Electronic Supplementary Material (ESI) for Journal of Analytical Atomic Spectrometry. This journal is © The Royal Society of Chemistry 2023

Supplementary information (S1)

## Isoclock: A free and novel routine for common Pb correction in U-Th-Pb data

reduction of LA-ICP-MS analysis

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August 6, 2023



## A. Figures of accessory mineral dating results processed with Isoclock.

Fig.S1 The Tera-Wasserburg diagrams of studied monazite and apatite after Isoclock processing (anchored common Pb values derived from the Stacey and Kramers (1975) Pb model). (a) Anomalously high common Pb spots are present in the Ts-Mnz monazite analysis. (b-e) Correction of anomalies for common Pb ("Cal <sup>204</sup>Pb") or filtering for discordant anomalies in RM, the unknowns yielded slightly varied results. However, not correcting for common Pb or abnormality filtering in RM can lead to offset results. (f)The results of monazite and apatite in the Xiangshan volcanic rocks processed by Isoclock software are consistent with the zircon U-Pb results.



Fig. S2 The Tera-Wasserburg diagrams of apatite and cassiterite after Iolite, Isoclock and U-Pb Saturn processing. (a-b) Result of MRC and BRZ apatite displayed on Tera-Wasserburg diagram after different software and common Pb correction in MAD. (c-f) Comparison of the MRC and BRZ <sup>208</sup>Pb/<sup>232</sup>Th ages obtained with Isoclock and Iolite shows that the "Cal <sup>204</sup>Pb" method yields E-consistent U-Pb and Th-Pb ages. (g-h) Comparison of different Pb correction or uncorrected method for cassiterite using Isoclock.



Fig. S3 The Tera-Wasserburg and corrected weighted mean<sup>206</sup>Pb/<sup>238</sup>U ages diagrams of studied apatite after Isoclock processing (anchored common Pb values derived from the Stacey and Kramers (1975) Pb model). Common Pb in standards were corrected by the "Cal <sup>204</sup>Pb" method and weighted mean ages were corrected by the <sup>207</sup>Pb method.



Fig. S4 The Tera-Wasserburg and corrected weighted mean <sup>206</sup>Pb/<sup>238</sup>U ages diagrams of studied wolframite after Isoclock processing (anchored common Pb values derived from the Stacey and Kramers (1975) Pb model). Common Pb in standards was corrected by the "Cal <sup>204</sup>Pb" method and weighted mean ages were corrected by the <sup>207</sup>Pb method.

## B. User Manual of Isoclock 2.0



Hydrothermal/Accessory Minerals U-Th-Pb Data processing for LA-ICPMS



## **User Manual of Isoclock 2.0**

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## I. Software operation procedures

#### 1.1 Start-up and functional block division

Windows users can also download and run the packaged exe file directly. Download

Isoclock 2.0.exe: https://www.researchgate.net/publication/371012414\_Isoclock20.

The demo video is available at:

https://www.researchgate.net/publication/371039144\_Demo\_of\_Isoclock20.

The following steps 1.1.1-1.1.5 is run before Brama source code runs for the first time.

1.1.1 Python 3.9 is necessary to run the code. Download from https://www.python.org/downloads/ and follow the installation (Fig.S5).



#### Fig. S5 Install Python 3.9.

- 1.1.2 Download or clone this repository (  $\tt https://github.com/sndjgm/Isoclock )$  .
- 1.1.3 Open terminal/cmd and navigate to the Brama folder (Fig. S6).
  - cd path/to/folder/ Isoclock

🖅 Run		×
	Type the name of a program, folder, document, or Internet resource, and Windows will open it for you.	V.
<u>O</u> pen:	cmd ~	Administrator: C:\WINDOWS\system32\cmd.exe
	This task will be created with administrative privileges.	Microsoft Windows [Version 10.0.19044.1889] (c) Microsoft Corporation. All rights reserved.
f ß		7 C:\Users\Administrator>
	OK Cancel <u>B</u> rowse	

Fig. S6 Open terminal/cmd and navigate to the Isoclock folder.

1.1.4 Instal python libraries required for Isoclock.

- pip install -r requirements.txt.
- 1.1.5 Run Isoclock from python.
  - python Isoclock.py

If everything is already installed, follow only steps1.1.5.

The main interface and functional partitions of the program are shown in Fig.S7 after

starting.

Isoclock v2.0 About Tools	– – ×
• Standard Corr. C Standard not Corr. (1)	C 207Pb(Std) C 204Pb(Std) C 208Pb(Std) C 204Pb(Std) (2)
Setting Standard     C Apatite(MAD-NEW)     C Cassiterite(AY-4	) C Zircon(91500) C Calcite(wc-1) (3)
G S&K	(4)
C Thermo C Agilent C Element	(5)
Input Path: D:/2.软件方法论文Isocloc Browse	Fractionation correction E(%): 3 (8)
Output Path: D:/2.软体方法论文Isocloc Browse	Export (Linear) Export (Average) C None C 207Pb C 208Pb C 204Pb C Cal 20(9)
Samples List Signal selection (7)	MRC - 14 :{MRC} Pb inclusion (10)
MAD-NEW - 8,csv MAD-NEW - 9,csv MRC - 1.csv MRC - 10,csv MRC - 11,csv MRC - 12,csv MRC - 13,csv MRC - 13,csv MRC - 15,csv MRC - 15,csv MRC - 15,csv MRC - 16,csv MRC - 16,csv	10 <sup>5</sup> 202Hd 204Pb 206Pb 205Pb 205Pb 203Pb 2232Th 238U 10 <sup>4</sup> 238U
All         Cancle         Delete         Comments:         Pb 204           RM         samples         Save	0 10 20 30 40 50 60 Time(s)

Fig. S7 Main interface and function partition

The software is divided into 7 functional areas. The main functional areas are outlined as follows.

### 2. General steps of data processing:

The software interface is divided into different functional areas according to color (Fig. S7).

 $\bigstar (1) \sim (2) \text{ Select Mode.}$ 

Calculation mode selection area (light steel blue and dark blue): If the standards contain relatively high common Pb (such as apatite, sphere, wolframite, etc.) which needs to be corrected, select the <standard Cor> button. Otherwise, select <standard not Cor> button (e.g., for most zircon).

Dark blue area (2) switches the method of standard common Pb correction methods.

Common Pb correction method based on <sup>207</sup>Pb and <sup>204</sup>Pb derived from Chew et al. (2014). <sup>208</sup>Pb correction method derived from Zack et al.(2011).

 $(3) \sim (4)$  Set standard sample

Standard setting area (turquoise and grey): Click the <Setting Standard> button and select "S&k" mode (Stacey and Kramers, 1975) or "User" mode to set the standard information.

Note: when selecting the corresponding method directly, it is necessary to ensure that the standard sample name is completely consistent with the software display name.

✤ (5) Select ICPMS instrument model.

The software provides three formats to choose from:

(a) **<Thermo>** mass spectrometer. The software does not need to provide a "List file"(Excel with two columns of file serial number and sample name), and the software can automatically extract the document serial number and sample name;

(b) **Agilent>** mass spectrometer. The file is stored in the 'sequence. CSV' file in the 'sequence. D' folder. It is necessary to provide the list format EXCEL file corresponding to the file sequence and sample name (the first column is the folder name, and the second column of the file is the sample or standard sample name);

(c) **<Element>** mass spectrometer. The "\*. Fin" format file stores the list sequence file, and the "\*. Fin2" format file stores the signal data.

✤ (6) Date input and output (light yellow):

Select the data input path and output path, and then click the <Load Data> button to import data. If <Agilent> is selected in step (3), the list file should be selected.Select the data input path and output path, and then click the <Load Data> button to import data.

Note: If **<Agilent>** is selected, you need to select the list file in the pop-up window.

✤ (7) Blank and sampling time settings (light purple):

Click the sample list on the left side of this area, and the signal diagram of the selected sample will be drawn in the area (10). Click the button <Set (All)> or < Set (Single)> to change the background and sampling time of selected or all signals.

In the "Comments" column, you can add annotations and remarks for the samples. By clicking the "Save" button, the comments will be exported to the result file.

✤ (8) Isotope ratio calculation (yellow-green):

Click <Fractionation Correction>button to generate the "result\_all. csv" and "Mean\_Cps.csv" file in the output directory.

The systematic uncertainty to be propagated can be entered in column " $\epsilon$ ". The default value is 3%. Uncertainty propagation refer to Horstwood et al. (2016).

✤ (9) Calculation of age results of samples (Saxe blue):

Click <Export (Liner)> to export the results of the calculated ages and isotope ratios of each sample with Sample-Standard-Bracketing method. No instrument drift correction is performed when the <Export (Average)> button is clicked.

The resulting file is named "cal\_age\_result\_L\*. xls" (Liner) or "cal\_age\_result\_A\*. xls" (average) (Fig. S8).

✤ (10) Signal diagram (white):

When the samples name in step (7) are selected, their signal diagram will be displayed here and automatically saved in the output directory.

SampleName	207Pb/206	28	206Pb/231	28	207Pb/23	28	208Pb/23:	25	208Pb/200	25	232Th/201	25	208Pb/204	28
GBW04420	0.04865	0.00073	0.01035	0.00027	0.06943	0.00207	-0.00015	6.91959	5.3E-05	7.5E-06	0	0	-55.2022	7.77121
GBW04420	0.04903	0.00073	0.01013	0.00026	0.06848	0.00203	-8.4E-05	4.114	3.9E-05	6.3E-06	0	0	-20.7367	3.30751
GBW04420	0.0487	0.00072	0.01119	0.00029	0.07517	0.00225	-0.00013	7.47153	6.1E-05	7.9E-06	0	0	158.982	20.685
GBW04420	0.04841	0.00061	0.00958	0.00025	0.06395	0.00183	-0.00049	52.371	0.00027	2.2E-05	8.48944	5.2E-06	45.8563	4.62953
GBW04420	0.04803	0.00069	0.01111	0.00031	0.0736	0.00232	#NUM!	#NUM!	3.2E-05	7.9E-06	0	0	-281.597	69.0111
GBW04420	0.04901	0.00079	0.00894	0.0002	0.06039	0.00164	-9.8E-05	13.6812	5.1E-05	9.9E-06	0	0	15.626	3.04804
GBW04420	0.04922	0.0007	0.01065	0.00022	0.0723	0.00179	-0.00017	13.7394	4.9E-05	6.7E-06	0	0	18.5625	2.63756
GBW04420	0.04878	0.0007	0.00895	0.00019	0.06022	0.00152	-5.5E-05	4.03773	6.6E-05	0.00001	0	0	26.3023	4.1602
GBW04420	0.04838	0.00076	0.01027	0.00015	0.06851	0.00145	-0.00029	20.8093	0.00019	2.5E-05	0	0	44.8235	7.15067
GBW04420	0.04856	0.00068	0.00862	0.00029	0.05775	0.0021	-0.00033	17.4518	9.8E-05	1.1E-05	0	0	12.8362	1.40998
GBW04420	0.04847	0.00064	0.01097	0.00026	0.07328	0.00198	#NUM!	#NUM!	4.7E-05	8.9E-06	0	0	-121.256	24.4517
GBW04420	0.0491	0.0007	0.01134	0.00032	0.07679	0.00241	-4.8E-05	5.31698	2.2E-05	5.6E-06	0	0	2.80409	0.68078
GBW04420	0.04896	0.00072	0.01112	0.0003	0.0751	0.00228	-7.1E-05	5.11945	5.2E-05	6.8E-06	0.4704	8.9E-07	-22.5528	2.84606
GBW04420	0.04808	0.00074	0.01085	0.00023	0.07189	0.00189	-0.00017	13.1518	9.6E-05	1.4E-05	1.24469	1.5E-06	1031.14	135.027
GBW04420	0.04835	0.00066	0.01088	0.00032	0.07254	0.00233	-0.00034	19.1255	8.7E-05	1E-05	0.55782	1.3E-06	13.3754	1.62798
GBW04420	0.0488	0.00068	0.01173	0.00029	0.07896	0.00223	-0.00017	8.97227	0.00013	1.3E-05	0	0	33.1283	3.31997
GBW04420	0.04815	0.00078	0.01085	0.00023	0.07203	0.00187	-7.7E-05	3.74507	7.9E-05	9E-06	#NUM!	#NUM!	11.1607	1.29952
GBW04420	0.04845	0.00072	0.01103	0.00027	0.0737	0.00211	-6.4E-05	4.32812	6.5E-05	6.7E-06	0.07701	3.7E-07	274.946	30.47
GBW04420	0.04841	0.00064	0.011	0.00022	0.07344	0.00177	-0.00015	11.8848	6.7E-05	1.1E-05	0	0	8.46403	1.57046
GBW04420	0.04781	0.00067	0.01176	0.00032	0.07753	0.00238	-6.1E-05	5.06623	3.8E-05	7.1E-06	0	0	9.07236	1.7496
GBW04420	0.04819	0.00071	0.01066	0.00025	0.07085	0.00195	-0.00013	5.84842	8.8E-05	9.3E-06	0	0	17.2545	1.74899
GBW04420	0.04788	0.00062	0.01143	0.00025	0.07543	0.00189	-0.0002	14.0437	4.8E-05	7.2E-06	0	0	-26.071	3.9657
GBW04420	0.04913	0.00073	0.01175	0.00023	0.0796	0.00194	-0.00012	9.46894	2.9E-05	5.1E-06	0	0	7.19651	1.30584
GBW04420	0.04834	0.00075	0.01121	0.00025	0.07468	0.00199	-6.7E-06	11903	7E-06	2.5E-06	0	0	6.24841	2.39495
GBW04420	0.04881	0.00061	0.01094	0.00028	0.07364	0.00207	-0.00018	10.3008	0.0002	1.6E-05	0	0	307.907	28.0788
GBW04420	0.04889	0.00063	0.01065	0.00021	0.07181	0.00165	-0 0002	14 2476	6 2E-05	1.1E-05	0	0	16 6864	2.58207
Cample	numbo	r colu	mn											
Sample number column						Isoto	pe rati	o and	error co					

										10 00 00														
										238U/206i	2s error	207Pb/206	2s error	Plotting pt	207Pb/235	2s error	206Pb/235	2s error	rho	208Pb/232Th	2s arror	208Pb/20	2s error	
206PD 2329	70.100	W/PD 23.	5	208Fb 23	25	Corrected f206	кад 206Р	25 1	erra-wasserburg Plot	98.60847	3.81446	0.048848	0.000729		0.069432	0.002072	0.010351	0.000409	0.905212	-0.00014983	6.919587	0.000053	7.47E-08	
66.3856	70422	68.1599	2.03385	0.30286	13987,1	0.00156	66.2826	2.61714		98.72796	3.885126	0.049034	0.000733		0.068479	0.00203	0.010129	0.000399	0.904966	-8.4029E-05	4.114005	3.93E-05	6.28E-06	
64.9663	65449	67.2549	1,99346	-0.16985	8315.67	0.00205	64.834	2.55134		89.33148	3.545738	0.048703	0.000721		0.075171	0.002248	0.011194	0.000444	0.907228	-0.00012688	7.47153	6.09E-05	7.92E-06	
71,7619	.86505	73 5951	2.20051	-0.25646	15102.6	0.00163	71.6457	2.84375		104.3808	4.138288	0.048406	0.000607		0.063954	0.001835	0.009582	0.00038	0.92286	-0.00048959	52.37102	0.000269	2.23E-05	
61.4765	.59233	62.9458	1.80596	-0.98982	105879	0.00126	61.3997	2.43354		89.97556	3.704976	0.048026	0.000689		0.073596	0.002321	0.011114	0.000458	0.916234	#NUM!	#NUM!	3.21E-05	7.9E-06	
71.2511	00973	72.106	2.27422	#NUM!	#NUM!	0.00078	71.1961	2.93168		111.8975	4.172434	0.049008	0.000788		0.060387	0.001643	0.008937	0.000333	0.884735	-9.7829E-05	13.6812		9.87E-06	
57.3541	1.2701	59.5362	1.62017	-0.19774	27654.1	0.00201	57.2391	2 13433		93.86134	3.416145	0.049219	0.000698		0.072301	0.001795	0.010654	0.000388	0.895957	-0.00017198	13.73936	4.89E-05	6.68E-06	
68.3169	1.4078	70.8806	1.75934	-0.34763	27772.7	0.00228	68 162	2.4808		111.6887	4.093335	0.048778	0.000701		0.060216	0.001519	0.008953	0.000328	0.8955	-5.4771E-05	4.037725	6.57E-05	0.00001	
57.4608	20966	59.3723	1.49773	-0.11071	8161.37	0.00172	57.3623	2.1023		97.36037	3.25/019	0.04838	0.00076		0.068515	0.001453	0.0102/1	0.000344	0.853355	-0.00029341	20.80928	0.000194	2.04E-00	
65.8742	97511	67.2888	1.42677	-0.59313	42066.4	0.00122	65.7941	2.20103		110.948	0.239123	0.040487	0.000844		0.00710	0.002097	0.008025	0.000389	0.931945	-0.00032744	17.4018	9.62E-05	1.0/E-00	
55.3591	86733	57 0081	2.06992	-0.66193	35279.8	0.00145	55,2789	2.4954		00 15220	3.452000	0.040000	0.000041		0.078706	0.00136	0.011244	0.00042	0.012402	A RATTE OF	#NUM:	4.0/E-00	6.63E-00	
70.3025	1.6736	71.8042	1.94047	#NUM!	#NUM!	0.00133	70.2094	2.68886		00.10020	2 825097	0.040000	0.000715		0.075097	0.002412	0.011125	0.000407	0.910720	7 09485 05	5.119452	5.2240-00	8 775 08	
72.7157	04971	75.1268	2.36005	-0.09799	10747.1	0.00213	72.5618	2.98701		92 20415	3 410297	0.048077	0.000745		0.071893	0.001892	0.010845	0.000440	0.887885	0.00017405	12 1518	9.57E-05	1.37E-05	
71.3182	92207	73.5252	2.23712	-0.1432	10347.9	0.00195	71.1797	2.87053		91 90264	3 850889	0.048348	0.000663		0.072535	0.00233	0.010881	0.000458	0.922872	-0.0003428	19 1255	8.85E-05	1.015-05	
69.5382	50433	70,4944	1.85489	-0 35183	26585	0.00084	69.4801	2.56982		85 22064	3 315919	0.048802	0.00068		0.078958	0.002227	0.011734	0.000457	0.909737		8 972285		1 25E-05	
69,7651	04065	71,1024	2.28358	-0.693	38663.5	0.00118	69.6831	2.9197		92,17918	3.382834	0.048152	0.000778		0.072028	0.00187	0.010848	0.000396	0.879169	-7.7264E-05	3.745073	7.89E-05	9.02E-06	
75.2034	86343	77.1647	2.17656	-0.35119	18136.5	0.00175	75.0723	2 92105		90.63792	3.524394	0.048448	0.000718		0.0737	0.002107	0.011033	0.000429	0.902882	-8.4024E-05	4.328116	6.53E-05	6.72E-06	
69.5569	.44387	70.6199	1.8331	-0.15617	7569.92	0.00093	69.4922	2.53518		90.88392	3.297295	0.048408	0.000643		0.07344	0.00177	0.011003	0.000399	0.902821	-0.00015106	11.88484	6.66E-05	1.11E-05	
70.7332	74983	72.2044	2.06404	-0.12941	8748.37	0.00131	70.6413	2.74684		85.0223	3.460672	0.047805	0.000872		0.077528	0.002379	0.011762	0.000479	0.916173	-8.1178E-05	5.066229	3.79E-05	7.1E-06	
70.5428	43925	71.9587	1.73436	-0.30534	24023.7	0.00126	70.4546	2.55611		93.78686	3.579568	0.048194	0.000709		0.070852	0.001952	0.010662	0.000407	0.900422	-0.00012592	5.848421	8.84E-05	9.26E-06	
75.3779	07357	75.8161	2.32633	-0.12366	10240.3	0.0005	75.3406	3.0666		87.5176	3.24122	0.047879	0.000624		0.075431	0.001894	0.011426	0.000423	0.908406	-0.00020489	14.04389	4.83E-05	7.16E-06	
68.3709	61321	69.508	1.91454	-0.25452	11821.7	0.00099	68.3037	2.60695		85.1111	3.054634	0.049133	0.000729		0.079598	0.00194	0.011749	0.000422	0.887353		9.46894	2.92E-05	5.14E-08	
73.2408	59052	73 8399	1.85366	-0.41418	28388 3	0.00059	73.1979	2 71089		89.2424	3.321344	0.048337	0.00075		0.07468	0.00199	0.011205	0.000417	0.888758	-6.6575E-06	1.119027	6.95E-06	2.53E-06	
75.2997	1.4834	77.765	1,89496	-0.24398	19140	0.00217	75 1371	2.69667		91.38684	3.591902	0.048807	0.000605		0.073637	0.002068	0.010942	0.00043	0.922452		10.3008		1.64E-05	
71.8332	58215	73.1313	1.9487	-0.01346	2261.81	0.00117	71.7498	2.67032		00.00208	0.01003	0.010002	0.000827		0.071805	0.001849	0.010852	0.00038	n.en2422	Lo.ocosozoz	14.24744	A 225 04	1,125,05	
70,1567	78153	72 153	2.02578	-0.37151	20822.1	0.00176	70.0139	2.75264			-	-					1				-	-		
68:3019	31041	70.4.11	1.61651	0.4004.0	28800.3	0.00187	68.1.5	267			_						1							
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#### Fig. S8 description of software data processing results

#### **Other Notes:**

- 1. Input folder and output folder cannot be the same.
- 2. Only the original data is stored in the input folder, and there can be no other data files (such as CSV file of non-signal data), otherwise the program will report an error!
- 3. After processing one sample at a time, restart the program and replace with a new output folder directory.
- 4. Note that <sup>206</sup>Pb, <sup>207</sup>Pb<sup>, 208</sup>Pb, <sup>232</sup>Th and <sup>238</sup>U are required items, otherwise an error will be reported.
- 5. When selecting the "Agilent" instrument, it is required to select the list file
- 6. when loading data. the first column is the folder name, the second column is the sample name, and the name of the list file worksheet must be "Sheet1".

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