**Abstract**

The application of stable isotope analysis (SIA) has rapidly expanded over the last two decades with technological developments such as cavity ring-down spectroscopy (CRDS) and off-axis integrated cavity output spectroscopy (OA-ICOS). Both instruments may provide a user with the ability to swiftly measure stable isotopes of hydrogen (1H, 2H) and oxygen (16O, 17O,18O), and thus provides the ability to measure advanced metrics like ∆17O (from the triple oxygen isotopes) and d-excess (from measurements of 2H and 18O). Additionally, both instruments provide cheaper and less labor-intensive alternatives to the traditional method of isotope ratio mass spectrometry for water sample analysis. While the use of CRDS and OA-ICOS instruments has become common in the fields of geochemistry, hydrology, and oceanography, these instruments remain uncommonly used in the fields of ecology and animal biology, despite potential to use these instruments to measure animal metabolism and water intake. The lack of relevant methodology for using these instruments to analyze biological materials and daunting post-processing of data are large barriers to these instruments being adopted by ecologists and biologists. To remedy this issue, I developed a highly automated Python script which allows a user to import raw data from a CRDS instrument and correct the raw measurements into a publishable format. I demonstrate the utility of this Python script using six datafiles from three cycles of measurements. I have uploaded this Python script as a data repository on Github for open access use. Future research should aim to develop similar tools for OA-ICOS instruments.

**Introduction**

An isotope is a variant of a chemical element that differs in the number of neutrons, and therefore, has a different atomic mass (IAEA, 2023). A stable isotope is an isotope that will not decay into another element (as opposed to a radioactive isotope; IAEA, 2023). For example, oxygen has three stable isotopes (O16, O17, O18; the number 18 signifies this variant of oxygen has 8 protons and 10 neutrons), whereas hydrogen only has one stable isotope (2H; deuterium) but does have a radioactive isotope as well (3H; tritium). Stable isotope analysis (SIA) is the assessment of the ratio of these isotopes in different samples to provide information about the sample (e.g., age of sample, historical climate the sample was found in, etc.) and SIA is a powerful tool that has been a staple of the fields of oceanography, geochemistry, and forensic sciences (Wostbrock et al. 2018; Landais et al. 2012; Ehleringer et al. 2008). Recently, the application of SIA has expanded to other fields such as ecology and animal biology (Newsome et al. 2007; Cucherousset & Villéger, 2015; Whiteman et al. 2019a). However, the incorporation of SIA to ecology and animal biology is often limited to carbon and nitrogen isotopes (Vander Zanden et al. 2016). In addition, many researchers in the fields of ecology and animal biology choose to send their samples to other institutions for analysis instead of completing their analyses in-house because of the expenses and logistics related to traditional SIA (Speakman, 1997). The development of advanced instrumentation such as cavity ring-down spectroscopy (CRDS) and off-axis integrated cavity output spectroscopy provide a potential solution to these setbacks for water samples (Thorsen et al. 2011; Melanson et al. 2018). In particular, CRDS is an affordable alternative to the long-standing traditional reliance on isotope ratio mass spectrometry (IRMS; Schauer et al. 2016). CRDS instruments, such as the Picarro L2140-*i*, provide high-precision measurements of hydrogen and oxygen stable isotopes in a fraction of the time required for IRMS analysis, and CRDS instruments possess automated functionality, allowing for a less labor-intensive process compared to IRMS (Schauer et al. 2016).

The capability of expanding the application of SIA to more frequently include oxygen and hydrogen would be highly beneficial to the fields of ecology and animal biology (Vander Zanden et al. 2016). Stable isotopes of oxygen and hydrogen (δ17O, δ18O, and δ2H) can provide information related to the sources of environmental water intake and to the animal’s body water pool (Vander Zanden et al. 2016; Whiteman et al. 2019b). For example, measurements of injected 2H and 18O tracers can reflect the size of the body water pool (Andrews et al. 1997) and metabolic rate (Speakman, 1997), natural abundance of 18O can reflect environmental water sources (Bryant and Froelich, 1995; Kohn, 1996), and a new application that simultaneously measures natural abundance of 16O, 17O, and 18O (i.e., Δ17O) can be used to infer relative changes in metabolic rate and water intake (Pack et al. 2013; Whiteman et al. 2019b; Sabat et al. 2021). A central premise for all these methods is that water is critical to animal biology (Hill et al. 2008). Most terrestrial animals are ~60-70% water by mass, and this body water comes from a combination of environmental sources (i.e., ingestion of preformed water by drinking or eating) and endogenous processes (e.g., newly-synthesized metabolic water, a byproduct of metabolic pathways; Kohn 1996; Hill et al. 2008). Analysis of a sample from an animal’s body water can thus provide insight related to their water intake and metabolism. A sample for analysis can be collected via blood plasma or serum samples (Speakman, 1997), but under the right circumstances (e.g., a trained animal in captivity) saliva and urine samples can be collected as well (Fancy et al. 1986). These samples can then be microdstilled to obtain a water sample that is safe for CRDS or OA-ICOS analysis (Nagy, 1983).

Since most analysis conducted using CRDS and OA-ICOS has been conducted within the fields of hydrology, geology, and plant science (Steig et al. 2014; Schauer et al. 2016), the methodology pertaining to analyses conducted via these instruments has been strategically developed in relation to these fields. In addition, currently available methodology included modifications to instruments to improve precision and throughput (Steig et al. 2014; Schauer et al. 2016). As a result, these methods have limited applicability to ecologists, animal biologists, and even plant scientists that analyze waters from very different systems than these other fields. Additionally, modified instrumentation and intensive post-measurement procedures deter potentially interested researchers that may have limited instrumentation experience. Adapting methodology to better suit the diverse range of fields that may use a CRDS or OA-ICOS instrument, while also simplifying procedures is necessary to expand the application of SIA of hydrogen and oxygen isotopes to the fields of ecology and animal biology.

To help expand the use of stable isotope analysis via CRDS to the fields of ecology and animal biology, I developed a Python (3.9.13) script to demonstrate the ease with which a researcher can correct and finalize data from a CRDS water analyzer instrument for publication. I uploaded this Python script, along with a series of datasheets that can be used to test the script, to the following open-access Github repository: <https://github.com/ZacharyTSteele/OEAS895/tree/master/Capstone_Project>

**Methods**

*Stable Isotope Measurement and Correction of Raw Measurements*

SIA data is reported in delta (δ) notation based on relative differences of isotopic ratios (as opposed to absolute ratios) between the sample and internationally-accepted standards (Steig et al. 2014; Schauer et al. 2016). In the case of hydrogen and oxygen isotopes, these standards are Vienna Mean Standard Ocean Water (VSMOW) and Standard Antarctic Light Precipitation Water (SLAP; Steig et al. 2014; Schauer et al. 2016). These standards provide for easy interlaboratory comparison of SIA measurements. An example is provided below for calculation of δ18O (Steig et al. 2014; Schauer et al. 2016):

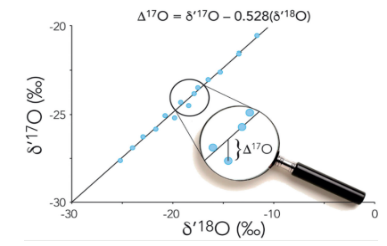
δ18Oraw = [ (18O / 16O)sample / (18O / 16O)VSMOW – 1 ] \* 1000 (1)

Once measurements of δ17O and δ18O are obtained (in per mil; ‰), Δ17O (calculated in either per mil or per meg; parts per million) is calculated as follows (Steig et al. 2014; Schauer et al. 2016):

Δ17Oraw = δ’17Oraw – 0.528\* δ’18Oraw (2)

When measurements of δ’17O and δ’18O (‘ indicates linearization) are plotted against each other (Figure 1), a near constant and predictable relationship is observed (hence the slope of 0.528 applied in Equation 2; Steig et al. 2014; Schauer et al. 2016). This relationship occurs because the isotopic variation of δ17O and δ18O is typically based on mass (i.e., via mass-dependent fractionation) and means that a sample with a high δ18O value is expected to also have a high δ17O value (Aron et al. 2021). However, there are small positive and negative deviations from this expected relationship, representing mass-independent fractionation (e.g., supersaturation, Rayleigh distillation, stratospheric intrusions, etc.; Aron et al. 2021) which are quantified as Δ17O (Whiteman et al. 2019b).

**Figure 1.** δ‘17O and δ‘18O represent the abundance of 17O and 18O relative to the abundance of 16O. Deviations from this slope (i.e., residuals) are represented as Δ17O (From Whiteman et al. 2019b; pg. 659; Figure 1).



When analyzing water samples via CRDS, VSMOW and SLAP can be measured consistently to correct measurements. However, since VSMOW and SLAP are expensive and only available in small volumes, many laboratories opt to measure VSMOW and SLAP seldomly, and instead use VSMOW and SLAP to validate in-house water standards that can then be used frequently during analyses (Whiteman et al. 2019b). As such, ‘instrument runs’ can be divided into either ‘standards runs’ or ‘analysis runs’. An instrument run is a segment of measurements on an instrument with a specific correction equation used to convert raw measurements to VSMOW-SLAP scale. Standards runs involve the measurement of VSMOW and SLAP, along with in-house standards and additional water samples to validate isotopic values of these waters on the VSMOW-SLAP scale using a correction equation. Once in-house standards have been validated on the VSMOW-SLAP scale, these in-house standards can then be used for proceeding analysis runs that include both water samples measured during the standards run (used as ‘control waters’ to provide additional validity to analysis runs) and water samples with unknown isotopic values (an example is provided in Table 1). Each analysis run will have a unique correction equation used to convert the raw measurements to VSMOW-SLAP scale. After a series of analysis runs, the user should conduct another standards run to re-validate in-house standards, and the cycle is repeated. Averages for isotope values for all water used within a lab should be recorded over time and stored at the top of the Python script provided. For example, in the provided code our lab has values for different water standards and samples used over a 2-year period. These values will be used for comparison during the standards run.

Conversion of raw δ values (e.g., δ18O) to VSMOW-SLAP scale can be accomplished by following two steps (both steps are shown for δ18O, but both are also applied to δ17O): the determination of a ‘stretching factor’, followed by the generation of an ‘offset value’ (Sharp 2007; Carter & Barwick 2018). First, a stretching factor is obtained by accounting for variation among laboratories in the measured value VSMOW and SLAP:

(δ18OVSMOW known – δ18OSLAP known) / (δ18OVSMOW measured – δ18OSLAP measured)= δ18Ostretching factor (3)

Second, an offset value is calculated, to account for variation among laboratories in the measured difference between VSMOW or SLAP:

δ18Ooffset value = δ18OVSMOW known – (δ18OVSMOW measured \* δ18Ostretching factor) (4)

This offset value can be calculated using either VSMOW or SLAP (Carter & Barwick 2018), or by calculating an offset for both VSMOW and SLAP and then dividing by two. Once an offset value and stretching factor have been determined, raw values can be corrected using the following equation:

δ18Ocorrected value = δ18Ostretching factor \* δ18Oraw value + δ18Ooffset value (5)

While Equations 3-5 are demonstrated for VSMOW and SLAP, these equations can also be used for in-house standards. For example, my lab uses standards provided by the United States Geological Survey (USGS) such as USGS47 and USGS50. Both USGS47 and USGS50 would simply replace VSMOW and SLAP in this equation and the isotopic values published by USGS (‘known’) would be used to calculate correction equations.

*Cleaning and Finalizing Raw CRDS Datasheets*

The Python script provided was developed using data from a Picarro L2140-*i.* The raw datasheet exported from this CRDS instrument contains various imperfections that the initial lines of the code for the standards run and analysis run clean. For example, blank spaces are frequent throughout the raw datasheet such as in the column names. The script is designed to automatically remove these blank spaces. In addition, the raw datasheet also contains numerous variables (columns) that contain advanced metrics that are likely irrelevant for ecological or biological purposes. The script for standards runs and analysis runs is designed to remove these variables so that data only contains the pertinent information: 1) raw and corrected measurements of δ17O, δ18O, Δ17O (these appear in the data as ‘d(17\_16)Mean’ for raw values and ‘d17O\_amended’ for example for δ17O); 2) raw and corrected measurements of δ2H (appears in the data as ‘d(2\_H)Mean’ for raw values and ‘2H\_amended’); and 3) measurements of the average water concentration for (in the code as ‘H2O\_Mean). Prior to removing additional variables, the script exports csv files for each water sample analyzed during either the standards or analysis run so that these can be revisited if the user needs to review these advanced metrics.

Once a datasheet has been cleaned and raw measurements have been corrected to VSMOW-SLAP scale, the script is designed to also remove measurements that have likely been influenced by the memory effect (similar to what was done prior to the creation of the stretching-offset, correction equation). At this point, a mean, standard deviation, and difference from the known or established value for δ17O, δ18O, and Δ17O is calculated for each relevant sample. This is displayed at the bottom of each individual dataframe. Then each dataframe is exported as a ‘sheet’ in a larger xlsx file. This larger xlsx file is designed to easily review data from a specific standards run and determine the precision and accuracy of measurements. If the measurements from the standards run are acceptable, the user can proceed to complete an analysis run using predetermined in-house water standards specific to their lab. Once this analysis run is completed, the raw data is exported from the CRDS instrument and exported into the Python script after the section in bold titled ‘analysis run’. The immediate step after this resets the values of the all the waters used for comparison during the standards run (those stored at the top of the code) so that they can be used for this analysis run and all proceeding analysis runs. The script for the analysis run proceeds in a similar fashion as the standards run but differs from the standards run when generating the correction equation (stretching-offset) because the in-house standards will be used in place of VSMOW and SLAP. In addition, the analysis run differs because later in the script, unknown samples (e.g., animal body water samples) will need to be differentiated from established samples. These is critical because a mean, standard deviation, and difference from the known or established value for δ17O, δ18O, and Δ17O will be calculated for established samples, but only a mean and standard deviation will be calculated for unknown samples because there is nothing to compare these samples with. The data for both the standards run and analysis run is exported as a final xlsx file in the same manner.

While the Python is script is designed to be as fully-automated as possible, a few lines of the code still need to be manually adjusted by the user. These lines are identified and described in Table 2.

**Data**

To provide support for this, I have provided three raw datasheets for both standards runs and analysis runs. Each standards run dataset is composed of ~600 measurements, while analysis runs typically are composed of 300-450 measurements. Each standards run datasheet is paired with an analysis run datasheet (e.g., ‘StandardsRun\_1’ is compatible with ‘AnalysisRun\_1’). Each pairing should demonstrate the following:

1) That generating a correction equation from VSMOW and SLAP measurements during standards runs should generate: a) δ17O values within 0.15‰ (per mi) of the known/established value; b) δ18O values within 0.3‰ of the known/established value c) Δ17O values within 0.015‰ of the known/established value;

2) That the finalized values from the standards run should be incorporated into the data environment such that it can be used to influence the proceeding analysis run;

3) That generating a correction equation from in-house water standards (in the provided code these are ‘USGS47’ and ‘USGS50’) with values established from the preceding standards run should generate: a) δ17O values within 0.15‰ of the known/established value b) δ18O values within 0.3‰ of the known/established value c) Δ17O values within 0.015‰ of the known/established value

I compared the six finalized xlsx files generated from this Python script to the original six xlsx files that were generated in an R (4.0.3) script that was more labor intensive and selective when generating correction equations to compare the precision and accuracy of δ17O, δ18O, and Δ17O values.

**Discussion**

This research demonstrates that raw data from a CRDS instrument can be seamlessly exported and then imported to a Python script that corrects and finalizes data in a publishable format. The script is nearly fully-automated but does require manual input for <10 sections of the code. The final product of the script produces isotope measurements that are comparable with those generated via a more labor intensive and scrutinous cleaning and correction process, although the values obtained from the automated method seem slightly less precise.

While the aim of this research was to produce a fully-automated script, several sections of the code continue to require manual entry. Some of these sections such as the importing of the data itself are justifiably difficult to automate and others such as the specified location to export csv and xlsx files will likely only need to be manually adjusted once and then should remain the same going forward. However, other sections like the removal of conditioning waters and setting the unknown and established waters could become automated by conducting modifications while operating the CRDS instrument itself. For example, while operating the instrument, the user has the opportunity to enter the name of the samples to be analyzed in the ‘Identifier 1’ section. However, an ‘Identifier 2’ section exists as well, which could be used to resolve this issue. The user could potentially enter ‘Conditioning’, ‘Established’, and ‘Unknown’ in the ‘Identifier 2’ section and then generate code to automatically separate samples into these sections based on this information.

The script provided generated highly accurate and precise data. However, the constraints of the automated process limited the ability to remove measurements that were biased or altered by the memory effect. In comparison, the more labor intensive and scrutinous approach using the R code was able to remove these measurements more effectively, which ultimately resulted in smaller final dataframes for each sample. As such, the R code approach, on average, generated data with smaller standard deviations for δ17O, δ18O, and Δ17O values compared to the Python script, and thus higher precision. However, the difference in precision was small. For example, for the Δ17O values the average precision for Δ17O values was ~8 per meg using the R code and ~11 per meg for the Python script. This could potentially be resolved by adjusting the current approach to automatically remove measurements by determining a cutoff line. For example, while the current cutoff line replicates removing all measurements outside of 1σ in an effort to not immediately remove potentially viable measurements, this could be adjusted to remove measurements outside of 1σ for this first round of removals, and the second round of removals could remove all measurements outside of 0.75σ.

**Conclusion**

Overall, the Python script generated provides a useful tool for finalizing data for ecologists and animal biologists new to CRDS instrumentation. While the Python script does not produce as highly precise data as more labor intensive and scrutinous approaches might, the Python script is able to finalize data in considerably less time and the script provided is less daunting than tackling the post-processing as a new user. While this project provides a route for CRDS users, future research should design a similar script for OA-ICOS instruments that also provide a great alternative to IRMS instruments.

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**Table 1**.Example of an analysis run completed on the Picarro L2140-*i*. Two in-house standards (VA01 and VA02) verified via internationally-accepted water standards were incorporated throughout the run to enable correction of raw measurements. Injection total refers to the total number of injections as the run progresses while number of injections refers to the number of injections for that particular item, with more injections required for analyzed samples that vary greatly in δ18O from the proceeding item. Autosampler job number refers to the order in which each item was listed for analysis. While a sample may have 30+ measurements, most of these measurements are removed due to the memory effect and only a select number of measurements remain for analysis.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Material being analyzed** | **Injection total** | **δ18O (‰)** | **Number of injections** | **Autosampler job number** | **Purpose** |
| Conditioning vial | 1-70 | ~ 0 | 70 | 1 | Warm-up instrument |
| Conditioning vial | 71-97 | ~ +4 | 27 | 2 | Positioningδ18O for in-house standard analysis |
| In-house standard (VA01) | 98-157 | ~ +8 | 60 | 3 | First of three points for correction equation |
| Control vial | 158-184 | ~ +4 | 27 | 4 | Further validation of data |
| Control vial | 185-211 | ~ -2 | 27 | 5 | Further validation of data & positioning δ18O for unknown samples |
| Distilled  Samples | 212-361 | ??? | 150 | 6-17 | Assessing isotopic values of unknown biological samples |
| Conditioning vial | 362-394 | ~ -4 | 33 | 18 | Positioning δ18O after running unknown samples |
| Control vial | 395-437 | ~ -10 | 43 | 19 | Further validation of data & positioning δ18O for in-house standard |
| In-house standard (VA02) | 438-470 | ~ -9 | 33 | 20 | Third point for correction equation |
| *Total Injections* | *470* |  |  |  |  |
| *Estimated run time* | *~ 72 hours* | |  |  |  |

**Table 2**. The Python script provided was designed to be as fully automated as possible. However, several sections of the script require manual input from the user, related to things such as importing and exporting data. These sections (in the Jupyter Notebook) are specified and a reason for the manual input is described.

|  |  |  |
| --- | --- | --- |
| **Number of manual inputs** | **Section** | **Reason for manual input** |
| 1 | Section 2 | Setting values for all waters run in the lab for comparison during standards run |
| 2 | Section 3 | Importing raw Standards datasheet |
| 3 | Section 37 | Setting a location for exporting sample csv files |
| 4 | Section 43 | Setting which conditioning water samples to remove |
| 5 | Section 46 | Setting a location for exporting final xlsx file |
| 6 | Section 48 | Importing raw analysis run datasheet |
| 7 | Sections 63-70 | Specifying in-house water standards |
| 8 | Sections 78-79 | Setting a location for exporting sample csv files and removing in-house standards from the list |
| 9 | Section 83 | Set which conditioning water samples to remove and set which waters are established versus unknown |
| 10 | Section 87 | Setting a location for exporting final xlsx file |