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Research paper

Data reporting standards for publication of U-series data for geochronology and timescale assessment in the earth sciences



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ABSTRACT

Uranium-series data provide essential dating and tracer tools for a broad spectrum of geologic processes. Data reported in U-series geochronology studies often contain insufficient information to completely assess the data collected. It is frequently not possible to calculate a date using the information provided or to re-calculate using different parameters, ultimately limiting the value of the data. The decay constants used are particularly important in that some of the relevant U-series isotopes have been revised. Here we provide a rationale for a minimum set of required data that will enable most calculations and facilitate later data comparisons. Along with these data reporting norms, we discuss additional metadata that will improve understanding of the data and also enhance the ability to re-interpret and assess them in the context of other studies. We posit that these recommendations will provide a foundation for increasing the longevity and usefulness of measurements in the discipline of U-series geochronology.

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1. Introduction

Uranium-series data are relied upon heavily to provide absolute, precise temporal frameworks for the pace, magnitude, and drivers of geological and climatological events over 10–10⁵ year time-scales. Examples of important applications include:

- (a) Understanding past climate change, the carbon cycle, sea level, ocean chemistry, and paleoclimate, all of which bear strongly on predictions of climate change vulnerability (Edwards et al., 1987; Henderson, 2002; Henderson and Slowey, 2000; Wang et al., 2001; Yokoyama et al., 2001),

- (b) Determining igneous and volcanic histories, e.g., eruption timing, the times scales over which magmas are produced and delivered to volcanoes, and the frequency and magnitudes of volcanic events in space and time on the planet (e.g., Reid et al., 1997; Rubin, 2001; Cooper et al., 2001; Zellmer et al., 2008; Sims et al., 2013),
- (c) Dating fossil teeth, bones, and cave paintings (e.g., Grun et al., 2014; Pike et al., 2002, 2012),
- (d) Calibration of the radiocarbon (carbon-14) system (Bard et al., 1990; Chiu et al., 2005; Reimer et al., 2013),
- (e) Neotectonics and landform evolution (e.g., Priewisch, et al., 2014).

Present data-reporting practices for U-series geochronology data (sometimes also referred to as U-Th or Th/U data) vary widely among publications, and the data provided are commonly

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incomplete. These practices present a challenge when attempting to create syntheses, particularly for U-Th and Ra-Th geochronology applications, where the goal is to make comparisons of U-series ages among different publications or to re-evaluate or re-interpret the data. These circumstances ultimately hinder the utility and longevity of the data as well as the ability to make scientific advances beyond those in the original study that generated them. Given the importance of U-series geochronology in several diverse disciplines and the continuing need to access, compile, and re-interpret data, there is a clear value to establishing baseline data-reporting norms.

This issue has been previously addressed in the context of general geochemistry data (Goldstein et al., 2003) as well as for specific sub-disciplines (e.g., Renne et al., 2009). As with other geochemical techniques, advances in instrumentation and analytical methodologies have enabled the production of a greater volume of data, typically with improved precision and accuracy. Coupled with these developments is the increasing ability of authors to publish more extensive suites of data in online supplements that are linked to journal publications and in open-access, independently maintained community databases. Despite these advances, in the absence of explicit community-endorsed data-reporting norms, the tendency for inconsistent and incomplete data reporting of U-series geochronological measurements continues.

Common problems encountered with U-series data-reporting share some similarities with those in other geochronology disciplines and fall into two main categories. The first is not including enough information about the analysis for reviewers and readers to evaluate the quality of the data relative to discipline practices. For instance, information about the relative ^{232}Th abundance can be used to determine the impact of the detrital Th correction on a U-Th date of a carbonate, and therefore its reliability. The second is that it is not always possible to calculate (or re-calculate) a U-series date using the information provided in published data tables because of omission of information on reference materials, external reproducibility, and measured isotopic values. In addition, the application of revised decay constants for ^{230}Th and ^{234}U (Cheng et al., 2000, 2013) has introduced systematic offsets among various sets of published U-series dates, further complicating data inter-comparisons.

We summarize below a proposed set of minimum data and metadata to serve as a community norm that, if provided when a dataset is published in a peer-reviewed journal article, will greatly aid in later reuse. We also encourage researchers to provide suggested additional items of information that would allow subsequent reanalysis. The guidelines in this paper arise out of consultation with end users and producers of U-series data over the course of several community-driven workshops. These discussions helped to define the need for this norm and provided guidance on how current data-reporting practices might be improved to leading practices that would support the needs of the wider community.

In addition to improving the longevity and utility of existing U-series data and facilitating editorial handling of manuscripts dealing with U-series measurements, our vision is that a norm will also facilitate seamless importing of new measured and older legacy data into emerging cyberinfrastructure like the NSF-funded database hosted at geochron.org.

2. General considerations

We have developed a guide that lists the components that we view as critical to report (required minimum data) versus those that are helpful (recommended data) (Table 1). First, we consider issues that are fairly universal across geochemical applications, and

second, we delve into the critical components to report for U-series applications. We note that while inclusion of all of the required components may lead to more larger tables, much of this information can be reported in the supplement to avoid taking up space in the manuscript.

2.1. Isotopes, ratios, activities and concentrations

There is a wide range of U-series isotopes and applications in the geosciences, but in this paper we limit the discussion to the four longest-lived and commonly applied members of the ^{238}U decay chain (^{238}U , ^{234}U , ^{230}Th , ^{226}Ra), ^{235}U and its daughter ^{231}Pa , and ^{232}Th , which is used as a normalizing isotope in ^{238}U – ^{230}Th geochronology much like ^{204}Pb and ^{86}Sr in U-Pb and Rb-Sr geochronology. Many of the principles and practices of the reporting norms we propose here can be extended to other U-series nuclides.

U-series isotopes are usually reported as activities (decays per unit time), atom abundances, and/or in concentration units. Though only certain ratios may be required to calculate a date, it is helpful to report all of the isotope ratios and concentrations measured, as these additional data may be useful in interpreting the data or using it for a different application. To facilitate data inter-comparisons, we advocate the use of SI units when possible for the reporting of all isotope abundances and sample masses, although application-specific modifications to the reported units are sometimes required to have reasonable numbers to present in tables. Units such as ppm ($\mu\text{g/g}$) and ppb (ng/g) for concentration and Bq/g (decays per second) or dpm (decays per minute) for specific activity are common in the U-series literature.

Before the advent of mass spectrometry (primarily the 1960s through 1980s, but continuing even to today), U-series isotopes were measured by alpha, beta, or gamma counting. Decay counting provides direct measurement of isotope activities, which are convenient units for U-series geochronology applications. Mass spectrometric analysis, on the other hand, measures the number of atoms of each isotope of interest present in a specimen. Their relative abundances are usually then converted to activities for data reporting and visualization using the appropriate decay constants. This underscores the importance of reporting which decay constant was employed for each isotope analyzed, because there have been several different values in use for many of these isotopes in the past two decades. Mass spectrometry is currently the favored form of analysis because it allows for smaller sample sizes and higher data precision than radiometric counting.

2.2. Uncertainties

Uncertainties should be reported for all parameters and should be included in all figures and tables since they are of key importance when making interpretations of the data. Reporting and plotting all uncertainties at the 2σ level is the common practice. When the type of uncertainty is clearly stated then useful comparisons among datasets can be made. We note that the term “uncertainty” represents the range of values within which the true value is asserted to lie and is therefore a more appropriate term to use in this context rather than the term “error”, which typically refers to the difference between a measurement and its accepted or true value. It is important to state whether uncertainties on reported dates include uncertainties in decay constants. To assess the calculation of dates, we recommend including a brief description of the uncertainty propagation for the results of isotope analyses and the computed ages. For example, explicitly state the specific software used to perform the date calculation including pertinent academic references, links to the software, version, and operating

Table 1

Checklist of minimum and recommended data to report for U-series ages. ☑ items are minimum required; ☐ items are recommended data.

General Considerations	
☐	Report all isotope ratios and concentrations measured
☑	Report uncertainties for all parameters
☐	Report uncertainties at 2σ level
☑	Clearly state whether uncertainties on ages include decay constant uncertainties
Minimum Data	
☑	Sample identifier (preferably one that is unique and persistent, such as an IGSN)
☑	Names, descriptions, and reference values of reference materials used
☑	Decay constants used
☑	Isotopes in spike and method of spike calibration
☑	Method of calibration for all activity or atom ratios reported (e.g., secular equilibrium or gravimetric)
☑	Activity or atom ratios for $^{230}\text{Th}/^{238}\text{U}$ (or $^{230}\text{Th}/^{234}\text{U}$) and $^{234}\text{U}/^{238}\text{U}$
☑	$^{230}\text{Th}/^{232}\text{Th}$ activity or atom ratio
☑	Details of procedures and values used to interpret ages using isochrons or other models
☑	Date of analysis or reference age, e.g., 1950
Recommended Data	
☐	Concentrations of ^{238}U , ^{234}U , ^{230}Th , ^{232}Th (plus ^{226}Ra and Ba, if measured)
☐	Description of sample preparation and chemical separations
☐	Description of data acquisition
☐	Description or measurements of sample preservation or mineralogy
☐	Bulk composition of sample and mineral phases (for silicates)
☐	Describe how ages were calculated (e.g., software package, assumptions, etc.)

system, as well as the assumptions employed in the numerical analysis of the data.

2.3. Significant figures

Data should be reported to the appropriate number of significant figures to facilitate both the recalculation of dates and integration with published data (e.g., to calculate rates and durations of processes) without incurring rounding errors. This is one advantage of online data archives, which can store long strings of digits easily to facilitate more precise recalculation of dates. We strongly encourage the practices of archiving data online and of storing unrounded values in these data archives to support reproducibility and future calculations, recognizing that this may lead to differences in appearance between data tables published in journals and the online archived versions.

2.4. Reference materials

Names, descriptions, and reference values (with citation) should be provided for any reference materials used. Additionally, the value obtained for the reference material should be reported, so that accuracy of the data can be better assessed.

3. Minimum U-series data reporting requirements

We consider the minimum data to comprise only the parameters required to reproduce the dates calculated for the samples as well as the basic sample information, as defined below. Some application-specific cases will require other data, such as detrital Th concentration and methods and values employed to make detrital Th corrections. In addition to the checklist of required minimum data and recommended items (Table 1), we provide three example data tables for applications with U-series measurements on corals, speleothems, and volcanic rocks (Tables 2–4). Not all of the required data need to be reported in tabular form, but common parameters can be given in footnotes to tables to make it easier for others to compile. Our intent is not to dictate the format of data reporting, but provide guidelines on information needed so that U-series dates can be re-calculated.

3.1. Basic sample information

Sample documentation is an important aspect of any data reporting norm, and we give below a U-series example of online tools available for this purpose. Reporting collection location coordinates with their datum and precision, the measuring technique, sample size and condition, and the specimen identifier as assigned by the sample collector are several necessary parameters.

Typically, each sample is assigned a sample identification name listed in a data table. An important component of data archiving is using a unique and persistent identifier providing the ability to link sample metadata with other geochemical analyses and to link multiple analyses to the same sample. The International GeoSample Number (IGSN), a traceable and persistent 9-character alphanumeric code, is such a unique identifier and is freely available to geoscientists at the System for Earth Sample Registration (SESAR, <http://www.geosamples.org/>; see also <http://www.igs.org> for background information). In the SESAR system, each IGSN records sample metadata such as the geographic location, sample type, field collection methodology, curator, current location of specimen (if not already exhausted by analysis), and images of the sample and outcrop. Additional domain-specific information can be included in the sample metadata to help contextualize the samples and to assist other users who may wish interpret the data.

The basic workflow for U-series sample identifier assignment can be summarized as follows: A specimen collected in the field receives an IGSN, which will be the parent to any subsamples. Each subsample will also be assigned a unique identifier, with a child relationship to the parent sample. This process can be iterated as more subsamples are taken, such as in closely spaced time series analysis of a speleothem or coral. The relationship between the primary parent specimen and all subsamples is explicitly preserved. In some instances, researchers may choose to assign the parent IGSN to a group of specimens taken from a single sampling location (such as a dredge, core, or other mode of sample collection). IGSNs are not exclusively for new samples, but can be assigned to samples with data that has already been published.

Regardless of the type of sample analyzed, we emphasize the importance of including geological context of the sample. In addition to location information, including latitude, longitude, elevation, datum, and the methodology and uncertainty for each of these, further description of outcrops, cores, and other geological

Table 2

Example of an acceptable data table for coral U-series ages. Values in parentheses are $\pm 2\sigma$ absolute uncertainties. Example data shown here are taken from Dutton et al. (2015).

IGSN	Analysis ID	^{238}U (ppm)	^{230}Th (ppt)	^{232}Th (ppb)	$[^{230}\text{Th}/^{232}\text{Th}]^a$	$[^{230}\text{Th}/^{238}\text{U}]^{a,b}$	$[^{234}\text{U}/^{238}\text{U}]^{a,c}$	Date (ka) ^d	$\delta^{234}\text{U}$ initial
IEDUT100H	SY-27a	2.247 (0.003)	28.105 (0.045)	0.511 (0.001)	10261 (25)	0.7697 (0.0017)	1.1030 (0.0008)	127.0 (0.6)	147.4 (0.8)
IEDUT100I	SY-27b	2.234 (0.003)	28.100 (0.083)	0.668 (0.002)	7855 (22)	0.7738 (0.0026)	1.1028 (0.0011)	128.3 (0.8)	147.7 (1.1)
IEDUT100J	SY-27c	2.290 (0.003)	28.635 (0.056)	0.680 (0.002)	7861 (17)	0.7694 (0.0019)	1.1024 (0.0014)	127.0 (0.7)	146.6 (1.4)
IEDUT100L	SY-36a	4.546 (0.004)	56.616 (0.233)	4.921 (0.017)	2157 (6)	0.7694 (0.0032)	1.1042 (0.0007)	126.6 (1.0)	149.1 (1.0)
IEDUT100M	SY-36b	4.372 (0.002)	54.500 (0.117)	16.303 (0.049)	627 (2)	0.7701 (0.0017)	1.1050 (0.0009)	126.6 (0.6)	150.2 (1.2)
IEDUT100N	SY-36c	4.403 (0.003)	54.791 (0.093)	42.681 (0.091)	241 (1)	0.7689 (0.0014)	1.1034 (0.0008)	126.6 (0.5)	147.9 (1.0)

^a Square brackets denote activity ratios.

^b Ratio determined using a Th-U spike calibrated to a secular equilibrium reference material (HU-1 aliquot at the ANU).

^c Ratio calibrated to a secular equilibrium reference material (HU-1 aliquot at the ANU).

^d Uncorrected, closed-system date calculated using the decay constants of Jaffey et al. (1971) for ^{238}U and Cheng et al. (2013) for ^{230}Th and ^{234}U . Ages are reported relative to the date of analysis, January 2010, and do not include uncertainties associated with decay constants.

Table 3

Example of an acceptable data table for speleothem U-Th ages with a detrital Th correction. All measurements are reported with $\pm 2\sigma$ absolute uncertainties.

IGSN	Dist. (mm)	^{238}U (ppm) ^a	^{232}Th (ppb)	$^{230}\text{Th}/^{232}\text{Th}$ (atomic $\times 10^{-6}$)	$[^{230}\text{Th}/^{238}\text{U}]_{\text{ACT}}$ (measured) ^b	$\delta^{234}\text{U}$ (measured) ^{c,d}	^{230}Th date (ka BP) (uncorrected) ^e	$\delta^{234}\text{U}_{\text{initial}}$ (corrected) ^{f,g}	^{230}Th date (ka BP) (corrected) ^{e,f}
SYN000001	3.2	10.87 \pm 0.11	22.5 \pm 0.1	12587 \pm 21	1.1549 \pm 0.0019	263.57 \pm 0.30	220.7 \pm 1.4	491.5 \pm 2.1	220.6 \pm 1.4
SYN000002	5.1	10.21 \pm 0.10	35.5 \pm 0.4	7537 \pm 10	1.1577 \pm 0.0016	262.99 \pm 0.17	222.6 \pm 1.0	493.2 \pm 1.6	222.5 \pm 1.0
SYN000003	7.5	10.32 \pm 0.10	126.1 \pm 1.4	2167.7 \pm 3.5	1.1606 \pm 0.0019	262.67 \pm 0.23	224.5 \pm 1.3	495.9 \pm 2.3	224.3 \pm 1.3
SYN000004	9.3	10.52 \pm 0.11	251.0 \pm 2.7	1102.6 \pm 1.1	1.1659 \pm 0.0012	262.64 \pm 0.29	227.5 \pm 1.1	501.0 \pm 3.2	227.2 \pm 1.2
SYN000005	11.8	11.63 \pm 0.12	94.2 \pm 1.3	3246.1 \pm 4.9	1.1666 \pm 0.0018	261.69 \pm 0.16	228.6 \pm 1.2	499.5 \pm 1.9	228.5 \pm 1.2
SYN000006	13.2	11.04 \pm 0.11	26.5 \pm 0.2	10955 \pm 13	1.1707 \pm 0.0013	260.93 \pm 0.26	231.5 \pm 1.2	501.8 \pm 1.7	231.5 \pm 1.2
SYN000007	15.6	12.35 \pm 0.12	455.4 \pm 3.8	717.18 \pm 0.87	1.1731 \pm 0.0014	260.76 \pm 0.31	233.1 \pm 1.3	506.4 \pm 4.6	232.6 \pm 1.4
SYN000008	17.2	12.49 \pm 0.12	235.8 \pm 2.6	1400.6 \pm 1.4	1.1772 \pm 0.0012	260.70 \pm 0.20	235.7 \pm 1.0	508.6 \pm 2.5	235.4 \pm 1.0
SYN000009	19.1	12.82 \pm 0.13	507.1 \pm 4.2	673.2 \pm 1.0	1.1790 \pm 0.0018	260.53 \pm 0.17	237.0 \pm 1.3	511.7 \pm 4.8	236.4 \pm 1.4
SYN000010	21.8	11.98 \pm 0.12	276.6 \pm 3.3	1159.9 \pm 1.6	1.1830 \pm 0.0016	259.25 \pm 0.26	240.5 \pm 1.4	512.9 \pm 3.2	240.2 \pm 1.4

All calculations use the decay constants of Jaffey et al., 1971 (^{238}U), Cheng et al., 2013 (^{234}U and ^{230}Th) and, Le Roux and Glendenin, 1963 (^{232}Th).

^a Reported uncertainties for ^{238}U concentrations are estimated at $\pm 1\%$ (2σ) due to uncertainties in tracer concentration. Analytical uncertainties in isotope ratios are smaller.

^b Ratio measured with a tracer calibrated against a gravimetric U-Th solution.

^c Ratio measured with a tracer calibrated to the $^{233}\text{U}/^{238}\text{U}$ of IRMM3636, which is 1.01906 (Verbruggen et al., 2008).

^d $\delta^{234}\text{U} = ([^{234}\text{U}/^{238}\text{U}]_{\text{activity}} - 1) \times 1000$.

^e Dates reported as ka Before Present (BP), where the Present is defined as the year 1950 CE.

^f corrected for detrital Th assuming an initial $[^{232}\text{Th}/^{238}\text{U}]_{\text{activity}} = 1.2 \pm 0.6$, $[^{234}\text{U}/^{238}\text{U}]_{\text{activity}} = 1.0 \pm 0.5$, and $[^{230}\text{Th}/^{238}\text{U}]_{\text{activity}} = 1.0 \pm 0.5$.

^g $\delta^{234}\text{U}_{\text{initial}}$ is corrected for radiogenic ingrowth and decay based on the detrital-corrected ^{230}Th date and also for detrital initial ^{234}U . Ages do not include uncertainties associated with the decay constants.

context information, including photographs can be included in the metadata associated with the IGSN of the sample. This information is important for primary interpretation of the ages, but also important for secondary applications of the data at a later time when someone may wish to reinterpret the data or use it for a different purpose than intended in the original study. Hence, more detailed metadata can easily translate to more robust interpretations and increased longevity and utility of the data and sample.

3.2. Isotopic tracers, decay constants, and isotope ratio calculations

Several pieces of information are essential to explain how any activity or atom ratios are calculated so that the data can be reprocessed with other decay constants at a later time: (1) the tracer spike composition (isotopes); (2) calibration method of isotope ratios (relative to gravimetric or secular equilibrium standards); (3) the decay constants employed (including a citation for the values used); and (4) the way in which each isotope ratio is converted into an activity ratio (see Tables 2–4). These parameters should be reported in each publication and not buried in a chain of citations, as is often the case. The rationale behind this list is explained below.

Decay constants and their associated half-lives of isotopes in the U-series decay chain have, at times, been updated. For example, the decay constants for both ^{230}Th and ^{234}U were updated in by Cheng

et al. (2000) and again by Cheng et al. (2013). This presents a situation where published U-series age data cannot be compared to newer ones without normalizing to the same set of decay constants. To perform this calculation requires the knowledge of how each activity ratio was derived. In the case of $^{230}\text{Th}/^{238}\text{U}$, activity ratios are typically determined using a Th-U spike (thermal ionization mass spectrometry (TIMS) or multi-collector inductively coupled plasma mass spectrometry (MC-ICPMS)). The spike ratio, in turn, can be calibrated using a gravimetric reference material, or a secular equilibrium reference material, or a combination (average) of these two approaches. If the $^{230}\text{Th}/^{238}\text{U}$ ratio was determined using a spike that has been calibrated to a secular equilibrium reference material, then the activity ratio of that reference material is still 1, even if the decay constant for ^{230}Th or ^{238}U gets revised. Hence no correction is required to the originally reported $^{230}\text{Th}/^{238}\text{U}$ activity ratio in this scenario. However, if the spike was calibrated using a gravimetric reference material, then the reported $^{230}\text{Th}/^{238}\text{U}$ activity ratio will need to be corrected to reflect the change in decay constants since the time of publication (e.g., see Cheng et al., 2000).

In addition, the calculation of activity or atom ratios for other isotopes needs to be defined. For example, the $^{234}\text{U}/^{238}\text{U}$ ratio can also be determined relative to a gravimetric reference material or a secular equilibrium reference material, regardless of how the corresponding $^{230}\text{Th}/^{238}\text{U}$ activity or atom ratio was determined. Therefore it is essential to clarify the calibration method for all

Table 4
Example data table for volcanic silicates. All measurements are reported with $\pm 2\sigma$ absolute uncertainties of last digit in parentheses. Example data shown here are taken from Zellmer et al. (2008).

IGSN	Sample ID ^a	Th (ppm)	U (ppm)	[²³⁸ U/ ²³² Th] ^{b,d}	[²³⁰ Th/ ²³² Th] ^{b,d}	[²³⁴ U/ ²³⁸ U] ^b	[²³⁰ Th] ^{b,c}	[²²⁶ Ra] ^{b,c}	[²²⁶ Ra/ ²³⁰ Th]	Ba (ppm) ^e	Eruption Year	Crystal assemblage Age (Kyr) ^f
KHR00023B	SAL643 (WR)	0.3902 (4)	0.1216 (5)	0.945 (4)	1.063 (12)	1.00 (0.3)	0.1013 (11)	0.147 (0.9)	1.451 (12)	37.87	1477	1.4 (0.3)
KHR10023B	SAL643 (Px)	0.01272 (2)	0.00424 (3)	1.012 (7)	1.063 (1)	n.d.	0.0033 (3)	0.0086 (4)	2.601 (44)	4.46		
KHR20023B	SAL643 (Pg)	0.003702 (4)	0.00376 (2)	3.083 (15)	n.d.	n.d.	n.d.	n.d.	n.d.	5.01		
KHR30023B	SAL643 (M)	0.097 (3)	0.0304 (1)	0.945 (5)	1.070 (9)	n.d.	0.255 (2)	0.156 (16)	0.611 (104)	6.66		
KHR00023A	SAL644 (WR)	15.89 (2)	4.715 (21)	0.900 (4)	1.028 (11)	1.002 (4)	3.993 (42)	4.424 (14)	1.108 (11)	495.3	1477	2.0 (+0.2, −0.1)
KHR10023A	SAL644 (M)	7.677 (8)	2.262 (1)	0.894 (4)	1.040 (12)	n.d.	1.950 (22)	1.502 (35)	0.770 (26)	54.88		
KHR000237	SAL647 (WR)	0.594 (7)	0.1823 (8)	0.931 (4)	1.061 (11)	1.001 (3)	0.154 (2)	0.206 (3)	1.335 (19)	61.04	871	n/a
KHR000236	SAL649 (WR)	17.84 (2)	5.27 (23)	0.897 (4)	1.045 (11)	1.000 (3)	4.555 (50)	4.681 (25)	1.028 (12)	466.2	871	3.2 (0.4)
KHR100236	SAL649 (Px)	3.661 (4)	1.059 (5)	0.878 (4)	1.038 (8)	n.d.	0.928 (8)	0.820 (16)	0.883 (21)	23.14		
KHR200236	SAL649 (Pg)	0.4662 (6)	0.1379 (6)	0.897 (4)	1.049 (8)	n.d.	0.1195 (10)	1.18 (8)	9.879 (68)	796		
KHR300236	SAL649 (M)	6.791 (7)	2.148 (13)	0.960 (6)	1.044 (10)	n.d.	1.733 (17)	1.541 (13)	0.890 (13)	51.65		

^a WR = Whole rock, Px = Pyroxene, Pg = Plagioclase, M = Magnetite.

^b Square brackets indicate activity ratios calculated from atomic abundances using the decay constants of Jaffey et al., 1971 (²³⁸U), and Meadows et al., 1980 (²³⁰Th), Holden, 1990, and using a $\lambda^{226}\text{Ra} = 4.332 \times 10^{-4} \text{ yr}^{-1}$.

^c Activity in units of dpm/g.

^d Ratio measured with a tracer calibrated against gravimetric U (CRM112-A) and Th solutions (Hawaii-Th1 and UCSC-A), see Rubin, 2001 for solution details.

^e Ba concentrations have an uncertainty of 0.1%.

^f Ages are reported in the row for the whole rock sample, relative to the year of analysis (2007). Ages do not include uncertainties associated with the decay constants.

activity or atom ratios that are reported. Analogous considerations apply to *in situ* analyses: no corrections to ²³⁰Th and ²³⁸U will be required when U-Th relative sensitivity factors are determined with respect to a secular equilibrium reference material, whereas ²³⁰Th/²³⁸U activity ratios will depend on the decay constants applied when calibrated against the Th/U ratio of a standard.

3.3. Isotope ratios and abundances

Sufficient information should be provided so that a date calculation can be performed from the reported data. For carbonate materials with initial ²³⁴U-²³⁸U disequilibrium, at least two isotope ratios that collectively include three isotopes, ²³⁸U, ²³⁴U, and ²³⁰Th, must be reported to perform a U-Th date calculation. For igneous materials in ²³⁴U-²³⁸U equilibrium, two isotopes, ²³⁸U and ²³⁰Th must be reported along with the normalizing isotope, ²³²Th, in ratio form. The Ra-Th age system is analogous, whereby ²²⁶Ra and ²³⁰Th must be reported, along with normalizing element Ba, when employed. Unfortunately, many publications include only a date or a date with incomplete isotope ratio information making recalculation of dates difficult to impossible. In past common practice, the choice of which isotope ratios to report usually depended on the specific analytical protocol performed. For example, alpha-counting data were reported as ²³⁰Th/²³⁴U and ²³⁴U/²³⁸U, whereas mass spectrometry measurements used the convention of reporting ²³⁰Th/²³⁸U and ²³⁴U/²³⁸U. However, in some laboratories where the ²³⁰Th isotope is measured relative to ²³⁴U rather than ²³⁸U on a mass spectrometer, ²³⁰Th/²³⁴U is reported in place of ²³⁰Th/²³⁸U. Because analytical protocols still vary between laboratories, this suggests two specific recommendations for reporting the isotope ratios of ²³⁸U, ²³⁴U and ²³⁰Th. First, report the activity or atom ratios for the isotopes measured directly on the mass spectrometer along with their associated 2σ analytical uncertainties.

Second, give any unreported activity or atom ratios and uncertainties for ²³⁰Th/²³⁸U and ²³⁴U/²³⁸U if not directly measured. Though not always strictly required to calculate a date, we suggest that the activity or atom ratio for ²³⁰Th/²³²Th be included as an essential minimum data-reporting parameter.

In addition to these three isotope ratios, the concentrations (g/g sample) of ²³⁸U, ²³⁴U, ²³⁰Th, and ²³²Th plus ²²⁶Ra and Ba, if measured along with their associated 2σ analytical uncertainties, should also be reported. Although ²³²Th is used directly in igneous applications (by comparing ²³⁰Th/²³²Th and ²³⁸U/²³²Th), it is not directly used in the date equation for carbonates. Nevertheless, because evaluating the presence of ²³²Th in a carbonate is critical to assess potential ²³⁰Th contamination, we have included this isotope as a minimum essential data reporting parameter. Terminology also needs to be defined, for example, where (²³⁰Th/²³⁸U)_A represents the activity ratio or in the case of reporting initial $\delta^{234}\text{U}$ values, which has variously been designated as $\delta^{234}\text{U}(0)$, $\delta^{234}\text{U}(T)$, $\delta^{234}\text{U}_i$, or $\delta^{234}\text{U}_{\text{init}}$ (Bard et al., 1990; Edwards et al., 2003; Richards and Dorale, 2003).

3.4. Dates and ages

For clarity, we adopt the convention that a “date” is calculated from the measurements and that an “age” is the interpretation of the date in the context of other facts. Uncorrected dates, sometimes referred to as conventional dates, should always be reported in addition to any corrected or otherwise interpreted date. This improves the transparency of the correction or interpretation relative to the uncorrected date. An example of an interpreted date (an age) is one that has been corrected in some way for detrital Th (²³²Th) contamination, a date that is determined from an average of multiple analyses measured from the same sample, or a date that is modeled using the measured isotope ratios, such as in open-system

model calculations for carbonates (e.g., Thompson et al., 2003). The methodology employed to calculate the age should be clearly articulated so that the method can be reproduced. This includes explicit definition of any constants or parameters used in the calculations such as assumed values for detrital Th corrections. To avoid confusion, there should be a clear distinction in the labeling of the numbers reported, for example: 'Date/Uncorrected Date/Conventional Date and 'Interpreted Age', where the interpreted age label can be modified with the technique used, e.g., 'Interpreted Open-system Age' or 'Interpreted Detrital Th-corrected Age'. Both types of ages should include their associated 2σ uncertainty.

For igneous systems, explicitly state assumptions and approximations used to derive an age. For instance, if external isochrons were employed to estimate the initial daughter/parent ratios, state how these estimates and their uncertainties were made. If internal isochrons were used, provide the isochron data itself (either graphically or in text form) that shows the goodness of fit. Also provide information on important assumptions such as Ba and Ra distribution coefficients and/or phase partitioning models for Ra and Ba if used (Blundy and Wood, 2003; Cooper, 2009; Cooper et al., 2001; Fabbrizio et al., 2009; Miller et al., 2007; Sims et al., 2013), or not (Rubin and Zellmer, 2009; Zellmer et al., 2008). In some cases, especially but not limited to higher silica magmas, different crystal phases may grow in sequence, or may grow slowly relative to the half-life of the daughter isotope being used for dating (^{226}Ra or ^{230}Th) (Sims et al., 2013). Such special conditions should be discussed and evaluated in the publication, as should evidence for different growth domains in single crystals.

3.5. Reference age

Though there is no convention for the reference age of a U-series date, the datum of what is considered 'the present' needs to be defined. There is precedent within the radiocarbon dating community for reporting ages relative to the year 1950 (Godwin, 1962). Noting the historical prevalence of this datum in both the radiocarbon and U-series dating literature, and also because it will continue to facilitate data inter-comparisons between these two dating methods, we strongly advocate the use of 1950 as the reference age.

There are effectively two ways to ensure proper definition of the reference age: (1) convert the calculated dates to a reference frame (e.g., years before 1950), or (2) report the date of analysis if dates are calculated using the isotope ratios measured on the day of analysis and not adjusted or corrected in anyway to normalize them to a common temporal reference frame. Defining the reference age is particularly important for very young samples and when measurements are made using spikes or reference materials containing isotopes with very short half-lives. Even for older samples with dates that are reported in thousands of years (ka), the reference frame should be made clear (e.g., normalized to 1950, 2000, or relative to date of analysis).

4. Recommended additional data

In addition to the minimum essential data that is required to recalculate a date, there is a suite of parameters commonly used to aid in the interpretation of the age, some of which are application specific. To be clear, just because these data are categorized as non-essential does not mean that they are not important and in some cases critical, to a robust age interpretation. Hence, it is best to think of the non-essential data as highly desirable or strongly encouraged.

4.1. Sample preparation and chemical separations

Full documentation of the sample preparation improves the transparency of the methodology and may provide potential explanations of disparate data for samples prepared or pre-treated in different ways. We recommend describing the processing of the sample for evaluation and eventual analysis. The form of the sample, e.g., powdered versus solid, should be specified along with any physical (slabbing, drilling, grinding, sonication, physical separations, heavy liquids, etc.) and chemical pre-treatments (e.g., rinses, acid leaches). If a citation is given for the methodology, a short summary of the method is appropriate along with any deviations to the cited methodology.

Analytical procedures used to separate and purify the elements of interest for isotope analysis should also be provided in sufficient detail for any knowledgeable practitioner to reproduce, and with sufficient information to understand the cleanliness and yield of the procedures. We recognize that there are several different protocols used for column chemistry (e.g., different resins and column geometries) to extract the isotopes of interest, and different processing methods for these apparatuses (resin used once or more than once, procedures for column cleaning between uses). Thus, we encourage the full reporting of column chemistry techniques to allow other workers to better evaluate data quality and applicability to a specific use. All reagents used in the procedures should be specified regarding grade, concentration, volume, and duration of treatment (for pre-treatment steps), as well as blank levels.

4.2. Data acquisition

The laboratory, instrumentation, and analytical protocol should be clearly defined. Where a citation is provided for the analytical protocol, any deviations should be explicitly stated. There are several important mass spectrometric parameters that should be discussed including sample introduction method, analysis routine (e.g., magnet settling, dwell times, and data cycles), washout parameters (for ICP-MS), method of mass bias corrections, ion counter gain correction, tailing corrections (i.e., from abundance sensitivity determination and monitoring) of baseline determination. For *in situ* analyses, information about sampling mode (e.g., rastering, spots, depth profiling), resulting sampling sizes (ideally including total analytical depth), and any beam-derived surficial cleaning procedures should be provided. Details of the sampling conditions should also be included: (1) e.g., for laser ablation-ICP-MS analyses: energy density/fluence, repetition rate, carrier gas and flow rate, ablation duration, and make-up gas flow; and (2) e.g., for SIMS analyses: primary ion beam current, secondary ion accelerating voltage and energy band pass, and mass resolution.

4.3. Th-U in carbonates

In all cases, we recommend that reported data include information that is potentially valuable in the interpretation of a calculated U-Th age. In addition to the measured isotopic ratios listed in Section 3, provide the initial uranium isotope composition (reported either as $^{234}\text{U}/^{238}\text{U}$ activity ratio or $\delta^{234}\text{U}$). For all carbonates, some type of quantitative and/or qualitative assessment of preservation is critical.

Additional data reported will depend upon the type of carbonate analyzed. At a minimum, coral data should include: taxonomic identification to the highest level possible and mineralogical assessment (e.g., % calcite or aragonite) including the methodology, uncertainty, and detection limits of the technique. Many fossil corals are dated for the purpose of sea level or paleoclimate reconstructions. For both of these purposes, the position of the coral

within the anatomy of the reef may be important to the interpretations. Regardless of the objective of the primary study, further description of the reef facies, associated reef biota, and paleodepth information are all valuable parameters that should be reported, where possible. Additional recommended metadata for coral U-series data that are collected for reconstructing sea level can be found in Hibbert et al. (2016). An example data table for the U-series geochemical information that should be reported is provided in Table 2. With respect to speleothem samples, the distance from the top of the speleothem should be included for each sample (Table 3) as well as a more detailed description of the sample placement within the specimen as well as the placement of the speleothem within the cave system. Other distinguishing features should be described, such as hiatuses and evidence for dissolution that can play into the interpretation of the data.

4.4. Th-U and Ra-Th in volcanic silicates

An example data table for U-series measurements on silicates has been provided (Table 4). Data requirements will depend on the type of material analyzed and the Th-U or Ra-Th dating method (e.g., internal mineral isochron, whole rock external isochron, single crystal dating). In all cases, the bulk composition and intrusive/extrusive condition of the sample should be provided by name (e.g., basalt, rhyolite) and distinguishing chemical characteristics that determine the name (e.g., Total Alkali vs. Silica, SiO₂, or MgO). Physical characteristics that can affect age interpretations such as alteration, rock textures, outcrop conditions (e.g., underwater, dry, near a roadside) should also be provided. For mineral isochrons, mineral phases should also be identified by name and composition, and information given about how the minerals were separated from the sample and purity of separates.

5. Data analysis

Sufficient information for readers to re-construct dates must be provided. In general, this means specifying the type of date reported, meaning an 'isochron date' for any U-series system (by either internal or external isochron approaches), a 'uncorrected (conventional) date' for the U-Th system, or an 'open-system date' for marine carbonates (see Section 3.4). The latter requires several additional pieces information, including the measured isotope ratios and a list of assumptions made in performing this correction.

Full traceability of the data requires specifying and citing, where possible, the software package used for data reduction and uncertainty propagation including its version and any pertinent references. If the uncertainty propagation is performed using in-house algorithms, then a brief description of these algorithms or an online repository of code would be helpful, both for the peer review and readers.

6. Data archiving

The preferred data archiving path follows the rigorous approaches developed over the last decade for geochemical and other geochronological analyses by major international data repositories such as those operated by the Interdisciplinary Earth Data Alliance (IEDA). The main components of this approach are unique sample identifiers that allow for both locating samples and amalgamating various sorts of data collected on the same sample, the use of standardized data schemas, naming conventions, extensible markup language (XML) and web services to exchange data among data generators, repositories, archives, and data manipulation software. Open access discoverability through various search approaches and interfaces is also crucial.

While we do not advocate for a specific repository and associated cyber infrastructure, we will point out that EarthChem, a part of IEDA, is one such group that has developed and uses such cyberinfrastructure for geoscience applications, in close interaction with the IEDA Geochron database, for the preservation and serving of age data of all sorts. This system (<http://geochron.org>) allows users to upload data in public or private modes, and users can invite other users to participate in a private group mode to view samples establishing a virtual space in which to share their samples and data. Within these first three modes, the user can update and change data sets as the analysis matures. There is a fourth mode where datasets become read-only and are published with a unique resource identifier (URI). Such datasets are also published to the EarthChem Library (<http://www.earthchem.org/library>), receive a DOI, and are archived in conjunction with the Columbia University Archives Digital Program.

7. Concluding remarks

The intention of these recommending these practices for data reporting is to encourage researchers and journal editors to collectively improve the utility and longevity of U-series data. These ideals have not been routine practice in the past, and in fact have perhaps rarely been attained, but adopting these practices as a routine part of the workflow in each laboratory will enable enhanced data sharing and interpretation. Ultimately such practices will facilitate online archiving and reprocessing of data. As has been witnessed in the U-Pb community, these capabilities, in turn, allow for larger scale data interlaboratory comparisons and synoptic studies that will be drivers of new theories and research directions (e.g., McKenzie et al., 2016).

While the initial transition to adopting these data reporting norms may require additional effort, the benefits in the long run will include a marked conservation of effort required to compile previously published data in a systematic and comparable way. To assist in the implementation of these data reporting norms, open-source, platform-independent software is presently under development by a subset of the author team to support seamless data uploading to community database, calculations (date determination, isochrons, etc.), visualizations (evolution diagrams, etc.), and—most relevant to this discussion—generation of data tables with templates that include all the required components proposed herein. While the development of this cyberinfrastructure is initially in response to user-based workshops, continued input from the community during the development stage is actively sought and will ultimately be a key factor for community buy-in. The main vehicle for continued conversation between the U-series community as well as those who are users of U-series data is a centralized website: www.useries.rocks. Standardization of data reporting will make U-series data more transparent to the larger earth sciences community and beyond as envisioned by the EarthCube project. This transparency will likely result in new scientific questions as scientists combine data sets from different disciplines in an effort to better understand our environment and its processes.

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