

Supplementary Information for:
A New Li/Mg Paleothermometer from Pteropod Shells

N. Keul¹, D. Garbe-Schönberg¹, V. Kitidis², G. Langer³, K.T.C.A. Peijnenburg^{4,5}

¹ *Institute of Geosciences, Christian-Albrechts-Universität zu Kiel, Ludewig-Meyn-Str.10, 24118 Kiel, Germany*

² *Plymouth Marine Laboratory, Plymouth, United Kingdom*

³ *Institute of Environmental Science and Technology (ICTA-UAB), Universitat Autònoma de Barcelona, 08193, Bellaterra, Spain*

⁴ *Naturalis Biodiversity Center, P.O. Box 9517, 2300 RA Leiden, The Netherlands*

⁵ *Institute for Biodiversity and Ecosystem Dynamics (IBED), University of Amsterdam, P.O. Box 94248, 1090 GE Amsterdam, The Netherlands*

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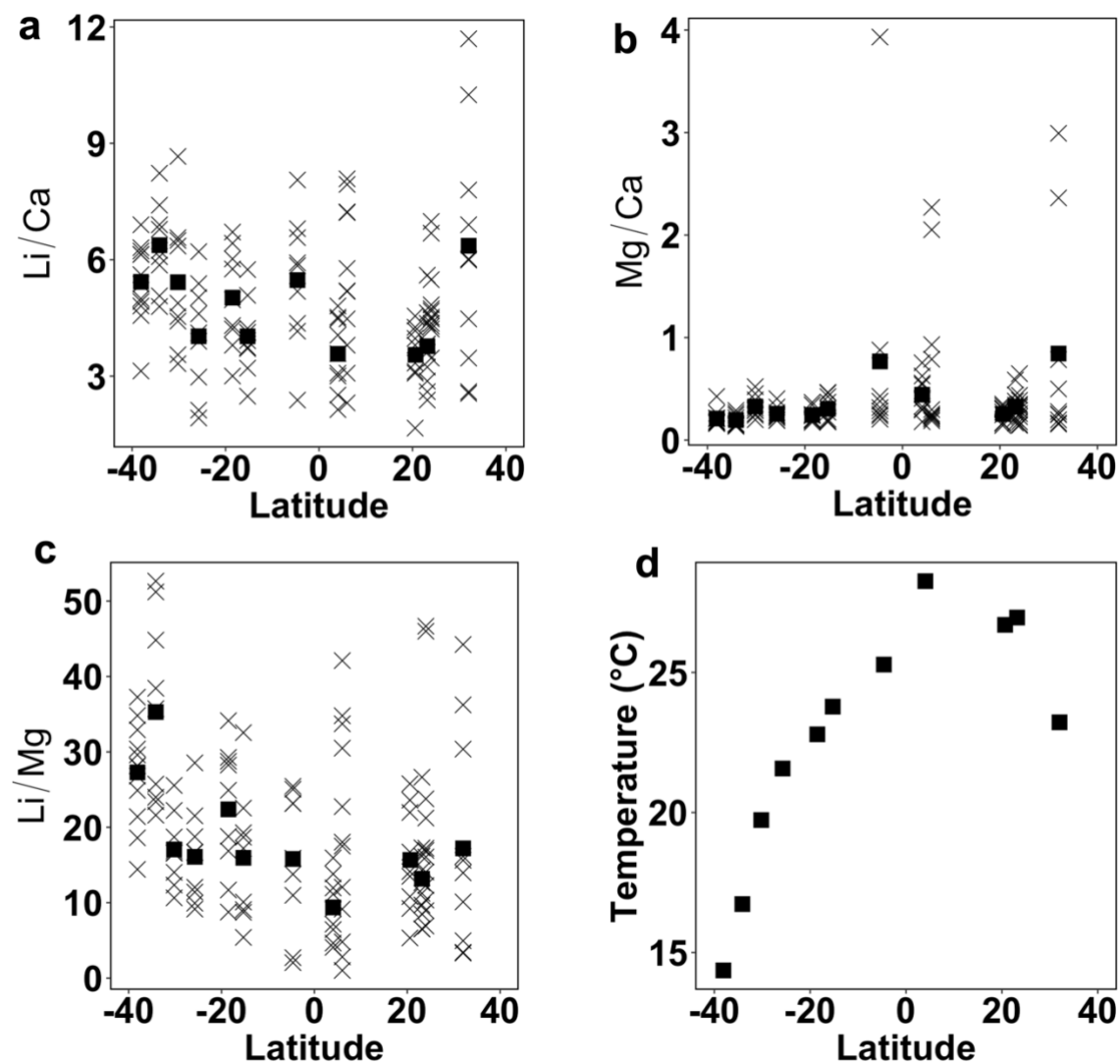


Figure S1. Distribution plots of (a) Li/Ca ($\mu\text{mol/mol}$), (b) Mg/Ca (mmol/mol), (c) Li/Mg ($\mu\text{mol/mmol}$) and (d) Temperature at 50m depth versus latitude in the Atlantic Ocean. Crosses depict individual measurements; Station averages are indicated by closed squares. Negative latitude denotes the southern hemisphere. Data can be found in Tab. 1.

pteropodID (internal)	cruise	Latitude	spot number	Li/Ca	Mg/Ca	Li/Mg
3722151A	AMT22	32.02	1	6.02	0.17	36.24
3822151B	AMT22	32.02	2	6.90	0.16	44.24
3922151C	AMT22	32.02	3	2.56	0.25	10.11
4022151D	AMT22	32.02	4	2.60	0.78	3.31
22151	pteropod avg.	32.02		4.52	0.34	23.47
4122152A	AMT22	32.02	1	5.99	0.20	30.37
4222152B	AMT22	32.02	2	4.48	0.28	16.14
4322152C	AMT22	32.02	3	3.46	0.25	13.96
22152	pteropod avg.	32.02		4.64	0.24	20.16
4422153A	AMT22	32.02	1	11.69	2.36	4.95
4422153B	AMT22	32.02	2	7.80	0.50	15.62
4522153C	AMT22	32.02	3	10.25	2.99	3.43
22153	pteropod avg.	32.02		9.91	1.95	8.00
2215	avg. station	32.02		6.36	0.84	17.21
	SE			1.78	0.55	4.70
1322231A	AMT22	23.16	1	2.38	0.17	14.30
1422231B	AMT22	23.16	2	3.83	0.34	11.24
1522231C	AMT22	23.16	3	3.23	0.38	8.50
1622231D	AMT22	23.16	4	2.60	0.27	9.69
22231	pteropod avg.	23.16		3.01	0.29	10.93
1722232A	AMT22	23.16	1	4.36	0.27	16.17
1822232B	AMT22	23.16	2	3.61	0.29	12.66
1922232C	AMT22	23.16	3	2.87	0.44	6.51
22232	pteropod avg.	23.16		3.61	0.33	11.78
2022233A	AMT22	23.16	1	5.60	0.21	26.64
2122233B	AMT22	23.16	2	4.63	0.27	17.27
2222233C	AMT22	23.16	3	3.83	0.59	6.53
22233	pteropod avg.	23.16		4.69	0.35	16.81
2223	avg. station	23.16		3.77	0.33	13.18
	SE			0.49	0.02	1.84
2322251A	AMT22	20.57	1	3.12	0.14	21.96
2422251B	AMT22	20.57	2	3.80	0.35	10.81
2522251C	AMT22	20.57	3	4.26	0.30	14.12
22251	pteropod avg.	20.57		3.72	0.26	15.63
2622252A	AMT22	20.57	1	4.17	0.16	25.77
2722252B	AMT22	20.57	2	3.34	0.25	13.50
2822252C	AMT22	20.57	3	3.08	0.33	9.23
22252	pteropod avg.	20.57		3.53	0.25	16.17
2922253A	AMT22	20.57	1	3.97	0.17	23.59

3022253B	AMT22	20.57	2	4.55	0.27	16.72
3122253C	AMT22	20.57	3	1.66	0.31	5.33
22253	pteropod avg.	20.57		3.39	0.25	15.21
2225	avg. station	20.57		3.55	0.25	15.67
	SE			0.10	0.01	0.28

3822371A	AMT22	4.03	1	3.00	0.33	9.21
3922371B	AMT22	4.03	2	4.48	0.63	7.16
4022371C	AMT22	4.03	3	2.51	0.54	4.64
22371	pteropod avg.	4.03		3.33	0.50	7.00
4122372A	AMT22	4.03	1	4.06	0.29	13.81
4222372B	AMT22	4.03	2	3.58	0.56	6.44
4322372C	AMT22	4.03	3	3.08	0.75	4.08
22372	pteropod avg.	4.03		3.57	0.53	8.11
4422373A	AMT22	4.03	1	2.14	0.18	11.96
4522373B	AMT22	4.03	2	4.81	0.30	15.94
4622373C	AMT22	4.03	3	4.52	0.41	11.13
22373	pteropod avg.	4.03		3.82	0.30	13.01
2237	avg. station	4.03		3.57	0.44	9.37
	SE			0.14	0.07	1.85

4722431A	AMT22	-4.62	1	4.36	0.32	13.78
4822431B	AMT22	-4.62	2	6.80	0.43	15.91
4922431C	AMT22	-4.62	3	5.85	0.25	23.16
22431	pteropod avg.	-4.62		5.67	0.33	17.62
5022432A	AMT22	-4.62	1	5.92	0.24	25.05
5122432B	AMT22	-4.62	2	4.16	0.38	10.98
5222432C	AMT22	-4.62	3	8.06	3.93	2.05
22432	pteropod avg.	-4.62		6.04	1.52	12.69
5322431A	AMT22	-4.62	1	5.18	0.20	25.43
5422431B	AMT22	-4.62	2	6.57	0.28	23.16
5522431C	AMT22	-4.62	3	2.38	0.88	2.71
22431	pteropod avg.	-4.62		4.71	0.46	17.10
2243	avg. station	-4.62		5.47	0.77	15.80
	SE			0.40	0.38	1.56

5622491A	AMT22	-15.29	1	3.21	0.19	17.20
5722491B	AMT22	-15.29	2	4.23	0.47	9.08
5822491C	AMT22	-15.29	3	2.48	0.46	5.40
22491	pteropod avg.	-15.29		3.31	0.37	10.56
6522492A	AMT22	-15.29	1	4.13	0.18	22.54
6622492B	AMT22	-15.29	2	3.74	0.37	10.09
6722492C	AMT22	-15.29	3	3.71	0.42	8.73

22492	pteropod avg.	-15.29		3.86	0.33	13.79
6822493A	AMT22	-15.29	1	5.75	0.18	32.55
6922493B	AMT22	-15.29	2	5.08	0.27	18.69
7022493C	AMT22	-15.29	3	3.91	0.20	19.28
22493	pteropod avg.	-15.29		4.91	0.22	23.51
2249	avg. station	-15.29		4.03	0.30	15.95
	SE			0.47	0.05	3.89

7122511A	AMT22	-18.52	1	3.80	0.20	18.79
7222511B	AMT22	-18.52	2	6.42	0.19	34.13
7322511C	AMT22	-18.52	3	4.30	0.37	11.68
22511	pteropod avg.	-18.52		4.84	0.25	21.54
7422512A	AMT22	-18.52	1	4.97	0.17	28.75
7522512B	AMT22	-18.52	2	5.76	0.20	29.27
7622512C	AMT22	-18.52	3	4.22	0.25	16.86
22512	pteropod avg.	-18.52		4.98	0.21	24.96
7722513A	AMT22	-18.52	1	6.02	0.24	24.91
7822513B	AMT22	-18.52	2	6.71	0.24	28.26
7922513C	AMT22	-18.52	3	3.00	0.34	8.76
22513	pteropod avg.	-18.52		5.25	0.27	20.64
2251	avg. station	-18.52		5.02	0.24	22.38
	SE			0.12	0.02	1.32

8022571A	AMT22	-25.75	1	2.12	0.23	9.15
8122571B	AMT22	-25.75	2	4.61	0.40	11.41
8222571C	AMT22	-25.75	3	5.02	0.27	18.75
22571	pteropod avg.	-25.75		3.92	0.30	13.10
8322572A	AMT22	-25.75	1	1.92	0.19	9.94
8422572B	AMT22	-25.75	2	5.39	0.32	16.71
8522572C	AMT22	-25.75	3	2.97	0.25	12.04
22572	pteropod avg.	-25.75		3.43	0.25	12.90
0422573A	AMT22	-25.75	1	4.11	0.19	21.52
0522573B	AMT22	-25.75	2	6.21	0.22	28.54
0622573C	AMT22	-25.75	3	3.90	0.23	16.65
22573	pteropod avg.	-25.75		4.74	0.21	22.24
2257	avg. station	-25.75		4.03	0.26	16.08
	SE			0.38	0.03	3.08

0722601A	AMT22	-30.2	1	6.57	0.26	25.55
0822601B	AMT22	-30.2	2	4.42	0.20	22.23
0922601C	AMT22	-30.2	3	6.50	0.39	16.56
22601	pteropod avg.	-30.2		5.83	0.28	21.45
1022602A	AMT22	-30.2	1	3.55	0.29	12.34

1122602B	AMT22	-30.2	2	4.88	0.29	16.88
1222602C	AMT22	-30.2	3	6.35	0.45	14.03
22602	pteropod avg.	-30.2		4.93	0.34	14.42
1322603A	AMT22	-30.2	1	3.32	0.31	10.64
1422603B	AMT22	-30.2	2	4.53	0.24	18.71
1522603C	AMT22	-30.2	3	8.66	0.52	16.62
22603	pteropod avg.	-30.2		5.51	0.36	15.32
2260	avg. station	-30.2		5.42	0.33	17.06
	SE			0.26	0.02	2.21

1622621A	AMT22	-34.15	1	4.79	0.13	35.73
1722621B	AMT22	-34.15	2	5.07	0.22	23.40
1822621C	AMT22	-34.15	3	5.86	0.24	23.99
22621	pteropod avg.	-34.15		5.24	0.20	27.71
1922622A	AMT22	-34.15	1	6.90	0.15	44.82
2022622B	AMT22	-34.15	2	8.23	0.16	52.64
2122622C	AMT22	-34.15	3	6.79	0.26	25.73
22622	pteropod avg.	-34.15		7.31	0.19	41.06
2222623A	AMT22	-34.15	1	6.08	0.16	38.44
2322623B	AMT22	-34.15	2	7.41	0.14	51.21
2422623C	AMT22	-34.15	3	6.24	0.29	21.61
22623	pteropod avg.	-34.15		6.57	0.20	37.09
2262	avg. station	-34.15		6.37	0.20	35.29
	SE			0.60	0.00	3.96

3122661A	AMT22	-38.11	1	4.56	0.16	28.13
3222661B	AMT22	-38.11	2	6.14	0.18	34.82
3322661C	AMT22	-38.11	3	4.81	0.16	29.61
3422661D	AMT22	-38.11	4	5.62	0.26	21.41
22661	pteropod avg.	-38.11		5.28	0.19	28.49
3522662A	AMT22	-38.11	1	3.13	0.17	18.60
3622662B	AMT22	-38.11	2	5.00	0.19	26.78
3722662C	AMT22	-38.11	3	6.31	0.21	30.38
3822662D	AMT22	-38.11	4	6.90	0.21	32.92
22662	pteropod avg.	-38.11		5.33	0.19	27.17
3922663A	AMT22	-38.11	1	6.22	0.17	37.26
4022663B	AMT22	-38.11	2	4.92	0.17	28.18
4122663C	AMT22	-38.11	3	5.37	0.22	24.89
4222663D	AMT22	-38.11	4	6.14	0.43	14.42
22663	pteropod avg.	-38.11		5.66	0.25	26.19
2266	avg. station	-38.11		5.43	0.21	27.28
	SE			0.12	0.02	0.67

Table S1: Trace elemental composition of individual laser spots. Columns contain: pteropod ID (for internal reference purposes), Station location information (cruise, Latitude), spot number on pteropod, trace elemental composition (Li/Ca in $\mu\text{mol/mol}$, Mg/Ca in mmol/mol , Li/Mg in $\mu\text{mol/ mmol}$). Average values for individual pteropods (bold), and station averages (bold, highlighted in purple), as well as standard error (SE, highlighted in purple) are calculated as well (SE).

<i>a</i> R^2 values for Li/Ca versus		
Depth (m)	Temperature	Salinity
2	0.45	<i>n.s.</i>
25	0.45	<i>n.s.</i>
50	0.42	<i>n.s.</i>
75	0.39	0.37
100	<i>n.s.</i>	<i>n.s.</i>
150	<i>n.s.</i>	<i>n.s.</i>
200	<i>n.s.</i>	<i>n.s.</i>
250	<i>n.s.</i>	<i>n.s.</i>
300	<i>n.s.</i>	<i>n.s.</i>

<i>b</i> R^2 values for Mg/Ca versus		
Depth (m)	Temperature	Salinity
2	<i>n.s.</i>	<i>n.s.</i>
25	<i>n.s.</i>	<i>n.s.</i>
50	<i>n.s.</i>	<i>n.s.</i>
75	<i>n.s.</i>	<i>n.s.</i>
100	<i>n.s.</i>	<i>n.s.</i>
150	<i>n.s.</i>	<i>n.s.</i>
200	<i>n.s.</i>	<i>n.s.</i>
250	<i>n.s.</i>	<i>n.s.</i>
300	<i>n.s.</i>	<i>n.s.</i>

Table S2. Statistical parameters for linear correlation between (a) average pteropod shell Li/Ca ($\mu\text{mol/mol}$) and (b) average pteropod shell Mg/Ca (mmol/mol) and selected water parameters: temperature ($^{\circ}\text{Celsius}$) and salinity. Regressions were performed against parameters at specific depths; the R^2 is reported when $p < 0.05$. *n.s.* indicates non-significant regressions ($p > 0.05$).

Station	Lat.	Long.	Temp.	Sal.	Li/Ca	Mg/Ca	Li/Mg	KD Mg *1000	KD Li *1000
15	32.02	-30.74	23.22	36.79	6.36	0.84	17.21	0.17	2.54
23	23.16	-40.60	26.96	37.43	3.77	0.33	13.18	0.06	1.51
25	20.67	-38.56	26.7	37.36	3.55	0.25	15.67	0.05	1.42
37	4.03	-26.47	28.26	35.70	3.57	0.44	9.37	0.09	1.43
42	-4.62	-25.00	25.28	36.12	5.47	0.77	15.80	0.15	2.19
48	-15.29	-25.13	23.78	37.23	4.03	0.30	15.95	0.06	1.61
50	-18.52	-25.10	22.79	36.95	5.02	0.24	22.38	0.05	2.01
56	-25.75	-24.99	21.57	36.67	4.03	0.26	16.08	0.05	1.61
60	-30.20	-27.92	19.73	36.16	5.42	0.33	17.06	0.06	2.17
62	-34.15	-33.49	16.73	35.60	6.37	0.20	35.29	0.04	2.55
66	-38.11	-39.33	14.36	35.04	5.43	0.21	27.28	0.04	2.17

Table S3: Partitioning coefficients for Li (K_{DLi}) and Mg (K_{DMg}). Depicted are: station location information (Lat.= Latitude, Long= Longitude), Temperature at 50m depth (Temp., in °C), Salinity at 50m depth (Sal.) and average trace elemental composition (Li/Ca in $\mu\text{mol/mol}$, Mg/Ca in mmol/mol , Li/Mg in $\mu\text{mol/mol}$) with the partitioning coefficients for Li (K_{DLi}) and Mg (K_{DMg}). For the calculation of K_{DLi} and K_{DMg} seawater values of 5.1 mol/mol for Mg/Ca (Lebrato et al., 2020) and 0.0025 mol/mol for Li/Ca were used (Hathorne et al., 2013).

References

- Hathorne, E. C., Felis, T., Suzuki, A., Kawahata, H. & Cabioch, G. Lithium in the aragonite skeletons of massive Porites corals: A new tool to reconstruct tropical sea surface temperatures. *Paleoceanography* 28, 143–152, doi:<https://doi.org/10.1029/2012PA002311> (2013).
- Lebrato, M. *et al.* Global variability in seawater Mg:Ca and Sr:Ca ratios in the modern ocean. *Proceedings of the National Academy of Sciences* **117**, 22281–22292, doi:10.1073/pnas.1918943117 (2020)