5677.70
1.2	36	675.31	279.48	5262.08
1.2	36	819.11	338.39	5916.73

Li in mg/L	Na in µg/L	Parameter setting C		
		Li 812.6 nm	Na 589.5 nm	H 486.1 nm
1.2	36	727.16	303.25	5686.65
1.2	44	798.74	398.23	6393.54
1.2	44	691.11	350.40	5433.16
1.2	44	680.57	343.90	5397.72
1.2	44	793.84	402.92	5905.33
1.2	44	773.58	388.64	5813.32
1.5	0	1112.43	31.38	5928.52
1.5	0	947.02	19.73	5418.79
1.5	0	895.98	18.27	5273.35
1.5	0	1101.03	21.85	5980.84
1.5	0	948.44	18.79	5233.07
1.5	9	1074.05	102.75	5609.03
1.5	9	1125.64	108.18	5843.01
1.5	9	989.79	98.50	5417.34
1.5	9	906.27	90.80	5305.57
1.5	9	1070.76	103.77	5682.26
1.5	18	930.65	160.05	4998.67
1.5	18	832.66	146.80	4925.53
1.5	18	793.09	141.98	4475.02
1.5	18	1108.92	194.07	5700.91
1.5	18	947.51	166.11	5255.36
1.5	27	923.97	230.75	4981.20
1.5	27	1136.02	282.17	5686.29
1.5	27	1205.56	300.53	5983.33
1.5	27	947.52	233.43	5290.65
1.5	27	1197.89	293.59	5828.62
1.5	36	975.59	312.44	5184.99
1.5	36	1119.33	362.26	5820.44
1.5	36	1038.24	339.65	5506.45
1.5	36	1219.32	394.00	6139.98
1.5	36	1115.03	369.73	5833.47
1.5	44	1071.86	434.31	5912.55
1.5	44	1117.79	452.90	6101.66
1.5	44	1009.42	406.98	5629.07
1.5	44	986.06	397.50	5406.44
1.5	44	997.27	407.28	5526.67
2.0	0	1358.73	24.46	5414.46
2.0	0	1793.47	27.05	6025.59
2.0	0	1700.93	23.02	5763.41
2.0	0	1709.77	21.74	5746.21
2.0	0	1758.32	23.62	6023.89
2.0	9	1718.56	111.34	5829.09
2.0	9	1849.25	124.31	6309.54
2.0	9	1707.78	115.34	5824.09
2.0	9	1724.34	114.12	5788.84
2.0	9	1459.51	100.40	5299.14
2.0	18	1428.66	176.20	5310.59
2.0	18	1729.57	211.08	5906.10
2.0	18	1518.27	183.14	5321.71
2.0	18	1535.41	185.03	5336.34

Li in mg/L	Na in µg/L	Parameter setting C		
		Li 812.6 nm	Na 589.5 nm	H 486.1 nm
2.0	18	1618.58	195.54	5594.29
2.0	27	1683.17	291.59	5837.49
2.0	27	1330.09	230.78	4939.22
2.0	27	1540.79	264.52	5449.04
2.0	27	1624.24	274.49	5568.36
2.0	27	1734.64	299.06	5987.99
2.0	36	1504.36	328.34	5441.48
2.0	36	1620.43	358.81	5613.21
2.0	36	1615.47	355.86	5702.00
2.0	36	1598.16	358.56	5836.56
2.0	36	1407.72	309.55	5176.20
2.0	44	1488.32	397.72	5530.29
2.0	44	1153.89	307.50	4730.04
2.0	44	1564.13	417.70	5531.76
2.0	44	1431.69	380.65	5101.04
2.0	44	1616.49	443.02	5741.28

Table A4 Intensities in a.u. of the long-term stability measurements of a lithium hydroxide solution containing 1 mg/L Li.

Time in min	Parameter setting A		Parameter setting D	
	Li 812.6 nm	H 486.1 nm	Li 670.7 nm	H 486.1 nm
0	2226.48	4543.94	2146.05	96.68
7	2286.57	4595.97	2165.92	96.34
14	2303.21	4607.71	2190.45	95.97
21	2464.85	4876.53	2146.72	95.44
28	2349.36	4667.21	1923.14	85.15
35	2168.62	4084.72	2056.90	90.40
42	2295.28	4363.98	2203.55	94.02
49	2293.75	4416.85	2131.48	93.77
56	2327.41	4509.87	2124.68	93.99
63	2406.20	4695.13	2208.60	98.55
70	2337.75	4565.89	2179.70	97.89
77	2416.52	4765.44	2078.16	92.23
84	2090.59	3970.47	1865.40	84.89
91	2216.77	4274.70	2003.50	89.10
98	2291.54	4384.85	1985.46	90.14
105	2259.06	4399.42	2110.55	95.72
112	2223.24	4461.44	2118.69	96.34
119	2325.65	4494.82	2138.51	96.85
126	2391.79	4764.33	2164.58	98.74
133	2407.29	4754.82	2236.26	100.79
140	2116.90	4077.46	1993.23	86.28
147	2235.28	4319.53	1988.38	89.45
154	2190.88	4269.16	2037.10	91.60
161	2277.52	4407.87	2032.61	91.94
168	2313.08	4526.04	2082.51	92.90
175	2324.08	4654.94	2089.68	94.78
182	2331.86	4442.21	2102.42	93.59
189	2131.34	3987.74	1957.39	85.58
196	2237.32	4139.86	2012.40	89.21

Time in min	Parameter setting A		Parameter setting D	
	Li 812.6 nm	H 486.1 nm	Li 670.7 nm	H 486.1 nm
203	2264.43	4257.55	2069.83	91.25
210	2206.44	4399.86	2102.09	95.19
217	2263.82	4483.94	2045.68	93.63
224	2269.45	4530.06	2159.44	96.87
231	2340.71	4540.59	2123.39	95.85
238	2255.28	4028.74	1934.85	85.61
245	2295.90	4204.27	2012.78	88.17
252	2210.94	4290.85	2036.76	88.82
259	2228.03	4354.41	2012.54	91.90
266	2349.95	4580.78	2131.90	95.24
273	2308.18	4532.91	2094.15	94.23
280	2314.05	4601.68	2127.62	97.26
287	2373.25	4789.35	2165.95	97.96
294	2209.70	4119.88	2255.42	98.59
301	2253.31	4226.07	2040.15	90.92
308	2261.84	4360.47	2023.40	91.73
315	2209.44	4351.02	2140.32	95.29
322	2357.85	4619.06	2173.33	97.71
329	2377.35	4652.74	2117.02	96.67
336	2396.27	4731.72	2240.48	100.10
343	2269.69	4069.46	2223.31	99.42
350	2319.96	4175.02	2066.47	90.43
357	2371.53	4443.02	2136.28	95.16
364	2363.29	4528.47	2191.71	96.43
371	2521.96	4647.91	2190.19	98.12
378	2394.16	4674.37	2232.67	97.45
385	2541.28	4840.79	2192.72	98.45
392	2341.46	4189.87	1956.54	87.37
399	2147.10	4203.13	2045.95	91.79
406	2349.40	4435.87	2105.16	94.92
413	2415.84	4634.58	2162.98	96.77
420	2416.87	4697.81	2161.48	97.36
427	2453.61	4693.65	2209.82	98.05
434	2389.84	4809.08	2219.82	99.36
441	2275.87	4209.04	1996.62	89.34
448	2354.93	4364.66	2082.73	90.97
455	2452.85	4565.03	2120.30	95.62
462	2410.95	4673.62	2247.44	98.33
469	2492.29	4746.03	2232.92	97.80
476	2520.14	4670.71	2270.65	99.95
483	2558.85	4979.96	2273.38	99.73
490	2365.30	4294.15	2064.95	91.12
497	2297.81	4254.18	2055.40	90.36
504	2374.44	4567.80	2145.15	95.67
511	2439.86	4798.20	2262.93	97.45
518	2466.35	4667.78	2240.39	96.77
525	2473.50	4782.99	2196.31	100.13
532	2586.36	4900.75	2333.68	99.98
539	2399.10	4346.84	2248.23	100.17
546	2398.71	4520.29	2185.81	95.27

Time in min	Parameter setting A		Parameter setting D	
	Li 812.6 nm	H 486.1 nm	Li 670.7 nm	H 486.1 nm
553	2483.20	4642.03	2192.44	95.21