Baseline modelling.

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The standard way of processing results from clumped isotope studies is the absolute reference frame [Dennis, et al., 2011]. This follows on the work of Huntington, et al. [2009] where Δ₄⁷ was plotted vs Δ₄⁷ and the reported Δ₄⁷ was corrected to δ₄⁷=0. He et al. [2012] showed that the slope of the Δ₄⁷ vs δ₄⁷ was a function of shifted baseline in the m/z 47 reading, and that the Δ₄⁷ vs δ₄⁷ function is not a true line but an arc. Measuring and correcting for the baseline offset minimized the slope, as well as deviation from a linear fit, and data from multiple equilibrated and heated (1000 °C) gases could be combined to calculate said slope. He et al. [2012] measures the baseline in every run, and others, e.g. Bernasconi et al., [2013] determine it periodically. Here we report using a model system to fit the residual baseline to the EG and HG data. That baseline can then be added to the measured baseline, either as a function of the measured baseline reading or the m/z 44 reading, during the calculation of the Δ₄⁷ value. The effective Δ₄⁷ vs δ₄⁷ slope should be zero, so the baseline correction does the correction to δ₄⁷=0.


