Editorial Comment #1:

The reviews (thanks to the reviewers and to the editor) are generally positive, but there are important comments and suggestions that should be taken into consideration during the revision. Looking forward to the revised manuscript

Response to Editorial Comment #1:

We are pleased that the reviews are generally positive, and we found the feedback very helpful. In our responses to each comment, we have explained the changes that can be expected in order to address the reviewers' and editors' comments. We thank the reviewers and the editors for the constructive changes they have suggested to this manuscript.

- Bronwen Konecky
On behalf of all authors

Response to SC1 (Editor Johannes Wagner):

We thank the Editor for examining the database serializations from a user point of view and providing us with this helpful feedback. Below, we detail the revisions we will undertake in order to clarify usage of the serializations, and to provide additional sample code for non-R users. The original comment is copied below in **bold text** and our responses appear in plain text.

- Bronwen Konecky
On behalf of all authors

I think you present a well prepared product worth publishing, however looking through the data I noticed a few points that could be clarified before publication.

- if I look at the 3 serialisations, I see that the R and matlab versions contain d, TS and sTS, however the python pickle only contains D and TS
>>> infile = open('iso2k0_14_2.pkl','rb')

>>> iso2k_dict = pickle.load(infile)
>>> iso2k_dict.keys()
dict_keys(['D', 'TS'])
does that have any relevance? please clarify

- directly regarding those: I have not found in the paper what D TS and sTS stand for. For the undiscerning user, this is confusing.

We thank the Reviewer for this very helpful observation; the three variables are indeed different and require explanation. We have therefore added the following short paragraph in section 6.2 (between lines 685-690 of the Discussion paper) describing the D, TS, and sTS variables. The text is below.

The MATLAB and R serializations contain three variables: 'D', 'TS', and 'sTS.' The variable 'D' includes site-level data for each dataset structured in the LiPD format. Datasets in 'D' often contain multiple variables (e.g. stable isotope, ancillary, and chronological data), and represent how LiPD data appear when loaded into the initial environment. For most users, however, a "flattened" version of the database is more useful. We have provided this as the 'TS' variable, where each entry contains an individual time series and its associated metadata. A slightly modified version of 'TS' is included with R and Matlab, called 'sTS', which is identical to TS except that the interpretation fields are split by scope ('isotope' or 'climate') in order to simplify querying, which may be preferable for some users. The Python serialization contains only 'D' and 'TS'.

- your dataset at figshare makes no mention of the ESSD paper and the data are not well described at the repository. Whoever stumbles uppon your data there will be at a loss. Could you add a little data description or a readme file to the repository? The

very good metadata spreadsheet you provide is also missing there.

Thank you for this suggestion. Text will be added to the Figshare page with a link to the ESSD paper where users can find a description of the database, metadata fields, and supplementary tables. Links will also be added to download the 3 sample codes.

NOAA-WDS is in the process of getting a DOI minted for Iso2k version 1.0.0 (the "final publication" and official release of the database). It is our intention for that NOAA-minted DOI to be the DOI that is published in the final ESSD publication, rather than the Figshare DOI. Recognizing that v.0.14.7 of the database will be available via the Figshare DOI in perpetuity, a note will be added to that Figshare page directing users to Iso2k v1.0.0 and all future updates via the NOAA-minted DOI, and the NOAA-WDS landing page.

**- lastly, for final publication, it would be very helpfull to provide a short sample code for
the other two serialisations as well (in a free matlab implementation like octave, and
python). I don't think they would have to be as extensive as the R sample. (This may
also resolve issue number one, maybe you handle the m files differently)**

We have created MATLAB and Python sample codes that replicate the example workflow in the original R sample code. The 3 sample codes are now available in a revised Supplementary Materials for this paper. The variable handling with Python is indeed a little different than with R and MATLAB, and the sample code now makes those procedures explicit. Thank you for this helpful suggestion!

Response to Anonymous Referee #1:

We thank the reviewer for the feedback and constructive comments on this manuscript. Below, we detail the revisions we will undertake in order to address the reviewer's comments. The original review is copied in **bold text** and our responses appear in plain text. We greatly appreciate the feedback and we believe the revised manuscript will be substantially improved.

- Bronwen Konecky
On behalf of all authors

The Iso2k database presented here represents a massive data synthesis effort and is a valuable contribution to our ability to effectively analyze regional and large-scale patterns in isotopic data. A random spot check of DOIs, LipD, and original data links, suggests that all the references are correct. This dataset will facilitate many new studies and will be well cited. The data quality of each individual record largely depends on the quality of the original work, but the authors are very thorough in providing the necessary metadata about each record that will allow users to evaluate the original data.

It is also good that the data links to the original author's study, since many of the datasets in the compilation are already posted on complementary data repositories like NOAA Paleoclimatology, and includes information on the original authors' interpretation of the isotopic signal. With this as with other data synthesis products, several records may be listed in multiple data synthesis products (e.g. SISAL for speleothems). The authors should be commended for section 6.5: we know that, for better or worse, scientific impact is measured in terms of citations, and so future work that simply cites Iso2k instead of the original studies risks undervaluing the scientific contributions of the researchers who generated the original data that forms the basis of the database, potentially influencing especially ECR career advancement. Providing the original citation information makes this easy.

We really thank the reviewer for recognizing the care we took to preserve the ability for original studies to be cited.

The effort to compile age control points from 'dark literature' is also commendable. I was slightly concerned to see the number of especially lacustrine records where authors did not make age control data available. I wonder if there is a way to permanently host a webform for authors to submit additional information that was requested as part of this version of the database but was not provided, but could be easily included in subsequent revisions. Might be easier than direct emails. This also applies to a few records I know have come out since this paper has been posted - for these large synthesis efforts finding an efficient way to update these databases seems key given the volume of data that is published in each year.

The Reviewer raises two important issues here, the submission of chronological data as well as the overall governance and procedure for submission of future datasets (paleo-isotopic data as well as age control data) to future versions of the Iso2k database.

We heartily agree that the submission of raw chronological data to public repositories should be standard operating procedure when authors submit datasets. Nowadays, many authors do indeed submit age control data in addition to their paleo-observation data, but for older publications this was not customary. We are very pleased to be able to now bring these chronological datasets to the publicly-available sphere.

A submission page for datasets not currently included in the Iso2k database is an excellent idea. A link to a LiPD entry template hosted through http://lipd.net/playground will be added to the official WDS-NOAA landing page for Iso2k, along with instructions for dataset submission. Because the Iso2k database was designed to use LiPD files, and the project was in direct coordination with LinkedEarth, these solutions are relatively straightforward from a technical perspective. When someone submits a new datasets as a LiPD files through http://lipd.net/playground, there is already an option to generate a "NOAA-ready" LiPD file so that users can then submit directly to the NOAA-WDS public repository, rather than having to fill out data entry templates separately. This will encourage broader submission of datasets to public repositories.

Long-term governance of the database and the procedure for community vetting and incorporation of new datasets to the Iso2k database are issues that require more than a technical fix. Those issues are currently being discussed by the group in consultation with other related PAGES groups and with the PAGES 2k coordination team. In the meantime, for purposes of this publication, we have added text to section 6.3 (line 715 of Discussion paper), with a reference to this section at the end of Section 1.3 (line 190), explaining the steps for dataset submission and stating that more detailed instructions and a link to a LiPD entry template will be added to the NOAA-WDS landing page when it is created.

6.3 Database updates, versioning scheme, and submission of new or updated datasets

This publication marks Version 1.0.0 of the Iso2k database (editors and reviewers: please note that you are reviewing version 0.14.7; this will become version 1.0.0 upon publication, following any edits during the review process). Following publication, the database will continue to evolve, as new datasets are added (both new studies and previous records that have been missed) and existing data or metadata are extended, or as necessary, corrected. Readers who know of missing datasets are asked to submit them directly through http://lipd.net/playground. Database users who find errors in individual datasets can submit proposed edits using the "Edit LiPD file" function at http://lipdverse.org/iso2k/current_version/, or they can use the "Report an issue" option for errors that apply to multiple datasets. More detailed instructions for dataset submission and a link to a LiPD entry template hosted through http://lipd.net/playground will be added to the WDS-NOAA landing page when they become available.

We thank the Reviewer again for these helpful suggestions.

Response to Anonymous Referee #2:

We thank the reviewer for the feedback and constructive comments on this manuscript. Below, we detail the revisions we will undertake in order to address the reviewer's comments. The original review is copied in **bold text** and our responses appear in plain text. We greatly appreciate the feedback and we believe the revised manuscript will be substantially improved.

- Bronwen Konecky
On behalf of all authors

Konecky et al. present a large compiled dataset of isotopic tracers of the hydrologic cycle spanning the last 2000 years. This database clearly represents a huge coordinated data synthesis effort, and the authors should be lauded for their efforts to provide a standardized metadata template to facilitate intercomparison across studies and proxy types. In addition, I appreciate the authors have gone through the effort to maintain a link between datasets and the original study/citation the data were derived from. My sense is that this dataset will be highly cited, and enable new studies of Common Era hydroclimate. Furthermore, the authors have provided a roadmap for how this dataset is to be versioned and built upon; the expectation is that it will only improve in quality and utility through time. Therefore, I recommend that this study be published after a few minor comments below are addressed.

We are pleased the reviewer found the database to be promising.

Minor "science" comments:

1. I understand that the discussion of controls on isotope ratios of the different "archive types" in section 3 are meant to be brief, as an exhaustive discussion of controls on each proxy type would increase the length of this paper several times over! However, I would argue for a slight expansion (and correction of small errors) in the description of controls on tree-ring cellulose. First, the 27‰ offset observed by Sternberg et al.1986 was between cellulose and water, not the cellulose precursors (L. 415-416). Cellulose synthesis from these precursors also permits exchange with water at carbonyl oxygens, so the offset between the isotope ratios of the precursors and water is likely to be different than the offset between cellulose and water, especially if the sugars are no longer in the leaf (as in tree rings).Second, I'm not sure that I understand what's meant by "as the biosynthetic fractionation is relatively constant" at L. 416 – leaf waters certainly vary in space and time rather dramatically (e.g., West et al. 2008 Plos One), and therefore, the sugars produced using these leaf waters would also have different isotope ratios. Third, some of the signal found in the leaf is dampened before being used in tree-ring cellulose as a fraction of oxygen in leaf-exported sugars exchange with xylem water in the trunk (e.g., Roden et al. 2000 GCA). Therefore, tree-ring cellulose d18O values reflect both changes in plant water sources through time (e.g., changes in xylem water isotope ratios) as well as changes in environmental conditions (e.g., more enrichment of leaf waters/sugars via a drier atmosphere, for example). Some of Paul Szejner's recent work

has shown this clearly for the North American Monsoon, for example (Szejner et al. 2016 JGR).

Thank you. We appreciate these points. The text on the biochemical fractionation has been corrected and improved. We clarify that variability in tree-ring cellulose 18O is primarily influenced by the 18O of source water and leaf water, which are influenced by climate and environmental factors. We replaced the paragraph from lines 410-421 of the Discussion paper with the new paragraph below:

The wood in tree rings (tree-ring cellulose) is one of the few terrestrial proxy archives that can be directly constrained to calendar years (McCarroll and Loader, 2004; Schweingruber, 2012). Information about climatic and environmental changes on seasonal-to-annual time scales is recorded in tree-ring cellulose $\delta^{18}O$. The $\delta^{18}O$ of tree-ring cellulose is influenced by (i) the $\delta^{18}O$ of source waters, and (ii) factors influencing $\delta^{18}O$ of the leaf water and (iii) a fractionation related to the isotopic exchange of carbonyl oxygen of cellulose intermediates with cellular waters (derived from enriched leaf water and unaltered xylem or source waters), resulting in an overall ~27‰ enrichment of cellulose $\delta^{18}O$ relative to cellular waters (Barbour et al., 2004; Gessler et al., 2014; Roden et al., 2000). This fractionation is regarded as a constant in mechanistic models (e.g., Cernusak et al., 2005; Roden et al., 2000) and so cellulose $\delta^{18}O$ variability mainly reflects the $\delta^{18}O$ of source water and leaf waters. The $\delta^{18}O$ of the source water is closely related to the $\delta^{18}O$ of precipitation-derived soil water (Bowen et al., 2019). As such, the primary climatic signal that controls $\delta^{18}O$ of tree-cellulose varies by location, depending on the climatic signals controlling precipitation $\delta^{18}O$ (Section 1.2). For example, tree-cellulose $\delta^{18}O$ records have been interpreted to reflect temperature at mid- to high-latitude sites (e.g., Churakova (Sidorova) et al., 2019; Porter et al., 2014; Saurer et al., 2002; Sidorova et al., 2012), and precipitation amount in tropical or monsoonal sites (Brienen et al., 2013; Managave et al., 2011). As the $\delta^{18}O$ of the soil water is also affected by evaporation of the soil water, precipitation minus evaporation (P-E) influences $\delta^{18}O$ tree-cellulose (Sano et al., 2012; Xu et al., 2018). Water vapour pressure deficit between the leaf intercellular space and the ambient atmosphere in conjunction with the leaf physiological traits control the extent of evaporative enrichment of the source water in ^{18}O in the leaf and hence $\delta^{18}O$ of the leaf water and tree-cellulose (Kahmen et al., 2011; Szejner et al., 2016).

Minor 'science' comment #2

L. 420 – could it also be the case that this cellulose d18O signal is due to changes in the d18O of the vapor that is the source of this precipitation? There's been a fair amount of work in the past decade that has suggested the relationship between local precipitation amount and d18O is fairly weak compared to precipitation processes (e.g.,microphysics) and moisture transport history (e.g., Dayem et al. 2010 EPSL, Konecky et al. 2019 GRL, Vimeux et al. 2011 EPSL, Bowen et al. 2019 among others).

We agree that cellulose d18O can reflect factors other than temperature and precipitation amount, such as moisture source, precipitation microphysics, and transport history. We revised the text here to clarify that the climatic controls on the d18O of cellulose are largely driven by the climatic controls on d18O of precipitation, which are discussed in Section 1.2. See the above revised paragraph. We also added a reference to section 1.2 and also added the reviewer's suggested citations to that section.

Minor technical comments:

1. Supplemental Table S2 - rows 769-778 seem to be missing a full reference for pub1.

These rows have a full reference for pub1 (Moreno et al., 2012, QSR, complete with doi). However, the formatting of special characters appears to have been incorrect, which may have led to problems viewing the publication reference. We fixed this as well as other special character errors in Supplemental Table S2.

2. L. 207: publicly-available -> publicly available

Fixed.

3. L. 411. Seasonal to annual -> seasonal-to-annual

This line was edited for clarity.

4. L. 451 - comma placement? The second half of this sentence doesn't seem to line up with the first.

The second half of the sentence L. 451 was rephrased. "...foraminifera calcite is systematic **i.e.** the δ18Osw can be reconstructed…"

5. L. 448 - seasonally-biased -> seasonally biased
Changed

6. L. 625 - what are these percentages based on? L. 621 suggests that the percentages in L. 625 should perhaps add to 100%

This is indeed a bit confusing as written. Therefore, we clarified the text in this paragraph so that the percentages are out of stable isotope records, rather than being out of all the records in the database (which included 255 ancillary records).

We thank the Reviewer again for these helpful suggestions.

2

The Iso2k Database: A global compilation of paleo-δ^{18}O and δ^2H records to aid understanding of Common Era climate

Bronwen L. Konecky[1], Nicholas P. McKay[2], Olga V. Churakova (Sidorova)[3], Laia Comas-Bru[4],

Emilie P. Dassié[5], Kristine L. DeLong[6], Georgina M. Falster[1], Matt J. Fischer[7], Matthew D. Jones[8],

Lukas Jonkers[9], Darrell S. Kaufman[2], Guillaume Leduc[10], Shreyas R. Managave[11], Belen Martrat[12],

Thomas Opel[13], Anais J. Orsi[14], Judson W. Partin[15], Hussein R. Sayani[16], Elizabeth K. Thomas[17],

Diane M. Thompson[18], Jonathan J. Tyler[19], Nerilie J. Abram[20], Alyssa R. Atwood[21], Olivier Cartapanis[22], Jessica L. Conroy[23], Mark A. Curran[24], Sylvia G. Dee[25], Michael Deininger[26], Dmitry V. Divine[27], Zoltán Kern[28], Trevor J. Porter[29], Samantha L. Stevenson[30], Lucien von Gunten[31], and Iso2k Project Members*

[1]Department of Earth and Planetary Sciences, Washington University, Saint Louis, Missouri, 63108, USA
[2]School of Earth and Sustainability, Northern Arizona University, Flagstaff, AZ, 86011, USA
[3]Institute of Ecology and Geography, Siberian Federal University, Krasnoyarsk, 660041, Russian Federation & Department of Forest Dynamics, Swiss Federal Institute for Forest, Snow and Landscape Research WSL, Birmensdorf, CH-8903, Switzerland
[4]School of Archaeology, Geography & Environmental Sciences, University of Reading, Reading, Berkshire, United Kingdom
[5]EPOC Laboratory, University of Bordeaux, France, 33615, France
[6]Department of Geography and Anthropology, Coastal Studies Institute, Louisiana State University, Baton Rouge, LA, 70803, USA
[7]NSTLI Environment, ANSTO, Sydney, NSW, 2234, Australia
[8]School of Geography, University of Nottingham, Nottingham, NG7 2RD, UK
[9]MARUM Center for Marine Environmental Sciences, Bremen University, Bremen, 28359, Germany
[10]Aix Marseille University, CNRS, IRD, INRAE, Coll France, CEREGE, Aix-en-Provence, 13545, France
[11]Earth and Climate Science, Indian Institute of Science Education and Research, Pune, Maharashtra, 411008, India
[12]Department of Environmental Chemistry, Spanish Council for Scientific Research (CSIC), Institute of Environmental Assessment and Water Research (IDAEA), Barcelona, Barcelona, 08034, Spain
[13]Polar Terrestrial Environmental Systems and PALICE Helmholtz Young Investigator Group, Alfred Wegener Institute Helmholtz Centre for Polar and Marine Research, Potsdam, 14473, Germany
[14]L-IPSL, CEA-CNRS-UVSQ-Université Paris Saclay, Laboratoire des Sciences du Climat et de L'Environnement, Gif Sur Yvette, 91191, France
[15]Institute for Geophysics, University of Texas at Austin, Austin, TX, 78758, USA
[16]School of Earth and Atmospheric Science, Georgia Institute of Technology, Atlanta, GA, 30332, USA
[17]Department of Geology, University at Buffalo, Buffalo, NY, 14260, USA

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[18]Department of Geosciences, University of Arizona, Tucson, Arizona, 85719, USA

[19]Department of Earth Sciences, The University of Adelaide, Adelaide, South Australia, 5005, Australia

[20]Research School of Earth Sciences and Centre of Excellence for Climate Extremes, Australian National University, Canberra, ACT, 2601, Australia

[21]Department of Earth, Ocean, and Atmospheric Sciences, Florida State University, Tallahassee, Florida, 32306, USA

[22]Institute of Geological Sciences & Oeschger Centre for Climate Change Research, University of Bern, Bern, CH-3012, Switzerland

[23]Department of Geology, University of Illinois at Urbana-Champaign, Urbana, IL, 61822, USA

[24]Australian Antarctic Division, Kingston, Tasmania, 7050, Australia

[25]Department of Earth, Environmental, and Planetary Sciences,, Rice University, Houston, Texas, 77005, USA

[26]Institute of Geosciences, Johannes Gutenberg University Mainz, Mainz, 55128, Germany

[27]Norwegian Polar Institute, Tromsø, 9296, Norway

[28]Institute for Geological and Geochemical Research, Research Centre for Astronomy and Earth Sciences, MTA Centre for Excellence, Budapest, H-1112, Hungary

[29]Department of Geography, University of Toronto - Mississauga, Mississauga, Ontario, L5L1C6, Canada

[30]Bren School of Environmental Science & Management, University of California, Santa Barbara, Santa Barbara, CA, 93106, USA

[31]PAGES International Project Office, Bern, 3012, Switzerland

Correspondence to: Bronwen L. Konecky (bkonecky@wustl.edu)

*A full list of authors appears at the end of the paper.

Abstract. Reconstructions of global hydroclimate during the Common Era (CE; the past ~2,000 years) are important for providing context for current and future global environmental change. Stable isotope ratios in water are quantitative indicators of hydroclimate on regional to global scales, and these signals are encoded in a wide range of natural geologic archives. Here we present the Iso2k database, a global compilation of previously published datasets from a variety of natural archives that record the stable oxygen ($\delta^{18}O$) or hydrogen (δ^2H) isotopic composition of environmental waters, which reflect hydroclimate changes over the CE. The Iso2k database contains 756 isotope records from the terrestrial and marine realms, including: glacier and ground ice (205); speleothems (68); corals, sclerosponges, and mollusks (145); wood (81); lake sediments and other terrestrial sediments (e.g., loess) (158); and marine sediments (99). Individual datasets have temporal resolutions ranging from sub-annual to centennial, and include chronological data where available. A fundamental feature of the database is its comprehensive metadata, which will assist both experts and non-experts in the interpretation of each record and in data synthesis. Key metadata fields have standardized vocabularies to facilitate comparisons across diverse archives and with climate model simulated fields. This is the first global-scale collection of water isotope proxy records from multiple types of geological and biological archives. It is suitable for evaluating hydroclimate processes through time and space using large-scale synthesis, model-data intercomparison and (paleo)data assimilation. The Iso2k database is available for download at: https://doi.org/10.25921/57j8-vs18 (Konecky and McKay, 2020) and is also accessible via through the NOAA/WDS Paleo Data landing page: https://www.ncdc.noaa.gov/paleo/study/29593.

2

1. Introduction

1.1 Progress and challenges in the synthesis of Common Era hydroclimate

The past ~2,000 years, otherwise known as the Common Era (CE), are an important research target for contextualizing modern climate change. Decades of paleoclimate research have yielded numerous records spanning all or part of this time period, making it sufficiently data-rich to assess the range of natural (internal and forced) climate variability prior to the industrial revolution. These records are also used in conjunction with climate model simulations to detect and attribute anthropogenic climate change. Over the past several years, large-scale data synthesis efforts within the international paleoclimate community have produced important constraints on regional to global surface air and ocean temperature patterns during the CE (McGregor et al., 2015; McKay and Kaufman, 2014; PAGES 2k Consortium, 2013, 2017, 2019; Tierney et al., 2015). However, progress on the synthesis of hydroclimate patterns has been limited (PAGES Hydro2k Consortium, 2017), despite the societal relevance of the changing water cycle (e.g., Kelley et al., 2015). The water cycle is a far more complex target than surface air and ocean temperature, and different proxy systems track different aspects of the water cycle in different ways (PAGES Hydro2k Consortium, 2017). For example, annual precipitation amount at any given location on the Earth's surface is governed not just by atmospheric processes that deliver moisture to the region, but also by topography, varying characteristics of storms and associated clouds, dynamics of the seasonal cycle, and variations in the contribution of extreme precipitation events to the water budget (Bowen et al., 2019).

Individual paleoclimatic proxy types are often sensitive to multiple aspects of the water cycle that can be difficult to disentangle, making it challenging to directly compare among proxy types. For example, precipitation amount in the Arctic could be inferred from two common precipitation proxies: grain size from lake sediments and accumulation rates from ice cores. Grain size fluctuations in lake sediments can track extreme precipitation and runoff events, but inter-lake comparison requires knowledge of lake morphometry and competing moisture source regions (Conroy et al., 2008; Kiefer and Karamperidou, 2019; Rodysill et al., 2019). Comparison of sedimentary grain size to snow accumulation rates would be uninformative without understanding how annual precipitation and dry season ablation, which both affect accumulation rates, are related to moisture delivery from extreme precipitation events (Hurley et al., 2016; Thompson et al., 1986). Snow accumulation rates can be strongly affected by air temperature, whereas grain size is generally not. Thus, although comparison of such heterogeneous hydroclimatic proxies is certainly possible, the lack of a common environmental signal to serve as a reconstruction target has been a major hindrance to the global reconstruction of hydroclimatic variables. These challenges have been further exacerbated by archive- and record-specific standards for data formatting, sampling resolution, metadata availability, and public archiving. These limitations may be addressed by creating a metadata-rich, multi-proxy, and multi-archive database of hydrological proxies united through standardized formatting and a common environmental signal: water isotopes.

1.2 The potential for a network of paleo-water isotope records to track past hydroclimate variations

25 In order to address these challenges, we focus here on the stable oxygen ($\delta^{18}O$) and hydrogen ($\delta^{2}H$) isotopic compositions of environmental waters such as precipitation, seawater, lake water, and soil and groundwater **[Figure 1]**. The stable isotopic compositions of such waters (here collectively referred to as "water isotopes") have long been used as integrative tracers of the modern water cycle (e.g., Bowen et al., 2019; Galewsky et al., 2016; Gat, 2010; Rozanski et al., 1993). The rare heavy isotopologues of water (e.g., $^{1}H_2^{18}O$, $^{1}H^{2}H^{16}O$) fractionate from their lighter, more common counterpart ($^{1}H_2^{16}O$) during

30 evaporation, condensation, and other phase changes, capturing an integrative history of parcels of water as they move through and among oceans, atmosphere, and land **[Figure 1]**. Global databases of isotopic measurements of modern precipitation (IAEA/WMO, 2019), rivers (Halder et al., 2015), seawater (LeGrande and Schmidt, 2006), and water vapor (Galewsky et al., 2016) have contributed considerably to our understanding of the contemporary water cycle on scales from micro (e.g., cloud microphysics) (Kurita et al., 2011) to mesoscale (e.g., hurricane dynamics) (Good et al., 2014; Kurita et

35 al., 2011) to global (e.g., residence time of atmospheric moisture) (Aggarwal et al., 2012). More recently, space-borne measurements of $^{1}H^{2}HO/^{1}H_2O$ in multiple levels in the atmosphere have identified the critical role of poorly-observed processes such as tropical rain re-evaporation (Aggarwal et al., 2012; Worden et al., 2007) and forest-atmospheric feedbacks (Wright et al., 2017). Together with climate and Earth system model simulations, which increasingly incorporate sophisticated water isotope tracers into their hydrologic schemes (Brady et al., 2019; Haese et al., 2013), water isotopes offer

40 observational constraints on processes that are otherwise difficult to identify or constrain (Brady et al., 2019; Nusbaumer et al., 2017).

In the paleoclimate realm, hydroclimate proxy records using water isotopes are commonly obtained from a variety of natural archives, including glaciers, ground ice, cave formations, corals, sclerosponges, mollusk shells, tree wood, lake sediments,

45 and marine sediments. Of all of the proxy types that are used to reconstruct past hydroclimate changes, water isotopes are arguably the most common, and certainly the most widely distributed geographically. A global, spatially distributed network of water isotope proxy records therefore has the potential to capture features of large-scale circulation patterns while minimizing site-specific influences from individual locations (Evans et al., 2013). Paired with an understanding of water cycle processes from modern observations and isotope-enabled model simulations, reconstructions of paleo-$\delta^{18}O$ and $\delta^{2}H$

50 from these archives can provide critical information about water vapor source and air mass transport history, precipitation amount and other characteristics, glacial ice volume changes, and temperature, prior to the beginning of instrumental climate observations (Bowen et al., 2019; Dayem et al., 2010; Galewsky et al., 2016; Konecky et al., 2019b). Further, Proxy System Models (Evans et al., 2013) are available for most water isotope proxies, facilitating direct comparison with paleoclimate model output and thus an improved understanding of the climate dynamics responsible for observed (spatial and temporal)

55 water isotope variability (Dee et al., 2015, 2018; Dolman and Laepple, 2018; Jones and Dee, 2018; Konecky et al., 2019a; Thompson et al., 2011).

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One of the obstacles to synthesizing hydroclimate-sensitive paleoclimate records has been a lack of standardized metadata at
60 the proxy system level that systematically encodes the important variables that are necessary for integrating records into a
multi-proxy synthesis, and interpreting the results. Although the paleoclimate community is in the process of defining and
adopting metadata conventions (Khider et al., 2019), the 'bare minimum' current standards (e.g., ISO 19115 for geographic
metadata) used by World Data System (WDS) repositories (e.g., NOAA Paleoclimatology, PANGAEA) are insufficient for
characterizing water isotope proxy systems in a way that can be reliably applied to large-scale paleo-hydroclimate syntheses.
65 One key example of this challenge is the temperature dependence of O- and H-isotopic fractionation, which has frequently
been exploited to reconstruct past temperature changes in locations where air or water temperature exerts first-order
influence on isotope ratios in precipitation and/or seawater (Kilbourne et al., 2008; Meyer et al., 2015; Porter et al., 2014).
Yet in most places, the influence of temperature on isotopic fractionation is only one of many factors that influence the $\delta^{18}O$
and δ^2H of precipitation (Liu et al., 2012; Thomas et al., 2018) and seawater (Conroy et al., 2017; Partin et al., 2012; Russon
70 et al., 2013). A network of water isotope records will inevitably contain information about air and water temperature, but
also other key hydroclimatic variables such as atmospheric moisture source changes and surface water evaporation. In order
to tap the full potential of water isotope proxy records in a large-scale synthesis, the metadata associated with such records
must be sufficient to capture at least a bare minimum of the complexity of the environmental signals that the records contain.

75 Additional metadata challenges have hindered progress in paleo-water isotope synthesis thus far. Most published datasets
shared outside WDS repositories follow non-uniform metadata standards or contain minimal metadata. Datasets are often
catalogued using different conventions (often at the authors' discretion), stored in varying formats (e.g., text, CSV, PDF),
and uploaded to different public or private (i.e., behind journal paywalls) repositories. Furthermore, datasets are frequently
archived without the raw chronological information that would be required to propagate age uncertainties if desired. These
80 challenges are common to any paleoclimate synthesis effort and are not unique to water isotopes (Atsawawaranunt et al.,
2018; Emile-Geay and Eshleman, 2013; PAGES 2k Consortium, 2017), but they exacerbate the challenge of hydroclimate-
specific metadata needs.

1.3 The PAGES Iso2k database
85 Here we introduce the Past Global Changes (PAGES) Iso2k database, a collection of 756 water isotope proxy records (i.e.,
individual time series) from 505 sites (geographic locations) covering all or part of the CE. The database has been assembled
by the PAGES Iso2k Project (hereafter "Iso2k"). The Iso2k database contains $\delta^{18}O$ and δ^2H-based paleoclimate records from
ten different archives: glacier and ground ice (205 records); speleothems (68 records); corals, sclerosponges, and mollusks
(145 records); wood (81 records); terrestrial and lake sediments (158 records); and marine sediments (99 records). Of these,
90 606 records are considered to be primary time series for each site **[Figure 2]** (see Section 2.4 and Supplementary Table 1).
To address the complexity of environmental signals preserved in these proxy records, the database contains detailed
metadata about each record's isotope systematics and proxy system context, as well as details about the original authors'

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climatic interpretation, chronological and analytical uncertainties, and other information required for robust data synthesis
and interpretation. Iso2k has developed a uniform framework suitable for all proxy archives in the database. The architecture
of the Iso2k database therefore provides a scalable foundation on which future multi-proxy hydroclimatic databases can be
built, for example incorporating non-isotopic proxy records such as the grain size and ice accumulation example in section
1.1.

The Iso2k database is the latest in a series of community-led paleoclimate data synthesis efforts endorsed by PAGES
(Atsawawaranunt et al., 2018; Kaufman et al., 2020; McGregor et al., 2015; McKay and Kaufman, 2014; PAGES 2k
Consortium, 2013, 2017; Tierney et al., 2015). The main distinguishing feature of the Iso2k database is that it is not
organized around one archive type, climate variable, or region; rather, it contains a systematic representation of the suite of
environmental signals preserved in the water isotopic composition of diverse paleoclimatic archives, with no *a priori*
assumptions about the underlying climatic interpretation of those signals. This novel approach yields a database that is
flexible enough to evaluate many different environmental parameters and processes during the CE, depending on
investigator interest. The Iso2k database also contains even more comprehensive metadata descriptions compared with
previous PAGES compilations (e.g., PAGES 2k Consortium, 2017). Database users can therefore filter for and process only
the records required for their research question of interest.

This data descriptor presents version 1.0.0 of the PAGES Iso2k database. We describe the collaborative process of
assembling the database (including quality control and validation), and outline the structure and contents of the database
(including data selection criteria, metadata, and chronological information). All data are provided in the Linked Paleo Data
(LiPD) format (McKay and Emile-Geay, 2016) and are machine readable across different platforms and operating systems.
We provide files with sample code to quickly explore the database using various programming languages and platforms (R,
Matlab, Python). The Iso2k database is available for download at: https://doi.org/10.25921/57j8-vs18 (Konecky and McKay,
2020). The database can also be accessed via the NOAA NCEI World Data Service for Paleoclimatology (WDS-NOAA)
landing page: https://www.ncdc.noaa.gov/paleo/study/29593. The WDS-NOAA landing page contains links to download the
serializations for R, MATLAB, and Python, as well as information on submission of new or revised datasets and other
instructions. More information on versioning, submission of new datasets, and other database updates can be found in
Section 6.3.

2. Methods
2.1 Collaborative model

Iso2k is a contribution to Phase 3 of the PAGES2k Network (PAGES 2k Network Coordinators, 2017). Calls for
participation in Iso2k were widely distributed, ensuring a representative cross-section of scientists from various disciplines
(Konecky et al., 2017, 2018, 2015; Partin et al., 2015). Iso2k built on the successes and challenges of previous PAGES2k

projects (Anchukaitis and McKay, 2014; Kaufman, 2014; PAGES 2k Consortium, 2017; PAGES Hydro2k Consortium, 2017) when deciding on the selection criteria (i.e., requirements for inclusion of records) and metadata fields necessary to make the database suitable for a wide range of applications. Most work was done remotely via teleconferences, with one in-person meeting at the 2017 PAGES Open Science Meeting in Zaragoza, Spain.

The workload for assembling the data and metadata was subdivided among working groups, representing one of the following archive types: marine sediment, marine carbonates (corals, mollusks, sclerosponges), glacier ice, ground ice, lake sediments, speleothems, and wood. This archive-based approach ensured that data were collated by researchers with an in-depth, process-based understanding of each proxy system.

2.2 Data aggregation and formatting

The database comprises publicly available water isotope proxy records that span all or part of the CE and meet the criteria outlined in Section 2.3. The database was compiled in two main stages. During the first stage, the archive teams obtained records, entered data, and compiled the extensive metadata outlined in Section 4. During the second stage, the data and metadata were extensively quality controlled following the procedure outlined in Section 2.4.

We used a variety of sources to identify records for inclusion in the database. We first extracted records that met our selection criteria (described in section 2.3.1) from existing data compilations, including the PAGES2k temperature database (PAGES 2k Consortium, 2017), the Arctic Holocene Transitions database (Sundqvist et al., 2014), the SISAL database (Atsawawaranunt et al., 2018). Archive teams then searched the literature and online data repositories (WDS-NOAA and PANGAEA) for additional suitable datasets. For records that had been published but not previously been made available in an online public repository (referred to as 'dark data'), datasets were digitized from publication tables, appendices, and supplementary materials. Datasets that were not available in their original publications were requested from the authors by email. If two or more email requests went unanswered the dataset was deemed not publicly available and therefore did not meet that criterion for inclusion in this database. Of the 606 primary timeseries in the database, more than 20% (128 records) are dark datasets that were added by Iso2k members and are now available in a public, online, machine-readable format for the first time. The vast majority of those datasets were from Wood or from Lake and Terrestrial Sediments (58 and 52, respectively), with an additional 14 from Glacier and Ground Ice, 2 from Marine Sediments, and 2 from Corals.

In addition to isotopic datasets, raw age control data (e.g., ^{14}C ages) were obtained for records where age-depth modeling is required (i.e., non annually-resolved records). Many isotopic datasets that were available through data repositories did not contain raw age control data, in which case we followed the dark data procedure described previously to obtain appropriate chronological data from the authors. For dark age control data, authors were emailed with a request for the data and a spreadsheet template in which chronological information could be added. Age control data from authors who did not respond

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to these requests could not be added to the database. Again, the majority of 'dark' age control data added to the Iso2k database was from the Lake Sediments archive (over 40 age control datasets are now publically available for the first time).

Metadata (Section 4) were obtained from the data source, extracted from the original publication, or requested from the original data generators (again, following the dark data procedure above). We note that even for datasets that were previously publicly available, the Iso2k database has expanded on these data by adding chronological data and compiling an extended suite of metadata not previously available in a consolidated format.

2.3 Record selection criteria

Records were screened by their respective archive teams to ensure that criteria for inclusion in the database were met. Criteria for inclusion in the database were formulated to optimize spatio-temporal coverage of the data, with the goal of building a comprehensive database of water isotope records that can be sub-sampled as needed to address diverse scientific questions. The selection criteria for data records to be included in the Iso2k database are as follows.

2.3.1 Record resolution and duration

The duration and temporal resolution of records included in the Iso2k database varies by archive type. For ~annually- or ~sub-annually-banded archives (corals, shells, sclerosponges, tree wood, varved lake and marine sediments, and glacier ice), the minimum record duration for inclusion in the database is 30 years. For all other archives (speleothems, non-varved lake and marine sediments), records must have a minimum duration of 200 years and contain at least five data points during the CE.

2.3.2 Chronological constraints

The PAGES2k temperature database (PAGES 2k Consortium, 2017) was used as a guide for minimum chronological control criteria. Records from annually-banded archives must be either cross-dated or layer-counted; records from non-annually banded archives must have at least one age control point near both the oldest and youngest portions of the record, with one additional age control point somewhere near the middle required for records longer than 1,000 years.

2.3.3 Peer review and public availability

To qualify for inclusion in the database, isotope records must be published in a peer-reviewed journal (i.e., not university published theses and dissertations). Records included in version 1.0 of the database had to be published and publicly available (see definition in Section 2.2) before 4 May 2018.

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2.3.4 Ancillary data

15   In some cases, paired geochemical measurements are also included in the Iso2k database to complement interpretation of the isotopic data, such as paired trace elemental measurements (e.g., Sr/Ca or Mg/Ca) that accompany some carbonate $\delta^{18}O$ records from corals, sclerosponges, and planktonic foraminifera, or $\delta^{13}C$ data that accompany some carbonate records. Derived isotopic data for deuterium excess (dxs) are also included for glacier and ground ice, where paired measurements of $\delta^{18}O$ or δ^2H allowed the original authors to calculate this additional hydroclimatic indicator. Similarly, derived values for the

20     $\delta^{18}O$ of seawater are available for coral and marine sediment records in cases where an independent temperature reconstruction was available for the same archive (e.g., Sr/Ca for corals and Mg/Ca for planktonic foraminifera). Where the paired carbonate $\delta^{18}O$ and Sr/Ca or Mg/Ca records can be used to infer the $\delta^{18}O$ of seawater (Cahyarini et al., 2008; Elderfield and Ganssen, 2000; Gagan et al., 1998), both time series ($\delta^{18}O$ measured directly on carbonate and $\delta^{18}O$ seawater calculated from paired records) as well as the ancillary, non-isotopic geochemical records are included in the database

25   (Section 4).

2.4 Quality control procedure

    Records considered to be a primary time series for their respective sites (Section 4; Table 6) were quality controlled to the highest degree possible, as described below. Primary time series were judged to be the one or two time series upon which the

30   original authors based their main climatic interpretations. For archives such as corals and speleothems, the primary time series are typically a composite of multiple records from a site or the latest of a series of modified records from a site, whereas for other archives the primary time series is one deemed to have the most robust climatic signal (e.g., for lake sediments, a biomarker of terrestrial versus mixed terrestrial/aquatic origin). Non-primary time series were quality controlled as much as possible and are included because they may contain valuable information for database users. Both data and

35   required metadata fields were screened for accuracy and completeness by one or more project members, with initials of the project member performing the final quality control (QC) check included in the Iso2k_QC_certification metadata field. Metadata fields that required standardized or controlled vocabularies were double checked to ensure those terms were adhered to (Section 4). During the quality control certification process, project members used a web-based data viewer (lipdverse.org) and other visualization tools to display the raw data and metadata.

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    Each metadata field in the database (Tables 1–7) has a quality control certification "level" from 1–3, defined as follows:

- **Level 1** fields are required metadata for inclusion in the Iso2k database. These fields are generalizable enough to be suitable for all archive types, and they are recommended as primary fields for filtering, sorting, and querying

45   records in the database. Level 1 required fields were subject to the highest QC standard. They follow standardized Iso2k vocabularies, where appropriate (Table 7); geographical data were checked against maps, and interpretation fields were checked against the original publication. Examples of level 1 metadata include geographical (ISO

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19115) and publication information (DOI), and the minimum required subset of isotope and proxy system
interpretation metadata fields (see Section 4).

- **Level 2** fields are highly useful, but not required, metadata fields in the Iso2k database. They may be used as secondary fields for further filtering, sorting, and querying records in the database; these fields may be particularly useful for certain archives, or to refine interpretations after an analysis has been performed. Examples of Level 2 fields include species name (marine and lake sediments and corals) and compound chain length for compound-specific δ^2H measurements (lake sediments). Terminology was standardized only where necessary and appropriate. In other cases, these fields contain freeform text with direct quotes from the original publications. During the QC certification process these fields were checked against the original publication for clarity and consistency.

- **Level 3** fields may be useful to some users of the Iso2k database but are not generally recommended as fields for filtering and sorting records in the database. Level 3 fields are not entered as standardized vocabularies and the information is sometimes not available in the original publications (thus, these fields are blank for many records). Examples of level 3 fields include information pertaining to the integration time of a proxy sensor.

- **Automatic fields:** The database also contains several automatically-generated fields that were computed directly from the data records following QC certification. Fields use standardized vocabularies and units. Examples include binary fields for whether the dataset contains raw chronological control data.

Ancillary data are not quality-controlled, but are included in LiPD format for reference.

3. Contents of Iso2k database

3.1 Archive types within the Iso2k database

The Iso2k database contains data from a variety of geological and biological archives. Following Proxy System terminology (Evans et al., 2013), each *archive* has one or more *sensors* that directly sense and incorporate *environmental* signals, i.e., the $\delta^{18}O$ and δ^2H of environmental waters, into their structures. Over time these sensors then form, are deposited into, or are otherwise imprinted upon an *archive* that is then subsampled and subjected to isotopic measurements or *observations*. In this section, we describe the key characteristics of the archives and sensors that are important for the interpretation of the paleohydrological signals that they preserve.

Corals, sclerosponges, and mollusks

Corals, sclerosponges, and mollusks (predominantly bivalves and gastropods) form hard body parts of calcium carbonate (aragonite or calcite) that record the conditions of the aquatic environment in which they live (see reviews of Black et al.,

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2019; Corrège, 2006; Druffel, 1997; Evans et al., 2013; Lough, 2010; Sadler et al., 2014; Surge and Schöne, 2005). Further,

85 except for sclerosponges (which are dated using U/Th geochronology), these aquatic carbonates contain annual banding structures, enabling precise chronology development. Reef-building corals represent the bulk of annually-resolved marine archives included in the Iso2k database. These corals are distributed in warm shallow waters throughout the tropical oceans, whereas sclerosponges (i.e., coralline sponges or Demospongiae) and mollusks are found worldwide, the latter in both estuarine and freshwater environments. Micro-sampling and laser ablation technologies allow for sub-annual to annual

90 sampling resolution in corals, mollusks, and sclerosponges for elemental (e.g., Sr/Ca, Mg/Ca) and isotopic analysis (δ^{18}O and δ^{13}C). When living samples are collected in modern waters, they contain environmental archives of the recent past (decades to several centuries), whereas dead, fossil, and archaeological material can be radiometrically dated to provide windows of past isotopic variability, some of which have been cross-dated with modern records (Black et al., 2019 and refs therein). The δ^{18}O signal in these archives represents a combination of linear, temperature-dependent isotopic fractionation,

95 as well as changes in the isotopic composition of the surrounding water (δ^{18}O$_w$) (Grottoli and Eakin, 2007; Rosenheim et al., 2005). In some regions, the temperature component dominates the δ^{18}O signal, whereas in other regions δ^{18}O$_w$ variability is the primary driver of the δ^{18}O variability and reflects hydrological and/or oceanographic processes such as vertical and horizontal advection or the freshwater endmember (Conroy et al., 2017; Russon et al., 2013; Stevenson et al., 2018). In some ocean settings, the close coupling between ocean-atmosphere variability leads to co-occurring cool and dry (or warm and

00 wet) anomalies that produce complementary isotopic anomalies (Carilli et al., 2014; Russon et al., 2013; Stevenson et al., 2015, 2018)(e.g., ENSO variability; Cobb et al., 2003). In estuarine or freshwater settings, mollusk δ^{18}O values are closely linked to the local precipitation-evaporation budget (Azzoug et al., 2012; Carré et al., 2019). Coral δ^{18}O and δ^{13}C contain a vital effect and coral δ^{18}O is offset from δ^{18}O$_w$, whereas mollusk and sclerosponge δ^{18}O is generally precipitated in equilibrium with environmental water. Some coral δ^{18}O records in the Iso2k database have had their mean δ^{18}O removed by

05 original authors for comparison and cross-dating with other coral records and this is noted in the metadata.

Glacier ice

Climate records from glacier ice are found primarily at high latitudes (Antarctica, Arctic) and high elevation sites (e.g., Andes, Himalayas) (Eichler et al., 2009; Meese et al., 1994). Glacier ice is formed from the accumulation of snow, which

10 over time compacts into a section of chronologically continuous layered ice. Cores drilled through layers of glacier ice preserve sub-annually to centennially resolved climate information, with resolution varying among records due to snow accumulation rates and laboratory sampling and analysis methods (Rasmussen et al., 2014). Ice cores are dated through a variety of methods; annual layer counting and alignment to volcanic horizons are the most common approaches for records spanning the CE (Sigl et al., 2014). This database contains records of δ^{18}O, δ^2H, and/or dxs of glacier ice. These proxies

15 reflect the isotopic composition of precipitation (snowfall and ice), which is highly correlated to local temperature but additionally reflects changes in moisture source and condensation processes (Goursaud et al., 2019). Physical processes such

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as isotopic diffusion in the firn, melt and infiltration, and compaction of ice layers generally smooths the seasonal to interannual signal of climate variability in glacier ice, and the potential influence of these processes is site specific.

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Ground ice (wedge ice and syngenetic pore ice)

Ground ice includes all types of ice found in permafrost; wedge ice and syngenetic pore ice hold the largest potential for paleoclimate reconstructions (Opel et al., 2018; Porter et al., 2016; Porter and Opel, 2020). Ice wedges in permafrost landscapes form via repetitive thermal contraction cracking in winter and infilling of frost cracks mostly by snowmelt in

25 spring (with potential minor contribution of snow and/or depth hoar). The integrated isotopic composition of the previous winter's snow pack is transferred into a single ice vein without additional isotopic fractionation due to rapid freezing in the permafrost. Thus, ice wedges preserve precipitation of the meteorological winter and spring, with $\delta^{18}O$ and δ^2H commonly interpreted as proxies for local air temperature (Meyer et al., 2015). Ice-wedge records are temporally constrained by radiocarbon dating of macrofossils or dissolved organic carbon in the ice. Conversely, pore ice in syngenetic permafrost

30 integrates precipitation that reaches the maximum thaw depth in the late summer. The pore ice seasonality is a function of the local precipitation climatology and residence time of active layer pore waters, and pore ice is enriched in heavy isotopes relative to the initial pore waters due to equilibrium fractionation during freezing (O'Neil, 1968). Because syngenetic pore ice formed within accumulating surface sediments, its age can be modeled based on a radiometrically constrained sediment age-depth profile. Syngenetic pore ice can be cored and sub-sampled in the same way as glacier ice (Porter et al., 2019).

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Lake sediments

Lake sediments may provide long and continuous records of past environmental change (Dee et al., 2018; Mills et al., 2017), and preserve a number of sensors for oxygen and hydrogen isotopes (e.g., Leng and Marshall, 2004). Carbonate minerals—precipitated inorganically from lake waters or in the shells of aquatic invertebrates—have been used as sensors for the

40 isotopic composition of lake water (e.g., Hodell et al., 2001; Morrill, 2004; Von Grafenstein et al., 1998). Additional proxies analysed with increasing frequency include biogenic silica, mostly from diatoms; e.g., (Chaplygin et al., 2016; Swann et al., 2018), cellulose (Heyng et al., 2014), chitinous invertebrate remains (Van Hardenbroek et al., 2018) and lipids (Konecky et al., 2019a; Sachse et al., 2012). Of these proxies, the oxygen isotope composition of carbonates and silicates is subject to temperature-dependent isotope fractionation during mineralisation, whereas the isotopic composition of organic materials is

45 generally not influenced by temperature (Rozanski et al., 2010). The compound-specific hydrogen isotopic composition of a lipid reflects the environment in which the organism producing the lipid grew. Lipids produced by aquatic macrophytes or algae reflect the isotopic composition of the lake water, whereas lipids produced by terrestrial plants reflect the isotopic composition of soil or leaf water (which is, in many cases, highly influenced by the isotopic composition of precipitation). Both types of lipids are preserved in lake sediments (Castañeda and Schouten, 2011; Rach et al., 2017; Thomas et al., 2016).

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For sensors that record the $\delta^{18}O$ or δ^2H of lake water, the climatic or hydrological change recorded in $\delta^{18}O$ or δ^2H depends primarily on the degree to which evaporation influences the lake's hydrological balance relative to other factors (Gibson et al., 2016; Morrill, 2004). In turn, the effect of evaporation on lake water isotopes largely depends on the residence time of water within the lake system, and the degree of hydrological 'closure' of the lake. In open lake systems—which often have surface water inflows and outflows, with a resulting short water residence time—lake waters often reflect the isotopic values of the inflowing waters, which itself generally approximates, a (sometimes) lagged, signal of the weighted mean of the isotopic composition of local precipitation (Jones et al., 2016; Tyler et al., 2007). In hydrologically closed lakes—often without surface outflows and where more water leaves the system through evaporation—the initial isotopic composition of inflowing waters is altered due to this evaporation, with the $\delta^{18}O$ or δ^2H of water increasing with increasing evaporation (Dean et al., 2015; Leng and Marshall, 2004).

Wood

The wood in tree rings (tree-ring cellulose) is one of the few terrestrial proxy archives that can be directly constrained to calendar years (McCarroll and Loader, 2004; Schweingruber, 2012). Information about climatic and environmental changes on seasonal-to-annual time scales is recorded in tree-ring cellulose $\delta^{18}O$. The $\delta^{18}O$ of tree-ring cellulose is influenced by (i) the $\delta^{18}O$ of source waters, (ii) factors influencing $\delta^{18}O$ of the leaf water, and (iii) a fractionation factor related to the isotopic exchange of carbonyl oxygen of cellulose intermediates with cellular waters. This fractionation is derived from enriched leaf water and unaltered xylem or source waters, and results in an overall ~27‰ enrichment of cellulose $\delta^{18}O$ relative to cellular waters (Barbour et al., 2004; Gessler et al., 2014; Roden et al., 2000). This fractionation is regarded as a constant in mechanistic models (e.g., Cernusak et al., 2005; Roden et al., 2000), such that cellulose $\delta^{18}O$ variability mainly reflects the $\delta^{18}O$ of source water and leaf waters. The $\delta^{18}O$ of the source water is closely related to the $\delta^{18}O$ of precipitation-derived soil water (Bowen et al., 2019). As such, the primary climatic signal that controls $\delta^{18}O$ of tree-ring cellulose varies by location, depending on the climatic signals controlling precipitation $\delta^{18}O$ (Section 1.2). For example, tree-cellulose $\delta^{18}O$ records have been interpreted to reflect temperature at mid- to high-latitude sites (e.g., Churakova (Sidorova) et al., 2019; Porter et al., 2014; Saurer et al., 2002; Sidorova et al., 2012), and precipitation amount in tropical or monsoonal sites (Brienen et al., 2013; Managave et al., 2011). As the $\delta^{18}O$ of the soil water is also affected by evaporation of the soil water, precipitation minus evaporation (P-E) influences $\delta^{18}O$ tree-cellulose (Sano et al., 2012; Xu et al., 2018).

The extent of evaporative enrichment of the source water in 18O in the leaf (and hence $\delta^{18}O$ of the leaf water and tree-cellulose) is controlled by the water vapour pressure deficit between the leaf intercellular space and the ambient atmosphere as well as leaf physiological traits (Kahmen et al., 2011; Szejner et al., 2016).

Speleothems

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Speleothems are secondary cave deposits that form when water percolates through carbonate bedrock. Both atmospheric CO_2 and CO_2 generated by plant root respiration and organic matter decomposition are dissolved into rainwater as it percolates through the soil, producing carbonic acid that rapidly dissociates to produce weakly acidic water. As this acidic water percolates through the bedrock, it dissolves carbonate until the water becomes supersaturated with respect to calcium and bicarbonate (Fairchild and Baker, 2012). When the percolating waters emerge in a cave, CO_2 degassing from the drip water to the cave atmosphere induces $CaCO_3$ precipitation, resulting in the formation of stalagmites and stalactites (Atkinson et al., 1978) that preserve the $\delta^{18}O$ signal of the waters that have percolated through from the surface (Lachniet, 2009). The $\delta^{18}O$ of the deposited carbonate therefore reflects the $\delta^{18}O$ of soil/groundwater that infiltrates, which is strongly influenced by the $\delta^{18}O$ of precipitation but with additional influences of aquifer mixing times, seasonality of infiltration, and in some cases extreme events (Moerman et al., 2014; Taylor et al., 2013) processes within the karst and cave, such as calcite precipitation prior to speleothem deposition and/or kinetic isotope effects, can alter the $\delta^{18}O$ of the deposited carbonate.

Although there are hydroclimatic limits on speleothem growth, speleothem distribution is largely constrained by the presence of carbonate bedrock (Fairchild and Baker, 2012). Speleothems form in a wide range of hydroclimate conditions, from extremely cold climates in Siberia to arid regions in the Middle East and Australia. The temporal resolution of speleothem paleoclimate series ranges from sub-annual to centennial, and primarily depends on the karst and cave environment. Due to the high precision of uranium-series dating, speleothems provide opportunities to determine the timing of regional hydrological response to global events and links to external forcing mechanisms (e.g., insolation changes) (Fischer, 2016). The different types of measurements made on speleothems—including $\delta^{18}O$, $\delta^{13}C$, and various trace elements— and their fluid inclusions can be used to reconstruct past changes in the hydrological cycle.

<u>Marine sediments</u>

Marine sediments contain two types of sensors that have widely been used for measuring water isotope variability: planktonic foraminifera and biomarkers. Planktonic foraminifera are unicellular zooplankton living in the upper hundreds of meters of the ocean. They build a calcite skeleton, which is preserved in the sediment. The $\delta^{18}O$ of planktonic foraminifera calcite reflects a spatially (and temporally) variable combination of temperature and $\delta^{18}O_{sw}$ (Urey, 1948) and to a lesser degree also the seawater carbonate ion concentration (Spero et al., 1997), although changes in the latter parameter are likely negligible during the CE. The temperature effect on the $\delta^{18}O$ of foraminifera calcite is systematic, i.e. the $\delta^{18}O_{sw}$ can be reconstructed using (species-specific) paleotemperature equations in conjunction with an independent estimate of calcification temperature based on Mg/Ca (Elderfield and Ganssen, 2000). Planktonic foraminifera have a short life cycle (about a month) and species-specific seasonal and depth habitat preferences (Jonkers and Kučera, 2015; Meilland et al., 2019), such that any planktonic foraminifera record bears an imprint of the ecology of the sensor (Jonkers and Kučera, 2017).

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Biomarkers in marine sediments are lipids synthesized either by marine photoautotrophs, which track past changes in surface seawater isotopic values, or from vascular plants, which track soil water isotopic values on an adjacent land mass (Sachse et al., 2012). Biomarkers are strongly affected by isotopic fractionation during lipid biosynthesis, and that fractionation is often assumed to be constant (Sachse et al., 2012). However, as for planktonic foraminifera, biomarker δ^2H values are also

35 affected by a combination of environmental parameters. The δ^2H values of C_{37} alkenones (synthesized by coccolithophorids) are impacted by fractionation that changes with salinity and growth rates (Schouten et al., 2006), which can mask changes in the δ^2H of seawater. The sources of leaf waxes are terrestrial plants, and the processes affecting leaf waxes in marine sediments are the same as in lake sediments but generally with longer associated time lags between the sensor recording the δ^2H of soil water and ultimate deposition in the marine sediment archive.

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4. Description of Iso2k metadata fields

The Iso2k database contains over 180 metadata fields. The 55 main fields are described in Tables 1–6; 23 of these were strictly quality-controlled following the Level 1 definition in Section 2.4. Entries for some required metadata fields were standardized with controlled vocabulary to allow users to easily query the database for records based on archive type, isotope

45 ratio (O or H), waters from which the isotope ratios are derived, materials on which the isotope ratios were measured, or the environmental parameter that controls isotopic variability **[Figure 1]**. Metadata fields describe the primary isotopic variable being inferred, i.e., the 'isotope interpretation' (e.g., the δ^2H of precipitation), the water from which it was inferred, i.e., 'inferred material' (e.g., soil water), the material that was actually measured, i.e., 'measured material' (e.g., long-chain *n*-alkane components of leaf waxes), and information about the original climate interpretation. Distinction between the archive

50 type **[Figure 2]**, inferred material **[Figure 3]**, and the isotope interpretation **[Figure 4]** allow for advanced analyses and straightforward data-model comparisons using the database. These metadata interpretation fields were derived from interpretations reported in the original publications. Below and in Tables 1–6, we describe key metadata fields in the database, including all Level 1 and Level 2 fields (see Section 2.4 for a description of levels). Table 7 provides standardized vocabularies and common terminologies. Table 8 provides selected chronological control metadata. Supplementary Table 1

55 gives key metadata for each primary time series (Section 2.4), including all Level 1 fields and selected additional Level 2 fields, and references to original publications (citations also listed in Supplementary Tables 2 and 3).

4.1 Entity metadata

The entity metadata fields provide basic information for each record, including the isotope measured, the archive type,

60 location (longitude, latitude, and elevation), start and end dates of each record, and both the DOI and citation for the original publication. Entries for *archiveType*, *paleoData_variableName*, and *paleoData_units* metadata fields are standardized (Table 7) across all archive types to facilitate easy querying and analyses. Each record is assigned a unique LiPD identifier, and all isotope records are assigned a unique Iso2k identifier. The alphanumeric Iso2k identifiers contain 11 characters and digits as follows: archive type (2 characters), year published (2 digits), first author's last name (2 characters), site name (2

65 characters), sample number (e.g., 00, 01, 02, 03…) for different cores or core composites from the same site, and letter (A, B, C…) for multiple time series derived from the same core. The paleoData_variableName indicates the variable measured for each archiveType, usually δ18O or δ2H. In some cases other paired geochemical measurements are included in the database to complement interpretation of the isotopic data (section 2.3.4). A list and detailed description of key entity metadata fields are provided in Table 1.

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4.2 Paleodata metadata

The paleodata metadata fields provide information for each proxy record; a detailed description of key paleodata metadata
75 fields are provided in Table 2. Measured and derived water isotope time series are identified using the
paleoData_variableType and *paleoData_description* fields, and should not be confused with the isotope interpretation
metadata fields (section 4.3), which more broadly refer to the way each proxy record is interpreted (e.g., speleothem
carbonate interpreted as a proxy for the δ^{18}O of precipitation). The variable description (*paleoData_description*) is the
general category of material that was measured for its isotopic ratio (e.g., carbonate or terrestrial biomarker). Further details
80 are given by *measurementMaterial*, which is a more specific description of what was measured (e.g., coral, glacier ice, lake
sediment), and *measurementMaterialDetail,* which provides further specificity of the *measurementMaterial*, such as mineral,
species, or compound. In contrast, the *inferredMaterial* field indicates the environmental source waters whose isotope
variability is inferred (e.g., precipitation, lake water, groundwater) **[Figure 1]**. The environmental source waters in the
inferredMaterial field are not meant to be highly specific (e.g., intracellular leaf water), but rather broad pools of
85 environmental waters that have direct analogs or counterparts in climate models.

4.3 Isotope interpretation metadata

The isotope interpretation metadata fields compile critical information about environmental variables that influence isotopic
variability within each record (Table 3). These fields indicate the environmental variable thought to exert dominant control
90 on isotopic variability of the inferred environmental source waters (*inferredMaterial*) of each record, the mathematical
relationship between the isotope interpretation variable and the isotope record, and the season(s) during which this
interpretation applies. All isotope interpretation fields in the database are prefaced by *isotopeInterpretation*. The
isotopeInterpretation1_variable field lists the primary driver of isotopic variability in the environmental source waters
according to the original publications, for example air temperature or relative humidity (Table 7). For records where multiple
95 variables can explain some fraction of the variability, the *isotopeInterpretation2* and *isotopeInterpretation3* fields are also
populated. The *isotopeInterpretation1_direction* is a field that gives the sign (positive or negative) of the relationship
between the isotope measurements and the environmental variable.

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The *isotopeInterpretation1_variableGroup* field is a simplified supergrouping of terms in the
isotopeInterpretation1_variable field in order to facilitate comparisons across different archives and realms, with three
options (temperature, isotopic composition of precipitation ['P_isotope'], or effective moisture). Controlled vocabulary for
metadata fields *isotopeInterpretation1_variable* and *isotopeInterpretation1_variableGroup* are standardized across all
archive types (Table 7).

The isotope interpretation metadata fields reflect the isotope systematics of the environmental source waters, and as such are
distinct from the climatic inferences that one can make from a proxy record (Section 4.4). In some publications, this
distinction is explicitly spelled out. For example, the cave drip water that becomes incorporated into the $\delta^{18}O$ of speleothem
carbonate in Borneo reflects the $\delta^{18}O$ of water mixed throughout an aquifer system over many months, which ultimately
reflects a smoothed version of precipitation $\delta^{18}O$ (Moerman et al., 2014). In that case, the *inferredMaterial* is
soil/groundwater and the *isotopeInterpretation1_variable* is $\delta^{18}O_{precipitation}$ ('P_isotope'). Separately, $\delta^{18}O_{precipitation}$ at that same
study site reflects multiple hydroclimatic processes such as moisture transport and precipitation amount that lend it a
regional imprint of the El Niño Southern Oscillation (ENSO) (Moerman et al., 2013), and so the climate interpretation of
speleothem $\delta^{18}O$ is related to ENSO, which would be described separately in the climate interpretation fields (Section 4.4).
In many publications, the isotope systematics of the environmental source waters and the climate interpretation are stated
implicitly rather than explicitly (e.g., by stating that the $\delta^{18}O$ of speleothem carbonate reflects monsoon intensity, or by
stating that it reflects local precipitation amount via the amount effect (Dansgaard, 1964). In these cases, the
isotopeInterpretation1_variable is still 'P_isotope' and information about the climatic interpretation is included in the
climate interpretation fields. These distinctions are critical for facilitating comparisons with isotope-enabled climate models,
where complex and nonstationary climate/isotope relationships can be examined directly.

For *isotopeInterpretation1_seasonality,* some proxy sensors and/or archives are interpreted to record a seasonally biased
signal whereas others may record climate at an annual or sub-annual resolution (e.g., corals, some speleothems,
sclerosponges, mollusks, wood). If the record is interpreted to be biased towards a specific season, the calendar months
corresponding to that season—generally given as the first letter of each month, unless clarification is necessary—are
recorded in the metadata field (e.g., MAM, DJFM, Jan). If the record represents an approximately mean annual signal,
'annual' is recorded in the seasonality field. For coral records, if the record has sub-annual resolution (e.g., sampled at
monthly or bimonthly intervals) but the overall record is not biased to any particular season, 'sub-annual' is recorded in the
metadata field.

4.4 Climate interpretation metadata

In contrast to the isotope interpretation (Table 3), climate interpretation metadata (Table 4) represent the original authors'
expert judgment about the primary climatic controls on the isotope ratios at their study site. Climate interpretation metadata

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specify either climatic variables (e.g., temperature, precipitation amount) or processes (e.g., the Pacific Decadal Oscillation, Asian monsoon intensity) that the authors interpreted to influence the isotopic composition of the proxy record, and as such, they are neither standardized nor quality controlled. These metadata are included as useful background information, but should not serve as a primary filter for users of the Iso2k database. A user might filter records based on the isotope interpretation field, then check the climate interpretation field for a qualitative understanding of which climatic processes may be important for the filtered set of records. For records where the *isotopeInterpretation2* and *isotopeInterpretation3* metadata are populated (Table 3), the corresponding *climateInterpretation2* and *climateInterpretation3* metadata may also be provided.

4.5 Queryable and standardized metadata

To make the database more user-friendly and queryable, some metadata fields contain logical flags (e.g., 0 or 1, true or false), cross-links (e.g., to a corresponding record ID in another PAGES2k database), or geographic labels (e.g., continent or ocean basin) that allow for easy sorting (Table 6). For example, if a record was included in the PAGES2k temperature database and reconstructions (Abram et al., 2016; Kaufman, 2014; PAGES 2k Consortium, 2017; Stenni et al., 2017; Tierney et al., 2015), that record is cross-linked to its associated PAGES2k ID wherever possible, permitting easy database query and analysis of records in only one database and those common to both databases. Approximately 15% of the records in the Iso2k database were also incorporated into other PAGES2k compilations with the most overlap occurring in coral records and high-latitude ice cores. For these records, the extensive metadata can be used to facilitate deeper analyses of the hydroclimatic signals contained in these mainly temperature-dominated isotopic records. For example, with coral $\delta^{18}O$ records, many of which are included in both the PAGES2k temperature and Iso2k databases, the isotope interpretation fields denote the relative influence of $\delta^{18}O_{sw}$ vs. temperature to the isotopic variability of the coral carbonate skeleton.

4.6 Chronological control data

Chronological or depth-age metadata provides essential chronological information for isotope records across all archive types, including an age model and the average temporal resolution for each isotope record. For non-annually banded records, age-depth models and radiometric dating information (Table 8) are included where available to facilitate independent age modeling. This information is stored in 'chronData' tables that are linked to the measured data ('paleoData') tables. If a record has raw chronology data in the database (e.g., radiometric age determinations), *hasChron* is set to 1; otherwise this parameter is 0. Similarly, if sample depth data are available (e.g., core depth), *hasPaleoDepth* is set to 1.

To support the information implicit within each record's age-depth model, chronological metadata are provided for all individual age constraints (when available) and these metadata are summarized in Table 8. If available, sample information (*thickness* and *labID*) is provided for all age constraints. Each age constraint that is not in radiocarbon years has *age* in calendar years before 1950 CE, and *ageUncertainty*. Radiocarbon age constraints have *age14C* in radiocarbon years before

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1950 CE and *age14Cuncertainty*. The *materialDated*, *reservoirAge14C*, and *reservoirAge14Cuncertainty* are also provided for radiocarbon age constraints to allow users to derive their own age-depth models if desired. For radiocarbon ages, we also provide *fractionModern*, *fractionModernUncertainty*, *delta13C* (of the material that was radiocarbon dated), and *delta13Cuncertainty* when available.

Several lake and marine sediment archives contain measurements of radiogenic isotopes—^{210}Pb, ^{137}Cs, and/or $^{239+240}$Pu—to constrain the age of the sediment at and near the surface/core top. Where applicable, we provide the isotope *activity* and the *activityUncertainty*. For ^{210}Pb measurements, the *supportedActivity* field is Y if the activity is supported by ^{210}Pb production in the surrounding matrix and N if the activity is not supported. The *x210PbModel* describes the type of model used to determine the age based on the radiogenic isotope measurements.

For carbonate systems such as speleothems and corals, U/Th dating is often used. Where available, chronological tables in the database contain information about the ^{238}U and ^{232}Th content (*U238*, *Th232*), the ^{230}Th/^{238}U activity ratio (*Th230_U238activity*), δ^{234}U (*d234U*), and their uncertainties (*U_Thactivity_error* and *d234U_error*). Fields such as the initial ^{234}U/^{238}U (*dU234intial*) and ^{230}Th/^{232}Th activity ratios (*Th230_Th232ratio*) are also included for correcting ages for the initial ^{234}U/^{238}U activity, and detrital thorium contamination, respectively.

The *useInAgeModel* is a binary field where Y indicates that age constraint was used in the published age model and N indicates that age constraint was not used in the published age model.

The amount and type of uncertainty in each chronology are provided in *paleoData_chronologyIntegrationTimeUncertainty* and *paleoData_chronologyIntegrationTimeUncertaintyType* respectively, while *paleoData_chronologyIntegrationTimeBasis* outlines how the chronology was constructed. By contrast, the *paleoData_sensorIntegrationTime*, *paleoData_sensorIntegrationTimeBasis*, *paleoData_sensorintegrationTimeUncertainty*, *paleoData_sensorIntegrationTimeUncertaintyType*, and *paleoData_sensorIntegrationTimeUnits* fields—where available—describe the amount of time over which a sample integrates isotopic values.

5. Key characteristics of Iso2k data records

5.1 Spatial, temporal, archival, and isotopic characteristics of data coverage

The Iso2k database contains 753 stable isotope (δ^{18}O, δ^2H) records from 505 unique sites. There are 10 archive types, including: 143 records from annually-banded skeletal carbonate marine archives (corals (n = 137), sclerosponges (n = 4), and mollusks (n = 2)); 204 from glacier ice (n = 200) and ground ice (n = 4); 158 from lake or terrestrial sediments; 99 from marine sediments; 68 from speleothems; and 81 from wood **[Figure 2a]**. 87% of the 753 stable isotope records in the database are δ^{18}O, and 13% are δ^2H, with 12 sites (~2%) having records of both isotope systems (derived from the same

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sensor in ice cores, or different sensors in lake sediments). In addition to the 753 stable isotope records, the database contains 255 records containing ancillary data (e.g., δ^{13}C, Mg/Ca, Sr/Ca). Of the 753 records, 606 are considered 'primary' δ^{18}O or δ^2H time series (Figure 2, Supplementary Table 1 and Section 2.4), including 101 records from annually-banded skeletal carbonate marine archives (corals (n = 95), sclerosponges (n = 4), and mollusks (n = 2)), 170 from glacier ice (n = 166) and

30   ground ice (n = 4), 114 from lake or terrestrial sediments, 95 from marine sediments, 47 from speleothems, and 79 from wood.

Spatial coverage of the sites in the database is global, but most sites are from the low latitudes and Northern Hemisphere mid-latitudes **[Figure 2a; Figure 4b]**. Data availability is low for most of the Southern Hemisphere, with the exception of

35   glacier ice records from Antarctica **[Figure 4b]**. The temporal coverage increases from about 250 proxy time series near the year 0 CE to more than 400 time series at the beginning of the twentieth century **[Figure 2b]**. The average length and resolution of each δ^{18}O time series vary considerably and are archive-dependent. Banded, biologically-derived archives (corals, sclerosponges, mollusks, and wood) offer the highest resolution (monthly to seasonal), and a temporal extent of between 24 years to 375 years for corals and 38 to 1030 years for tree records (timespan is the 2.5–97.5% quantiles). Layer-

40   counted archives such as glacier ice generally offer annual resolution and a time span between 41–1979 years. Other archives have lower resolution, but provide more continuous coverage across the CE. The median resolution of records is 12 years/sample for speleothems, 25 years/sample for lake sediments, 28 years/sample for marine sediments, and 97 years/sample for ground ice, and the median time span of records in these archives is >1200 years. These lower resolution time series almost exclusively make up the records in the database prior to ~1700 CE, preventing the characteristic drop in

45   coverage in older time periods observed in and described by other PAGES2k compilations (PAGES 2k Consortium, 2013).

The records in the Iso2k Database capture many aspects of hydroclimate **[Figure 4]**. The first-order interpretation (*isotopeInterpretation1_variable*) for 44% of the δ^{18}O and δ^2H records in the database is 'P_isotope', meaning that δ^{18}O and δ^2H of the inferred material (ice, soil water, seawater, etc.) is primarily driven by the δ^{18}O and δ^2H of precipitation. The first-

50   order interpretation for 26% of the records in the database is 'T_water' or 'T_air', meaning that the temperature of water or air is the primary driver of δ^{18}O and δ^2H of the inferred material. Finally, 24% of records in the database are primarily driven by some aspect of evaporation or evapotranspiration, collectively referred to as 'Effective Moisture' in the *isotopeInterpretation1_variableGroup* category. This category includes 'd18O_seawater' (driven by ocean circulation and by precipitation/evaporation at the sea surface), 'ET' (evapo-transpiration), 'I_E' (infiltration/evaporation), and 'P_E'

55   (precipitation/evaporation) entries for *isotopeinterpretation1_variable*.

5.2 Validation

There is currently no existing observational dataset of isotope ratios in all major pools of the water cycle that can serve as a true validation of the Iso2k database. However, the vast majority of ice records in the Iso2k database have an inferred

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material of 'precipitation' and a first-order isotope interpretation of 'P_isotope'. For these records, the δ^{18}O averaged for the twentieth century (all data points after 1900 CE) provides a reasonable match with the observed annual average δ^{18}O of

'75   precipitation from the Global Network of Isotopes in Precipitation (GNIP) (Terzer et al., 2013) **[Figure 5]**. This provides confidence that the isotopic data contained in the Iso2k database can reasonably be used for analyses such as calculation of latitudinal gradients in δ^{18}O over the CE, even before accounting for seasonal biases and other transformations within the proxy system. We note that while other proxy data types such as speleothems and leaf wax biomarkers are sensitive to P_isotope (and *isotopeinterpretation1_variable* for many of these records is listed as 'P_isotope'; Figure 4), their most direct

'80   inferred materials are meteoric waters such as soil water or groundwater rather than precipitation; further, water isotope values are fractionated by proxy sensors, such that they are not as directly comparable to the GNIP database.

6. Usage notes

6.1 General applications

'85   The Iso2k database is the most comprehensive database of paleo-water isotope records to date for the CE. For the first time, this database allows investigation of spatial and temporal hydroclimate variability from regional to global scales across multiple proxy systems. Using the 'inferred material' metadata, the database can be directly compared with the output of climate models, allowing investigation of the water cycle in far greater depth than was previously possible.

'90   Alongside the data itself, the detailed 'isotope interpretation' metadata fields are the foundation of this database. These fields allow users to understand the processes reflected in the isotope data, and filter the database according to particular scientific questions. For example, a user may be interested in the temporal variability of isotope records driven primarily by changes in effective moisture, and the Iso2k standardized vocabulary means that it is straightforward to filter for these records. Note that for many records in the database, isotopic variability is affected by more than one variable and these secondary

'95   influences may not be trivial when conducting meta-analyses. Although only '*isotopeinterpretation1*' fields have been quality-controlled to the highest level, the subsequent isotope interpretation fields also contain well-curated information that is important for data interpretation.

6.2 Example workflow for filtering and querying data records

'00   Records in the Iso2k database are provided as published (i.e., not re-calibrated or validated). This preserves the large amount of information contained within water isotope proxy measurements that would be lost if condensed to reconstruct discrete variables. Rather, we leave it to the database users to filter and assess records as needed.

The MATLAB and R serializations contain three variables: 'D', 'TS', and 'sTS.' The variable 'D' includes site-level data for

'05   each dataset structured in the LiPD format. Datasets in 'D' often contain multiple variables (e.g., stable isotope, ancillary, and chronological data), and represent how LiPD data appear when loaded into the initial environment. For most users,

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however, a "flattened" version of the database is more useful. We have provided this as the 'TS' variable, where each entry contains an individual time series and its associated metadata. A slightly modified version of 'TS' is included with R and Matlab, called 'sTS', which is identical to TS except that the interpretation fields are split by scope ('isotope' or 'climate') in order to simplify querying, which may be preferable for some users. The Python serialization contains only 'D' and 'TS' because tools to split by scope were unavailable.

For initial querying of the database, in nearly all cases, we recommend first filtering by the following:

1. variableName = 'd18O' or 'd2H' (excludes any non-isotopic data)
2. paleoData_units = 'permil' (excludes records published as z-scores or anomalies)
3. paleoData_iso2kPrimaryTimeseries = 'TRUE' (includes only primary time series for each site)

Additional filtering of records should be performed using Level 1 or Level 2 fields. For example:

- isotopeInterpretation1_variable = 'P_isotope' (includes only records where the first-order control of isotopic variability is the isotopic composition of precipitation)
- paleoData_description = 'carbonate' or 'terrestrial biomarker' or 'tree ring cellulose' (to extract terrestrial archives sensitive to P_isotope aside from ice cores), or:
- paleoData_inferredMaterial = 'groundwater' or 'soil water' or 'lake water' (accomplishes similar results to the above)

Additional filtering of records may be useful with other Level 2 fields, for example:

- climateInterpretation1_variable = contains 'P' or 'Precipitation_amount' or 'P_amount' (to extract only records where authors' primary climatic interpretation was based on the amount effect)

The sample R, MATLAB, and Python codes provided with this dataset (Supplementary Material) provides a similar example to users.

6.3 Database updates, versioning scheme, and submission of new or updated datasets

This publication marks Version 1.0.0 of the Iso2k database (editors and reviewers: please note that you are reviewing version 0.14.7; this will become version 1.0.0 upon publication, following any edits during the review process). Following publication, the database will continue to evolve, as new datasets are added (both new studies and previous records that have been missed) and existing data or metadata are extended, or as necessary, corrected. Readers who know of missing datasets are asked to submit them directly through http://lipd.net/playground. Database users who find errors in individual datasets can submit proposed edits using the "Edit LiPD file" function at http://lipdverse.org/iso2k/current_version/, or they can use the "Report an issue" option for errors that apply to multiple datasets. More detailed instructions for dataset submission and

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a link to a LiPD entry template hosted through http://lipd.net/playground will be added to the WDS-NOAA landing page (https://www.ncdc.noaa.gov/paleo/study/29593) when they become available.

As the database updates, it will be versioned following the scheme used by other PAGES data collections (Kaufman et al., 2020; McKay and Kaufman, 2014; PAGES 2k Consortium, 2013, 2017), with the following format: X1.X2.X3, where X1, X2 and X3 are incrementing integers. When X1 increases, X2 and X3 reset to zero. When X2 increases, X3 resets to zero. X1 represents the number of publications describing the database. X2 increments each time the set of records in the database changes (addition or removal of a dataset). X3 increments when the data or metadata within the dataset change, but the set of records remains the same. Upon updates, extensions or corrections to the database, rather than issuing errata to this publication, changes will be included in subsequent versions of the database and updated and described through the online data repository.

6.4 Availability of data and code

Following the previous PAGES2k and the Temperature 12k data compilations (Kaufman et al., 2020; PAGES 2k Consortium, 2017), the Iso2k database employs the Linked Paleo Data (LiPD) format (McKay and Emile-Geay, 2016), with serializations available for R, MATLAB, and Python. The LiPD format is machine-readable, with codebases to facilitate input, output, visualization, and data manipulation in R, Python and Matlab. Simple visualization and data access (both as LiPD and csv files) is available through the LiPDverse at http://lipdverse.org/iso2k/current_version/. The LiPDverse additionally houses other paleoclimate records and compilations that may be of interest to users of the Iso2k database. The serializations contain all LiPD files included in the current version of the Iso2k database. Serializations of the database can be downloaded from https://doi.org/10.25921/57j8-vs18 (Konecky and McKay, 2020) and from the WDS-NOAA Paleo Data landing page: https://www.ncdc.noaa.gov/paleo/study/29593. We recommend accessing the database through the WDS-NOAA landing page in order to find up-to-date instructions on using the database.

6.5 Citation

This Iso2k data descriptor should be cited when the database is used in whole or in part, including its metadata fields, for subsequent studies. We encourage users of the database to not only cite the Iso2k data product but also the original publications of the underlying primary data (Supplementary Tables 2 and 3). Citation of both the Iso2k data product and the underlying studies is particularly encouraged when analyses make explicit use of individual records or small subsets of records, even though citation of >400 original studies may not be practical if the entire Iso2k database is used.

7. Conclusions and anticipated applications of the Iso2k database

The global extent, quantity and quality of metadata included in the Iso2k database allow examination of the multiple variables that impact water isotopes, including moisture source and transport history, temperature, and precipitation amount.

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These multivariate controls mean that water isotopes contain a wealth of information about climate. Importantly, water isotope signals contained in proxy archives can be modified by local environmental processes such as evaporation, biosynthetic fractionation, bioturbation in sediments, or diffusion. These archive- or proxy-specific transformations therefore additionally allow for reconstruction of water balance (E:P), different forms of drought (e.g., meteorological, hydrological or soil moisture), and relative humidity (Rach et al., 2017). It is difficult to tease apart the effects of multiple variables in a single proxy record, but this global compilation of water isotope proxy records from a range of archives will help to overcome this barrier, facilitating extraction of common signals from the noise of individual proxies, and providing insights into different aspects of the hydrological cycle at a range of spatial and temporal scales.

The Iso2k database also provides an unprecedented direct comparison for state-of-the-art water isotope-enabled climate models. Many data-model comparison efforts compare climate model variables such as temperature and precipitation to paleoclimate data; the latter is often a complex and nonlinear signal integration of multiple climate influences, and uncertainties arise from the assumptions that must be made(Dee et al., 2016)(Dee et al., 2016; Evans et al., 2013). Comparing water isotope fields from climate model outputs to isotope proxy records of the same components of the water cycle circumvents these uncertainties, providing a more direct comparison of proxies and model simulations in the same units. Model validation on this relatively level playing field will improve estimates of climate models' ability to simulate changes in hydroclimate on long timescales. For those archives that further filter the isotopic signal, proxy system models can aid data model comparison (Dee et al., 2015, 2018; Jones and Dee, 2018). Therefore, the Iso2k database will not only enable global-scale comparisons with isotope-enabled climate models, but may also serve as an input database for paleoclimate data assimilation reconstructions such as the Last Millennium Reanalysis (Hakim et al., 2016; Steiger et al., 2014) and the Paleo Hydrodynamics Data Assimilation (Steiger et al., 2018).

Tables

Table 1: Key entity metadata (*bold = Level 1 or required fields in database, *italics are references to other metadata or variable in the database*)

Variable	Name of field in database	Additional description	QC Level
Archive type	***archiveType**	Type of proxy archive (Table 2 and Table 7).	1
Latitude	***geo_latitude**	Site latitude in decimal degrees (-90 to +90).	1
Longitude	***geo_longitude**	Longitude in decimal degrees (-180 to +180).	1
Elevation	***geo_elevation**	Site elevation in meters relative to mean sea level (- below sea level, + above sea level).	1
Site name	***geo_siteName**	Name of the site, locality of nearest geopolitical center/municipality if applicable (i.e., islands retain their names).	1
Dataset ID	***dataSetName**	Iso2k-specific identifier assigned to all isotope records from a given site and publication.	1
Unique record ID	**•paleoData_iso2kUI**	Unique Iso2k identifier assigned to each isotope record to distinguish among records when more than one record exists in the original publication.	1
LiPD ID	***paleoData_TSid**	Unique LiPD file identifier for each time series in the database.	1
Variable name	***paleoData_variableName**	Variable measured (e.g., $\delta^{18}O$, $\delta^{2}H$). See Table 2 for more metadata and Table 7.	1
Variable units	***paleoData_units**	Units for *paleoData_variableName* (e.g., permil). See Table 2 for more metadata and Table 7.	1
LiPD link	***lipdverseLink**	Link to LiPDverse webpage.	1
Maximum year	maxYear	Maximum (most recent) year of each isotope record in calendar year (CE). See Table 8 for more chronology metadata.	auto
Minimum year	minYear	Minimum (earliest) date of each isotope record in calendar year (CE). See Table 8 for more chronology metadata.	auto

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Publication DOI	pub1_doi	Digital Object Identifier for the first publication presenting the isotope record.	1
Publication citation	pub1_citation	Citation for the first publication presenting the isotope record.	3
Dataset DOI	datasetDOI	Digital object identifier for dataset assigned by original authors if available.	3
Dataset URL	paleoData_WDSPaleoUrl	URL linking back to records obtained from the NOAA NCEI data repository	3

Table 2: Key paleodata metadata (*bold = Level 1 or required fields in database, *italics are references to other metadata or variable*)

Variable	Name of field in database	Description	QC Level
Variable description	***paleoData_description**	Human-readable description of *paleodata variableName* (e.g., carbonate, δ^{18}O of glacier ice).	1
Measurement material	***paleoData_measurementMaterial**	Type of material in which *paleodata_variableName* was measured (e.g., coral, cellulose, biomarkers).	1
Measurement material detail	paleoData_measurementMaterialDetail	Free-form text with additional information about *paleoData_measurementMaterial*.	2
Inferred material	***paleoData_inferredMaterial**	Source water whose isotope variability is inferred (e.g., surface seawater, lake water, precipitation). See Table 7.	1
Inferred material group	***paleoData_inferredMaterialGroup**	Supergroup of inferred material, see Table 7 for controlled vocabulary. See Table 7.	1
Archive genus	paleoData_archiveGenus	Genus name of the archive, if available.	3
Archive species	paleoData_archiveSpecies	Species name of the archive, if available.	3
Values (data field)	paleoData_values	Field containing isotope time series or other measurements for each paleorecord.	3
Analytical uncertainty	paleoData_uncertaintyAnalytical	Analytical uncertainty in the measured variable when provided by the original publication; based on long-term precision of an internal standard of known value.	3
Analytical reproducibility	paleoData_uncertaintyReproducibility	Analytical reproducibility in the measured variable when provided by the original publication; based on repeat measurements of replicate samples, transects or cores from the same site.	3
Equilibrium evidence	paleoData_equilibriumEvidence	Indicates whether equilibrium conditions were present when the archive formed.	2

		Indicates whether the isotope value was measured directly, temporally interpolated (e.g., from age tie points for annually-banded archives), or inferred (e.g., seawater isotopic variability, inferred from paired $\delta^{18}O$ and Sr/Ca or $\delta^{18}O$ and Mg/Ca in marine sediments). This information is also incorporated into paleoData_description.	3
Variable type	paleoData_variableType		
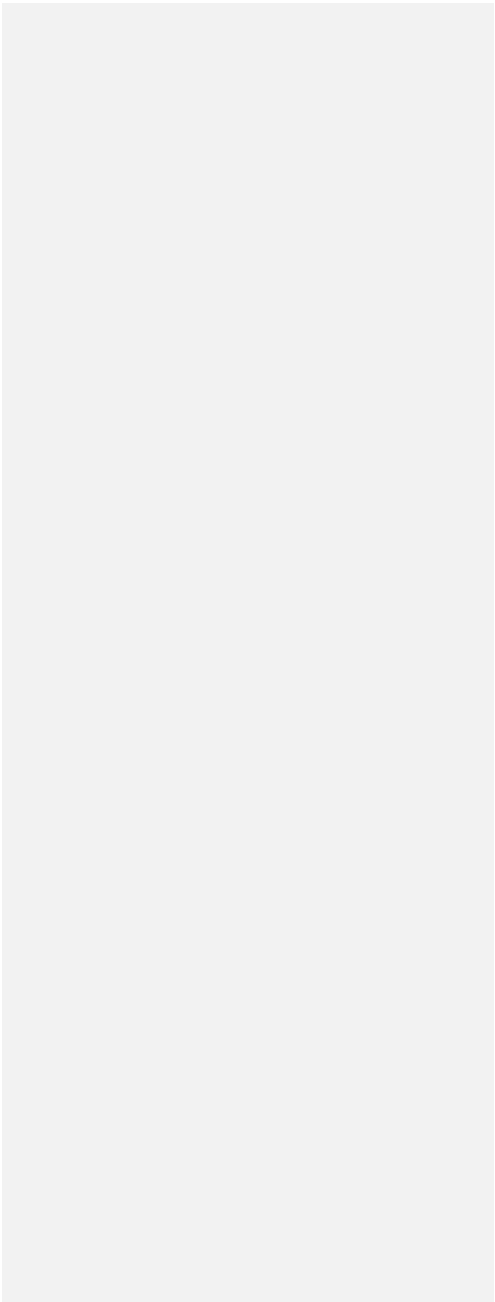
Table 3: Key isotope interpretation metadata (*bold = Level 1 or required fields in database, *italics are references to other metadata or variable*)

Variable	Name of field in database	Description	QC Level
Primary isotope interpretation	***isotopeInterpretation1_variable**	Variable that controls isotopic variability within the record (e.g., 'Temperature_air', 'd18O seawater'). See Table 7.	1
Direction of relationship	***isotopeInterpretation1_direction**	Sign ('positive' or 'negative') of the relationship between the isotope values and the isotope interpretation variable. For example, a record with a temperature interpretation may have a decrease in $\delta^{18}O$, that corresponds to an increase in temperature.	1
Interpretation group	***isotopeInterpretation1_variableGroup**	Supergroup of isotope interpretations (one of temperature, effective moisture, or precipitation isotope ratio). See Table 7.	1
Mathematical relation	isotopeInterpretation1_mathematicalRelation	Type of relationship between isotope and climate variable ('linear' or 'nonlinear').	2
Seasonality	isotopeInterpretation1_seasonality	The calendar months the isotope interpretation applies to is given as first initial of the months or as 'annual' or 'sub-annual' where applicable (e.g., corals, speleothems).	2
Basis	isotopeInterpretation1_basis	Basis for the isotope interpretation of each record as stated in the original publication (text or citation maybe given).	2
Coefficient	isotopeInterpretation1_coefficient	Numerical coefficient with interpretation variable.	2
Fraction	isotopeinterpretation1_fraction	Fraction of variance explained by given climate variable.	2

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Table 4: Key climate interpretation metadata

Variable	Name of field in database	Description	QC Level
Primary climate interpretation	climateInterpretation1_variable	Climate variables interpreted in each record (queryable freeform text with quotes from original publications; e.g., 'salinity', 'temperature').	2
Primary climate interpretation detail	climateInterpretation1_variableDetail	Provides more information about the climate variable (e.g., sea surface for temperature or salinity).	2
Climate interpretation relationship direction	climateInterpretation1_direction	Sign ('positive' or 'negative') of the relationship between the isotope ratios and climate variable. For example, a record with a temperature interpretation may have a decrease in $\delta^{18}O$, that corresponds to an increase in temperature.	2
Climate interpretation basis	climateInterpretation1_basis	Basis for climate interpretation of each record as stated in the original publication.	2

Table 5: Key depth-age metadata (*bold = Level 1/required fields in database)

<u>Variable</u>	<u>Name of field in database</u>	<u>Description</u>	<u>QC Level</u>
Year (data field)	***year**	Field containing year data (units are CE) for the paleorecord.	1
Year units	***yearUnits**	Units of year data (CE).	1
Depth (data field)	depth	Depth in archive (e.g., in sediment core, stalagmite).	2
Depth units	depthUnits	Units of depth measurements.	2
Chronological integration time	paleoData_chronologyIntegrationTime	Average temporal resolution of each record in years/measurement.	3
Chronological integration time units	paleoData_chronologyIntegrationTimeUnits	Units for the *paleoData_chronologyIntegrationTime* field.	3

Table 6: Selected queryable metadata (*bold = Level 1/required fields in database)

Variable	Name of field in database	Description	QC Level
Has chronology?	hasChron	Indicates whether chronology data for the isotope record are available in the database.	auto
Record included in previous PAGES2k compilation?	paleoData_inCompilation	Indicates whether the record was used in earlier PAGES2k databases.	2
Ocean2k ID	paleoData_ocean2kID	Ocean2k unique ID for records included in both databases.	2
PAGES2k Dataset ID	paleoData_pages2kID	PAGES2k temperature dataset ID for records included in both databases.	2
QC Certification	***paleoData_iso2kCertification**	Initials of Iso2k Project Member that QC'ed the record.	1
Iso2k primary time series for dataset	***paleoData_iso2kPrimaryTimeseries**	For sites with multiple time series (e.g., caves with multiple stalagmites and a final composite), this time series should be primarily used ('TRUE' or 'FALSE').	1
PAGES2k region	geo_pages2kRegion	The continental (e.g., 'SAm' for South America) or ocean (i.e., Ocean) regions corresponding to the PAGES2k or Ocean2k temperature reconstructions for the records included in those data compilations.	3
Ocean region	geo_ocean	The ocean region (e.g., Pacific) corresponding to the record site.	3

Table 7: Standardized controlled vocabulary options for metadata fields in the Iso2k database (Standardized labels show labels used in Iso2k Database, parentheses expand any abbreviations)

Metadata Field	Standardized labels
archiveType	coral, glacier_ice, ground_ice, lake_sediment, marine_sediment, mollusk_shells, terrestrial_sediment, speleothem, sclerosponge, wood
paleoData_variableName	d2H, d18O
paleoData_units	permil, zscore, permil_anomaly (specify relative to), PC (principal component)
isotopeInterpretation1_direction	positive, negative
isotopeInterpretation1_variable	T_water, d18O_seawater, P_E (precipitation/evaporation), I_E (input/evaporation), P_isotope, T_air, relative humidity, Veg (vegetation dynamics), ET (evapotranspiration: soilwater)
isotopeInterpretation1_variableGroup	- Temperature (comprising T_water, T_air) - EffectiveMoisture (comprising d18O_seawater, P_E, I_E, relative humidity, Veg, ET) - P_isotope
isotopeInterpretation1_inferredMaterial	Surface seawater (1 thermocline), subsurface seater, precipitation, lake water, soil water, lagoon water, groundwater
paleoData_inferredMaterialGroup	- Surface water (comprising surface seawater, lake water, lagoon water, subsurface seawater) - Precipitation - Soil/leaf water (comprising soil water, groundwater)
paleoData measurementMaterial (*Level 2 QCed, not fully standardized*)	Coral, mollusk, ostracod, gastropod, glacier ice, aquatic or terrestrial biomarkers (n-alkane, n-alkanoic acid, dinosterol, botryococcene), planktonic foraminifera, cellulose, carbonate, or bulk carbonate

Table 8: Key chronological metadata

Variable	Name of field in database	Description
Age	age	Age in calendar years before 1950 CE (after any dating technique-specific corrections have been applied).
Age Uncertainty	ageUncertainty	1 standard deviation uncertainty of calendar age.
Radiocarbon Age	age14C	Age in radiocarbon years before 1950 CE.
Radiocarbon Age Uncertainty	age14Cuncertainty	One standard deviation uncertainty of radiocarbon age in years.
Fraction modern ^{14}C activity	fractionModern	Fraction of modern radiocarbon activity.
Fraction modern ^{14}C activity uncertainty	fractionModernUncertainty	One standard deviation uncertainty of fraction of modern radiocarbon activity.
δ^{13}C	delta13C	δ^{13}C of material analyzed for radiocarbon.
δ^{13}C uncertainty	delta13Cuncertainty	One standard deviation uncertainty of δ^{13}C of material analyzed for radiocarbon.
Thickness	thickness	Thickness of the layer analyzed for the age constraint.
Lab Identifier	labID	Unique identifier provided by lab where age analysis was conducted.
Material Dated	materialDated	For radiocarbon age constraints, the material dated.
Activity	activity	^{210}Pb, $^{239+240}$Pu or ^{137}Cs activity.
Activity Uncertainty	activityUncertainty	^{210}Pb, $^{239+240}$Pu or ^{137}Cs activity uncertainty.
Supported Activity	supportedActivity	"Y" if supported ^{210}Pb activity, "N" if unsupported ^{210}Pb activity.
^{210}Pb model	x210PbModel	Model used to convert ^{210}Pb activity to age (e.g., constant rate of supply).
^{14}C reservoir age	reservoirAge14C	^{14}C reservoir age.
^{14}C reservoir age uncertainty	reservoirAge14CUncertainty	^{14}C reservoir age uncertainty.
U/Th depth	depthUTh	Mid-point depth of the sub-sample drilled for U-Th age.

U/Th sample ID	sampleID	Sample ID for the U-Th age measured.
U/Th sample weight	weight	Weight of powder analyzed for U-Th age in mg.
^{238}U content	U238	^{238}U content of the sub-sample in ppb.
^{238}U error	U238_error	Analytical uncertainty of ^{238}U in ppb.
^{232}Th content	Th232	^{232}Th content of the sub-sample in ppt.
^{232}Th error	Th232_error	Analytical uncertainty of ^{232}Th in ppt.
d234U ratio	d234U	d234U ratio measured in the subsample.
d234U error	d234U_error	Analytical uncertainty of d234U.
$^{230}Th/^{238}U$ activity	Th230_U238activity	$[^{230}Th/^{238}U]$ activity measured in the subsample.
$^{230}Th/^{238}U$ activity error	U_Thactivity_error	Analytical uncertainty of ^{230}Th-^{238}U activity.
$^{230}Th/^{232}Th$ ratio	Th230_Th232ratio	$[^{230}Th/^{232}Th]$ ratio in the subsample in ppm.
$^{230}Th/^{232}Th$ ratio error	Thratio_error	Analytical uncertainty of ^{230}Th-^{232}Th ratio in ppm.
Uncorrected U/Th age	AgeUncorrected	Uncorrected U-Th age of the subsample in years ago.
Uncorrected U/Th age uncertainty	AgeUncorr_error	Analytical uncertainty of uncorrected Age in years.
Corrected U/Th age uncertainty	AgeCorr_error	Uncertainty of corrected age (includes Th correction) in years.
Initial d234U	dU234initial	Calculated initial d234U ratio in the subsample.
Initial d234U error	dU234i_error	Analytical uncertainty of calculated d234U initial.
Use in age model?	useInAgeModel	"Y" if this age constraint was used in the published age model, "N" if not.

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Acknowledgments

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Team list

The "Iso2k Project members" group author includes: Kerstin Braun (Institute of Human Origins, Arizona State University, Tempe, Arizona, 85287, USA), Matthieu Carré (LOCEAN Laboratory, Sorbonne Universités (UPMC)-CNRS-IRD-MNHN, Paris, 75005, France), Alessandro Incarbona (Department of Earth and Marine Sciences, Palermo University, Palermo, 90134, Italy), Nikita Kaushal (Department of Earth Sciences, University of Oxford, Oxford, Oxfordshire, OX1 3AN, United Kingdom), Robert M. Klaebe (Department of Earth Sciences, The University of Adelaide, Adelaide, South Australia, 5005, Australia), Hannah R. Kolus (School of Earth and Sustainability, Northern Arizona University, Flagstaff, AZ, 86011, USA), P. Graham Mortyn (ICTA and Dept. of Geography, Universitat Autonoma de Barcelona (UAB), Bellaterra, 08193, Spain), Andrew D. Moy (Australian Antarctic Division, Kingston, Tasmania, 7050, Australia), Heidi A. Roop (Climate Impacts Group, University of Washington, Seattle, WA, 98195, USA), Marie-Alexandrine Sicre (LOCEAN Laboratory, Sorbonne Universités (UPMC)-CNRS-IRD-MNHN, Paris, 75005, France), and Kei Yoshimura (Institute of Industrial Science, The University of Tokyo, Kashiwa, Chiba, 2778574).

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Author contributions

Author contributions are as follows. BLK directed the Iso2k Project. NPM built and managed the Iso2k database. BLK, NPM, OVC, EPD, KLD, DSK, GL, SRM, BM, AJO, JWP, HRS, EKT, DMT, JJT, OC, MAC designed the database (including development of metadata fields, data selection criteria). OVC, LCB, EPD, MDJ, LJ, DSK, GL, SRM, BM, TO, AJO, JWP, HRS, EKT, DMT, JJT, DVD, TJP coordinated an archive team. BLK, NPM, OVC, LCB, EPD, KLD, GMF, MJF, MDJ, LJ, DSK, GL, SRM, BM, TO, AJO, JWP, HRS, EKT, DMT, JJT, AA, OC, MD, DVD, TJP, KB, MC, NK, RMK, HRK, PGM, ADM, HAR, MAS assembled or entered datasets and/or metadata into database. BLK, NPM, OVC, LCB, EPD, KLD, GMF, MJF, MDJ, LJ, DSK, GL, SRM, BM, TO, AJO, JWP, HRS, EKT, DMT, JJT, AA, JLC, MAC, DVD, ZK, TJP, MC, AI, PGM, ADM, MAS performed quality control, term standardization, database cleaning, and/or QC certification. BLK, OVC, LCB, EPD, KLD, MJF, MDJ, LJ, DSK, GL, SRM, BM, TO, AJO, JWP, HRS, EKT, DMT, JJT, AA, JLC, MAC, DVD, ZK, TJP, PGM, ADM, MAS located missing isotopic and/or chronological datasets. BLK, NPM, GMF, MJF, MDJ analyzed data and generated figures for this manuscript. BLK, NPM, OVC, LCB, KLD, GMF, MJF, MDJ, LJ, DSK, GL, BM, TO, HRS, EKT, DMT, JJT, NJA, AA, JLC, SGD, ZK, TJP, SS, MC wrote the manuscript text. BM,

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Competing interests

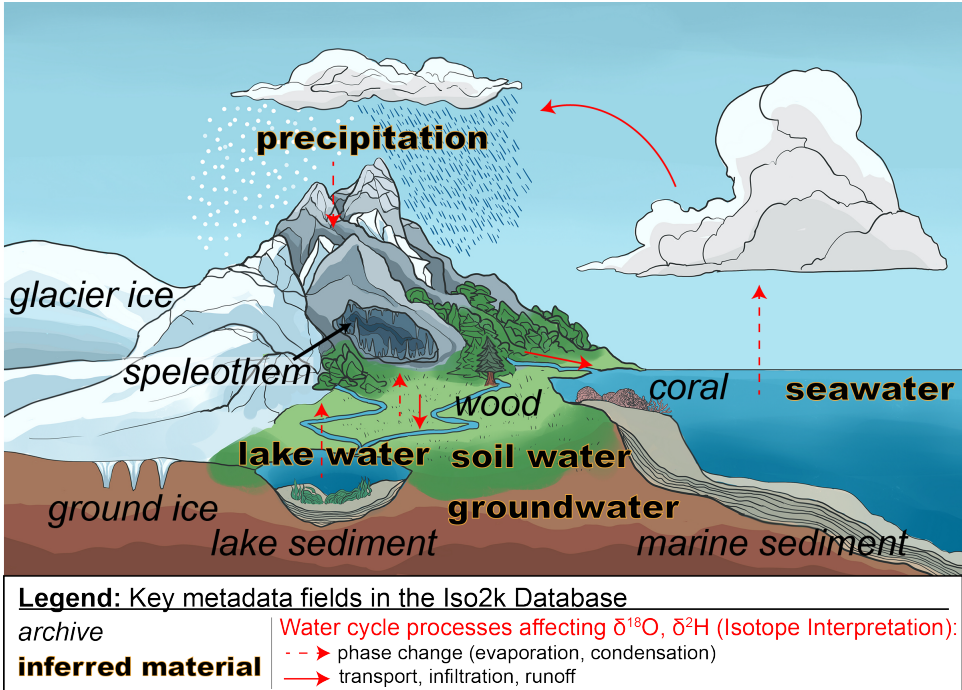The authors declare no competing interests.

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Figure 1. Schematic illustration of the global water cycle and key metadata fields in the Iso2k database. In the Iso2k database, the histories (including phase changes and transport; 'Isotope Interpretation'; red text and arrows) of different pools of environmental waters ('inferred material'; black bold text) can be inferred by interpretation of proxy records from different archives ('archive,' italic text). Base illustration by Helen Xiu, Washington University.

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a) **Iso2k network version 1.0.0 (606 records from 487 sites)**

Legend:
- Coral (95)
- GlacierIce (166)
- GroundIce (4)
- LakeSediment (112)
- MarineSediment (95)
- MolluskShells (2)
- Sclerosponge (4)
- Speleothem (47)
- TerrestrialSediment (2)
- Wood (79)
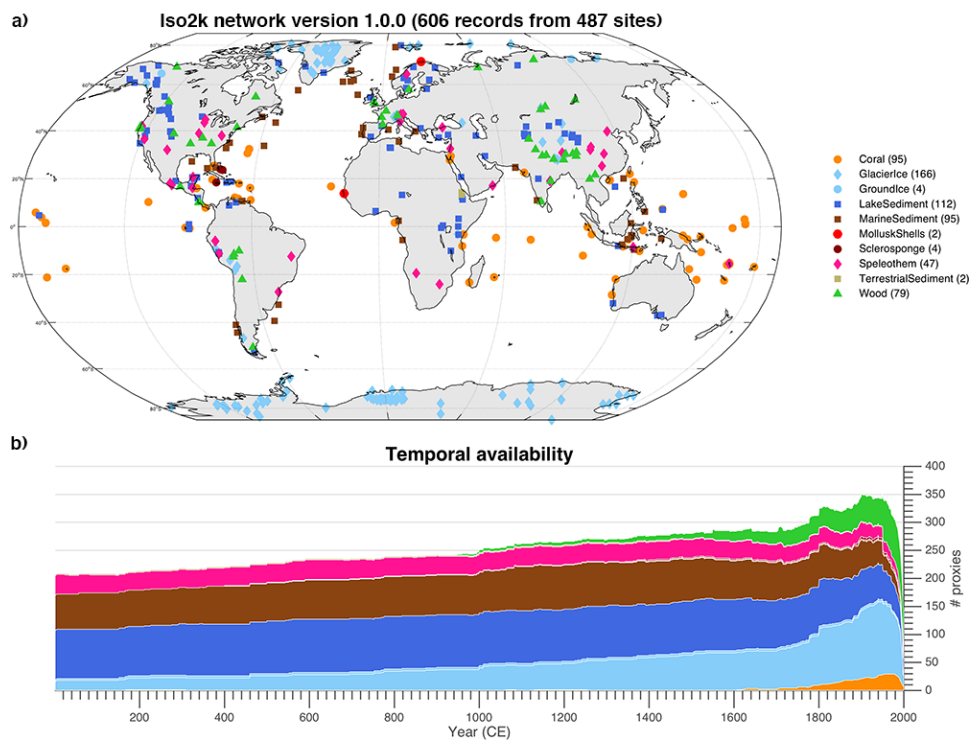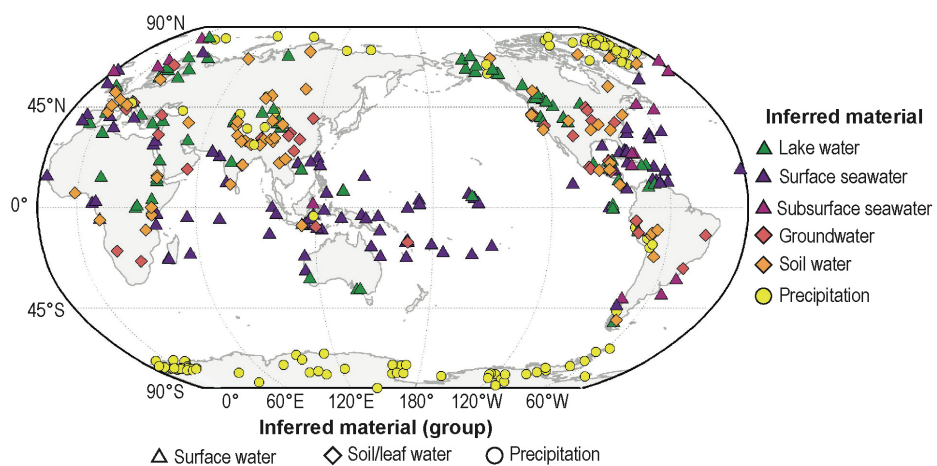
b) **Temporal availability**

Year (CE)

proxies

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Figure 2. The Iso2k database version 1.0.0. a) Spatial distribution of "primary time series" records in the Iso2k database. Symbols represent records from different archives. b) Availability of records in the Iso2k database over time during the past 2,000 years.

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Figure 3. Map of records in the Iso2k database with colours representing the 'Inferred Material' metadata field (Section 4.2) for each record (primary time series only; see Section 2.4). Symbols correspond to the inferred material supergroups.
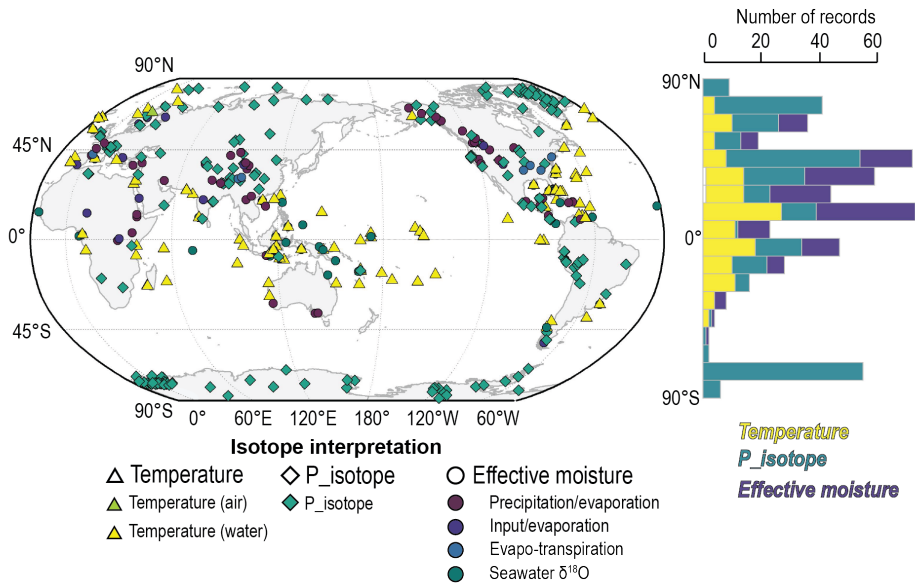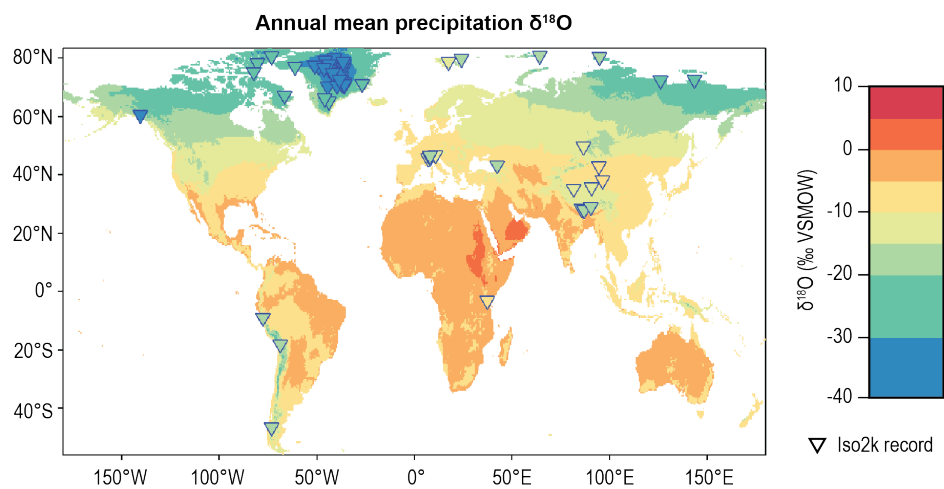
Figure 4. Left: Map of records in the Iso2k database with colours representing the first-order 'Isotope Interpretation' metadata field for each record (primary timeseries only; see Section 2.4). Symbols correspond to the three isotope interpretation 'supergroupings' (see Sections 4.3 and 5.1). Right: Bar chart showing the latitudinal distribution of records in the Iso2k database. Each bar represents ten degrees of latitude.

| Deleted: a) |
| Deleted: b). |

Figure 5. Average δ¹⁸O from glacier and ground ice records in the Iso2k database (symbols), calculated as the average value since 1900 CE, compared with mean annual δ¹⁸O from the Global Network of Isotopes in Precipitation (GNIP) (shading) (Terzer et al., 2013). Antarctica is excluded from this map due to the scarcity of GNIP stations.

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