Long-term precision and accuracy of clumped isotope measurements

DAVID BAJNAI[1], JENS FIEBIG[1], NIKLAS LÖFFLER[2], KATHARINA METHNER[2], EMILIJA KRSNIK[2], CHARLOTTE PRUD'HOMME[3], SVEN HOFMANN[1]

[1]Institute of Geosciences, Goethe University Frankfurt, DE (david.bajnai@em.uni-frankfurt.de)
[2]Senckenberg BIK-F, Frankfurt am Main, DE
[3]Max Plank Institute of Chemistry, Mainz, DE

The clumped isotope thermometer method became popular in recent years. Its main advantage is that it can reconstruct carbonate precipitation temperatures, *i.e.,* palaeoseawater temperatures, without independent information on the parent waters. Since measurements are still time consuming and expensive, laboratories restrain to make only a few replicate analyses per samples. Changes in phosphoric acid concentration, vacuum, the efficiency of CO_2 purification, ion source effects cause long-term variations in the reproducibility of Δ_{47} analyses. The accuracy and precision of Δ_{47} of samples that have been replicated only a few times are especially affected. Here we compare the performance of two gas source isotope ratio mass spectrometers (MAT253 and 253 Plus), and two sample preparation techniques (manual and automated) to assess how the reproducibility changes using different setups and to investigate ways to further advance Δ_{47} analyses.

We tested the following setup: (1) We carried out clumped isotope analyses (carbonates and equilibrated gases) on a MAT253, directly connected to an automated purification line where analyte CO_2 gases are purified using subsequent -80 °C ethanol and liquid nitrogen traps and a He-GC column and carbonates are on-line reacted at 90 °C. Such measurements were run over the course of three years (2) We analysed manually prepared equilibrated CO_2 (25 °C and 1000 °C) gases on a 253 Plus equipped with high-ohmic resistors. (3) We measured equilibrated gases and carbonate standards that were prepared using the automated line (HAL) on a 253 Plus.

Here, the external standard deviations of sample Δ_{47} and Δ_{48} are presented. Also, we performed Monte Carlo-type simulations to assess the confidence levels of the standard error ranges when averaging 3-15 replicate analyses.