The stable and clumped isotopic composition of bulk samples of dense calcite from the ventral margin of the shells was measured at the University of Michigan Stable Isotope Laboratory. Sample preparation was performed on a manual extraction line following Defliese et al. (2015), with the temperature of the PorapakTM trap increased to avoid fractionating stable isotope values (Petersen et al., 2016). 5mg aliquots of carbonate powder were reacted at 75°C in a common acid bath for 15 minutes. Water was removed from resultant CO2 in two cryogenic separation steps with LN2-cooled 1-propanol traps held below -80°C. Next, CO2 was passed through a PorapakTM trap held between -10°C and -15°C to remove organics and other contaminants, as well as being exposed to silver wool to remove sulphur compounds. Finally, clean CO2 was transferred to the mass spectrometer for analysis.

Sample CO2 was analysed on a ThermoFinnegan MAT253 equipped with cups to measure m/z 44-49. Each sample was analysed for 5 acquisitions of 12 cycles each, with pressure adjustment at the beginning of each acquisition setting the m/z 44 beam to 16V. Heated (1000°C) and H2O-equilibrated (25°C) gas standards and two in-house carbonate standards (Carrara Marble and Aragonitic Bahamanian Ooids) were run alongside carbonate unknowns. All gas and carbonate standard data is presented along with carbonate unknowns in supplementary data. Five individual gas standard points were eliminated from use in data correction due to various preparation issues (heated gases never heated, elevated Δ48 values relative to other standard gases, indicating contamination). One additional gas standard was a significant outlier from preceding and following samples, and was eliminated so as not to cause artificial large swings in reference frame parameters. All removed gases are indicated in red in supplementary data table.

Gas standards were used to convert unknowns into the absolute reference frame (Dennis et al., 2011). In-house carbonate standards were monitored to identify accuracy of the reference frame and were not used in the reference frame construction. All shells analysed in this study for their clumped isotopic composition are made of calcite, so δ18Owater values were calculated using the calcite-H2O equation of Kim and O’Neil (1997).

Each unknown was measured 3-4 times each and an average of all replicates was taken. Internal error on δ18O and δ13C is presented as 1 standard deviation of these replicates, whereas internal error on Δ47, temperature, and δ18Owater values is presented as 1 standard error of these replicates. Often the typical reproducibility of carbonate standards measured many times is more representative of true error than the internal error on a single sample. We calculate an external error as the larger of the internal error or the long-term standard deviation of carbonate standards (1sd on Δ47 = 0.011‰) divided by the square root of the number of replicates. For 3 and 4 replicates this is 0.0064‰ and 0.0055‰, respectively for Δ47. For samples in this study, in all cases the external error was equal to the internal error.

Each sample was analysed for 5 acquisitions of 12 cycles each and calibrated relative to heated (1000°C) and H2O-equilibrated (25°C) gas standards and two in-house carbonate standards (Carrara Marble and Aragonitic Bahamanian Ooids). Gas standards were used to convert unknowns into the absolute reference frame (Dennis et al., 2011) and carbonate standards (Carrara Marble and Aragonitic Bahamanian Ooids) were used to quantify reproducibility of reacted samples. δ18Owater values were calculated using the calcite-H2O equation of Hays and Grossman (1991). External long term reproducibility error on the Δ47 value was found to be 0.011‰ (1σ), based on measurements of carbonate standards

Clumped isotope data (raw voltage data) was processed twice – once using the typically used Santrock/Gonfiantini parameters given by Huntington et al. (2009) and once using the updated Brand parameters recommended by Daeron et al. (2016) and Schauer et al. (2016) (denoted by ‘BR’ in supplemental data table).

In the case of the Santrock/Gonfiantini parameter analysis, Δ47 values were corrected using an acid fractionation factor of +0.067‰ for the 75°C reaction temperature (Defliese et al., 2015) and converted to temperature using the 70-100°C high temperature compilation calibration shown in Equation 6 of Defliese et al. 2015. In the case of the Brand parameter analysis, we use the published calibration equation of Kelson et al. (2017) (Equation 1), which is given for samples reacted at 90°C. To convert our data into a 90°C framework, we used an acid fractionation factor of –0.015‰, which is the difference between the 75°C and 90°C fractionation factors of Defliese et al. (2015).

We present the data here using the updated Brand parameters in order to allow for recalculation of temperatures in the future as calibration equations using Brand parameters become more plentiful. For now, we prefer to use the Santrock/Gonfiantini parameters and Defliese et al. (2015) calibration, as this calibration study was carried out in the same lab and using the same preparation methods as the unknowns in this study. Inter-lab calibration differences continue to occur in the clumped isotope community. Use of Brand parameters may begin to resolve some of these differences (Kelson et al., 2017; Schauer et al., 2016; Daeron et al., 2016). However, until the establishment of a ‘universal calibration’ applicable to all labs, or until a calibration equation is presented using Brand parameters and samples measured at the University of Michigan, we feel the best approach is to keep consistency between methodology of preparation and data analysis between unknowns and calibration samples, and thus present the Santrock/Gonfiantini data in the main manuscript.

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