

This document provides: i) aragonite partition coefficients from Oxford Cave experiments (Day et al., 2021); ii) a visual comparison of partition coefficients from Jamieson et al. (2016), Wassenburg et al. (2016) and Day et al. (2021).

This initial text is brief, but feel free to e-mail me with questions (chris.day@earth.ox.ac.uk), and I plan to expand on this information in the near future.

## 1. Aragonite partition coefficients from Oxford Cave experiments

In the Day et al. (2021) study, a subset of 20°C experiments precipitated aragonite as a result of increasing  $[Mg_{solution}]$  to values that are equal to those of the beaker experiments of Marriott et al. (2004). These aragonite partition coefficients can be calculated from the published solution and solid measurements in tables 1 and 2 of Day et al. (2021). For convenience they are also provided here in table 1 below.

Whilst this is a small dataset, the advantage of these results is that the aragonite is grown under controlled conditions, with measurements made for both  $X/Ca_{solution}$  and  $X/Ca_{solid}$ , as is required for  $D(X) = \frac{X/Ca_{solid}}{X/Ca_{solution}}$ .

Chris Theaker conducted additional aragonite experiments (in prep).

T	interval	pH <sub>0</sub>	Solution [Mg]	D(Li)	D(Mg)	D(Co)	D(Sr)	D(Cd)	D(Ba)	D(U)	Mineralogy
<sup>o</sup> C	s		mol/L								
20	10.1	7.4	6.5x10 <sup>-5</sup>	3.2x10 <sup>-3</sup>	2.5x10 <sup>-2</sup>	9.1x10 <sup>-1</sup>	1.0x10 <sup>-1</sup>	2.2x10 <sup>-1</sup>	1.6x10 <sup>-1</sup>	2.7x10 <sup>-1</sup>	calcite
20	10.2	7.5	2.5x10 <sup>-3</sup>	1.3x10 <sup>-2</sup>	2.1x10 <sup>-2</sup>	1.1x10 <sup>0</sup>	2.0x10 <sup>-1</sup>	2.1x10 <sup>-1</sup>	2.8x10 <sup>-1</sup>	2.2x10 <sup>-1</sup>	highMg calcite
20	10.2	7.7	4.7x10 <sup>-3</sup>	5.8x10 <sup>-3</sup>	1.0x10 <sup>-3</sup>	7.0x10 <sup>-1</sup>	9.9x10 <sup>-1</sup>	3.7x10 <sup>0</sup>	1.2x10 <sup>0</sup>	1.7x10 <sup>0</sup>	aragonite

Table 1: Aragonite partition coefficients calculated from tables 1 and 2 of Day et al. (2021). These partition coefficients apply to a subset of experiments at 20 °C, that investigated the effect of  $[Mg]_{solution}$  on carbonate precipitation.

## 2. Visual comparison of partition coefficients from Jamieson et al. (2016), Wassenburg et al. (2016) and Day et al. (2021)

The extensive studies of Jamieson et al. (2016) and Wassenburg et al. (2016) have many data points and carefully discuss mechanisms that can cause shifts between calcite and aragonite within an individual sample. The partition coefficients from Day et al. (2021) are from a single experiment, but from aragonite growing in controlled conditions for which measurements are available for both the solid and the solution composition. There is encouraging agreement between the D(X) of all of these studies. Chris Theaker has completed more aragonite-specific experiments in the Oxford Cave, that will be available in due course.

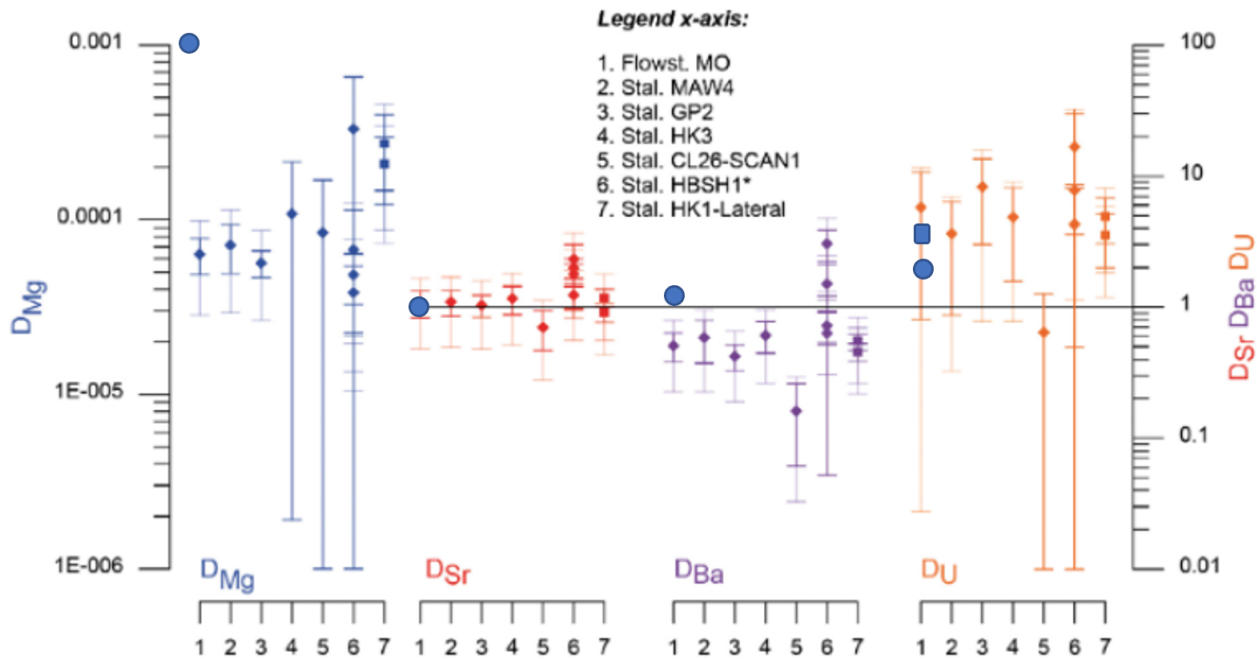


Figure 1: Figure adapted from Wassenburg et al. (2016) to include  $D(X)_{\text{aragonite}}$  from Jamieson et al. (2016) and from Day et al. (2021).

### Bibliography

Day, C. C., Pogge von Strandmann, P. A., Mason, A. J., jul 2021. Lithium isotopes and partition coefficients in inorganic carbonates: Proxy calibration for weathering reconstruction. *Geochimica et Cosmochimica Acta* 305, 243–262.

Jamieson, R. A., Baldini, J. U., Brett, M. J., Taylor, J., Ridley, H. E., Ottley, C. J., Pruffer, K. M., Wassenburg, J. A., Scholz, D., Breitenbach, S. F., 2016. Intra- and inter-annual uranium concentration variability in a Belizean stalagmite controlled by prior aragonite precipitation: A new tool for reconstructing hydro-climate using aragonitic speleothems. *Geochimica et Cosmochimica Acta* 190, 332–346.

Marriott, C. S., Henderson, G. M., Belshaw, N. S., Tudhope, A. W., May 2004. Temperature dependence of  $\delta^7\text{Li}$ ,  $\delta^{44}\text{Ca}$  and Li/Ca during growth of calcium carbonate. *Earth and Planetary Science Letters* 222 (2), 615–624.

Wassenburg, J. A., Scholz, D., Jochum, K. P., Cheng, H., Oster, J., Immenhauser, A., Richter, D. K., Häger, T., Jamieson, R. A., Baldini, J. U., Hoffmann, D., Breitenbach, S. F., 2016. Determination of aragonite trace element distribution coefficients from speleothem calcite–aragonite transitions. *Geochimica et Cosmochimica Acta* 190, 347–367.