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Metrological issues we would rather not dwell on: how we report and think about triple oxygen compositions

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Triple oxygen isotope studies are widely applicable and particulary powerful when used to link the compositions of different chemical species (water, carbonates, silicates, sulfates). In theory, comparing the triple oxygen compositions of different molecules is straightforward as long as all of them are expressed relative to a common reference (VSMOW in this case). In practice, however, we must contend with the fact that triple oxygen analyses rely on different analytical protocols and instrumentation and that constraining the relative compositions of reference materials (RMs) with different chemistries (e.g., carbonate vs water vs silicate RMs) is critical yet challenging.

Here we attempt to shed light on some possible causes for the discrepancies in the $\Delta^{17}O$ values of the main carbonate RMs relative to the VSMOW-SLAP scale measured using different mass spectrometric and/or spectroscopic approaches. Taking the example of a new dataset constraining "equilibrium" triple oxygen fractionation between water and calcite, we also interrogate the choices we make when reporting and interpreting such data. We conclude that despite the theoretical appeal of thinking purely in terms of compositions relative to VSMOW and fractionation exponents (θ values), a more careful/robust approach would be (1) to include reports of triple oxygen compositions relative to same-nature RMs (carbonate samples vs carbonate RMs, etc.), effectively separating purely metrological issues (the relative $\Delta^{17}O$ values of the various RMs) from purely analytical ones (how we standardize our measurements), and (2) to favor thinking in terms of changes/differences in cap-delta values rather than fractionation exponents.