Link to website: <u>https://gitlab.com/SophieBenaroya/olivine-opx-spinel-geothermo-oxybarometer</u>

Instructions for using the olivine-orthopyroxene-spinel geothermo-oxybarometer:

1. Download the 'oos_input.xslx' file by clicking on the name, which will take you to the download link for the file. In this file, you will add the chemical data and calculation conditions (i.e. pressure, and temperature if you previously calculated it). DO NOT RENAME THIS FILE!

븢 😑 🔍 Search GitLab	Z			o ~ D 11 ~	· 🖸 🕫 - 🏈 -
Olivine-Opx-Spinel geoth		Sophie Reparava > Olivine-Onx-Spinel geothermo-ovybarometer			
Project information					
Repository		Olivine-Opx-Spinel geothermo-	oxybarometer ⊕	_ ~ ☆ Star 0 양 Fork 0	
D Issues 0		Project ID: 43594747 🚯			
11 Merge requests 0		-0- 35 Commits 🖇 1 Branch 🧷 0 Tags 🕞 195 KB Project S	Storage		
CI/CD				•	
Deployments		Opload New File		08454f7c [t	
Packages and registries		 Sophie Benaroya authored 1 day ago 			
Infrastructure		main ~ olivine-opx-spinel-geothermo-oxybarometer /	+ ~	Find file Web IDE V da V Clone V	
- Monitor					
🗠 Analytics		README Add LICENSE Add CHANGELOG	Add CONTRIBUTING Add Kubernetes cluster E Set u	CI/CD Add Wiki 🔯 Configure Integrations	
📮 Wiki		Name	Last commit	Last update	
X Snippets		🖝 Dockerfile	Replace Dockerfile	2 months ago	
🥴 Settings		OOS_Al-in-olivine.ipynb	Upload New File	1 day ago	
		OOS_Fe-Mg_spinel_olivine.ipynb	Upload New File	1 day ago	
		TH DEADME md	Update README.md	1 day ago	
	oos_input.xlsx	a oos_input.xlsx	Upload New File	1 day ago	
😝 😑 🔍 Search GitLab	Γ			• • • • •	· 🖻 @•• 🏈 •
Olivine-Opx-Spinel geoth		Sophie Benaroya >) Olivine-Opx-Spinel geothermo-oxybarometer			
Project information					
Repository		Upload New File		08454f7c [
Merce requests		 Sopnie Benaroya authored 1 day ago 			
CI/CD		main v olivine-opx-spinel-geothermo-oxybarometer / o	oos_input.xlsx	Find file Blame History Permalink	
Φ Security and Compliance					
@ Deployments		🔁 oos_input.xlsx 🎼 19.02 KiB		Open in Web IDE V Replace Delete	
Packages and registries					
lnfrastructure					
Monitor			*		
Analytics			Download (19.02 KiB)		
U Wiki					
Solutions					
Securitys					

In 'oos_input.xslx', you can label the rows (column B) however you wish. In columns C – L, add the oxide data for spinel (in weight %). In M - U, add data for orthopyroxene, and in V - AD, add data for olivine. All compositional cells (C - AD) require a value. If you do not have a value, for example, you did not measure P₂O₅ wt.% in olivine, put a 0 in that cell.

E	÷	و بر المراجع ال مراجع المراجع ال														æ															
Fil	-	Home In	sert Pag	e Layout	Formula	s Dat	a Revi	ew V	iew Ac	robat 🤇	? Tell me	what you	want to de																		
1°	жc	ut	Verdana		11 - A	=	= =	87 -	🔐 Wrap 1	iext	Genera	al				Norma	12	Normal	2 2	Normal		Bad	G	ood		÷	>	Σ	AutoSum	AT	Q
Past	- 1 <u>6</u> C	opy *	BIL	B.	- 8 -	A - ≡		•= •=	🗮 Merge	& Center 🔹		%,	10 .00	Conditional	I Format a	Neutra	d	Calculat	ion	Check Ce	:11]	Explanate	ory Ir	iput	* -	Insert	Delete Form	iat 🎍	Fill *	Sort &	Find &
	Clipbe	oard r	. –	Font		5		Aliana	tent		5	Number	5	Formatting	 lable * 				Style	es.							Cells		Ed	Filter * :	Select *
AEI		*	×	<i>f</i> × R€	sults																										
- 4	A	8		с	D	E	F	G	н	1	1	K	L	м	N	0	P	Q	R	s	т	U	v	w	x	Y	Z	AA	AB	AC	AD
1	Index	Lal	ol	sioz	TIO2	AI203	Cr203	SI FeO	MnO	MaQ	CaO	Fe203	V203	sinz	TIO2	A 203	Orti	nopyrox FeO	MnO	MaO	CaO	Na2O	sioz	TIO2	AI203	Cr203	Olivine	MnO	MaO	CaO	P205
3	1	COL		SIGE	nor	ALCOS	CILOS	100	THIO	ngo	cuo	TCLOD		SIGE	nor	ALCO	CILOS	100	Fillo	ngo	cuo	HULO	DIGT	nor	ALCO	CILOS	100		ngo	cuo	1205
4	2																														
5	3																														
6	4																														
7	5																														
8	6																														
9	7																														
10	8																														
12	10																														
13	11																														
14	12																														
15	13																														
16	14																														
17	15																														
18	16																														
19	17																														
20	18																														
21	19																														
28	21																														
24	22																														
25	23																														
26	24																														
27	25																														
28	26																														
29	27																														
30	28																														
31	29																														
32	30																														
34	82																														
35	33																														
36	34																														
37	35																														
38	36																														
39	37																														
40	38																														
41	39																														
92	40			1										1									1								

3. Add in calculation conditions. In cell AJ add the pressure (in bars) that the minerals formed at. Cell AK allows you to input a temperature (in kelvin) to use for the geobarometry calculations; if you do not have a previously determined temperature you would like to use, leave this blank, and the notebook will calculate a temperature for you.



4. Go back to GitLab and click the 'launch binder' tab near the bottom of the page, which will take you to the repository interface. Please note that it can take a few minutes for binder to launch the first time you use it on your device, so be patient!





^ ♡ 4× ENG 11:26

5. Once launched, you will be brought to the ENKI-server page. You will likely get an error saying 'Directory not found,' which you can dismiss. Then, hit the green button at the bottom of the screen called 'Close this screen' to be taken to JupyterLab.

ENKI Server
Kelone to the ENKI server More and the formation and resources to help you use the ENKI server effectively. You can always return here by clicking ENKI Information on the Commands palette or by clicking the ENKI Info Iauncher button. To the the project website, see ENKI and the ENKI server effectively. You can always return here by clicking ENKI Information on the Commands palette or by clicking the ENKI Info Iauncher button. To the the project website, see ENKI and the ENKI Information on the Commands palette or by clicking the ENKI Info Iauncher button. To ENKI server shull on top of a JuppterLab computing environment. If you have never used JuppterLab, please consult the excellent JuppterLab User Guide at Read The Dock. The Information project website, see accessible from the ENKI pleate (scable in the lefthand pane after you does the page). Experimentation Code responsion (FLNK) is located at Glidal (ENKI-point) Code responsion (FLNK) is located at Glidal (ENKI-point) Code responsion (FLNK) is pleated as a data store for accumulating memplating and queying plase equalibrium calculations (includes interfaces to Berman, Holland and Powell, Storude, MELTS: and DEXI Code responsion Code res
Copyright © ENKI-portaLorg Close this screen
ENKI Server
Welcome to the ENKI server This page contains some basic information and resources to help you use the ENKI server effectively. You can always return here by clicking ENKI Information on the Commands palette or by clicking the ENKI Info Isuncher button. To the project website, see ENKI Portal. Welcome to fuel yupertab computing environment. If you have never used Jupytertab, please consult the excellent Jupytertab User Guide at Read The Docs. To learn hor to use software provided on the server, view the video tutorials on the ENKI Portal You base this page. Dependencies Rependencies Dependencies Dependencies Description
Copyright 5 ENIS spotatorg Close this screen

= = 🧿 🚍 🔒 📴 🛤 🖬

∧ ∰ d× ENG 11:30

6. You are now in JupyterLab! The main screen in front of you is the 'Launcher'; this is where the notebook will appear. To the left of this, you will see a folder titled 'work'; open this folder. Open it. There will be five files in the folder; two of which are Jupyter notebook files ending in .ipynb. One file, titled "OOS Fe-Mg spinel olivine.ipynb" uses the olivine-spinel geothermometer from Jianping et al. (1995), while the file titled "OOS Al-in-olivine.ipynb" uses the Al-in-olivine geothermometer from Coogan et al. (2014) and Wan et al. (2008). Both notebooks use the same geobarometer, the olivine-orthopyroxene, spinel barometer from Sack and Ghiorso. Double-click on the file of interest.

Filter files by name	Ŧ	Ŷ
Napor Last Modified	Notebook	10
Mare: work 2 days ago Name: work Created: 2023-05-03 1129-23 Modified: 2023-05-03 1129-23 Modified: 2023-05-01 13:10-29	Pyton 3 (sylteme)	
	Sonsole	
*	Pyton 3 (sykeme)	
	Other	
	Sull Info LATEX Emitting Marideonn File Python File R File Storic Contextual Heigh	
Simple 💽 0 🛐 0 🏟 Mem: 95.79 / 2048.00 MB	へ 見 de BMG	5
		U
File Edit View Run Kernel Tabs Settings Help	4	°o
File Edit View Run Kernel Table Settings Help H D D C Ø Ø Ø Filter files by name Q Ø Ø Ø	+ work	°¢ ë
File Edit View Run Kernel Tabs Settings Help File Edit View Run Kernel Tabs Comparison Filter files by name Filter files by name Last Modified Dockerfie 2 days ago	* work Notebook	\$
File Edit View Run Kernel Tabs Settings Help Image: Setting Setti	work Image: Constraint of the second seco	°0
C File Edit View Run Kernel Tabs Settings Help C Ther files by name Q Filer files by name Q C There is a Modified C Dockerfile 2 days ago © OS_Alfin- C Dockerfile 2 days ago ♥ READMEEM 2 days ago	work R Notebook Image: Console Image: Console	\$
File Edit View Run Kernel Tabs Settings Help Image: Setting Se	work Notebook Projektivnik R Sonscle	°0
File Edit View Run Kernel Tabs Settings Help Image: Setting Se	work Notebook Privania R R R R R R R Privania R R	°0 8
Clauncher File Edit View Run Kernel Tabs Settings Help Clauncher Filter files by name Clauncher Filter files by name Clauncher	vork Notebook Providing Providing R R Providing R Providing R R R R R	\$
File Edit View Run Kernel Tabs Settings Help Image: Setting Se	w w Image: Concle	ŝ
File Edit View Run Kernel Tabs Settings Help Image: Setting Se	vok Image: Source of the so	°0 8
File Edit View Run Kernel Tabs Settings Help Image: Setting Se	vet	°0 8
File Edit View Run Kernel Table Settings Help Image: Comparison of the syname <	<section-header></section-header>	°0 8

へ に d× ENG 11:31 - 開4)

📲 🛱 🧿 🚍 😫 😰 🛤 📲

7. Before running the notebook, you must upload your version of oos_input.xslx to Jupyter Lab. To do this, go back to the left panel where you launched the notebook, and hit the third button from the left with the upwards-facing arrow symbol (if you hover over it, it will say 'Upload files'). You will get a pop-up asking if you want to overwrite the oos_input file that already exists; say yes.

0	File Edit View I	Run Kernel Tabs	Settings Help		
	+ b	± C	☑ Launcher	+	Ŷ¢
ENKI	Filter files by name	e Upicao riles		work	ø
	Name 🔺	Last Modified 2 days ago		Notebook	
	OOS_Al-in OOS_Fe+M	2 days ago 2 days ago			
	Cos_input.x	2 days ago 2 days ago		Python 3 R (pykeme)	
*				>. Console	
				Python 3 (cyskemet)	
				Other	
				Image: Second	
S	imple 🔵 🛛 🚦	0 🛞 Mem: 95.7	79 / 2048.00 MB		
-	ਸ 🧿 🛙	8 	Ai 🗾	> 200 年1000 - 2000	11:33 03/05/2023 🐴



8. Return to the notebook tab – it's time to run it! Don't worry about all the lines of code you see; you will not have to interact with them. To run the code, hit the play button in the tab at the top (it looks like an arrowhead). If you hover over the symbol, it will say, 'Run the selected cells and advance.'



9. Scroll to the bottom, and hit the 'Upload' button. Navigate to your oos_input.xslx file and select it. Hit continue.



10. The calculators are now running! A file called 'oos_output.xslx' will begin to generate. At the bottom of the screen, you will see a pane with information about your session. This includes the kernel used and the amount of memory used to run the calculations. If next to the 'Python3 (ipykernel)' it says 'Busy', then the calculations are running. Wait until it says 'Idle' before downloading the output file to ensure you will have all the results.



11. The output file will contain all the initial data you used and the results for each row in columns AE - AI. In column AE you will find the temperature (in Celsius) calculated by the olivine-spinel geothermometer. If you input your own temperature, the output will simply be the temperature (in Celsius) you listed. In columns AF – AI, you will find the

oxybarometer results. These include the absolute log fO_2 (in column AF), the fO_2 relative to the Quartz-Fayalite-Magnetite buffer as defined by Frost (1991), listed as 'd QFM' (in column AG), the fO_2 relative to the Iron-Wustite buffer as defined by Euster and Wones (1982), listed as 'd IW' (in column AH), and the fO_2 relative to the Nickle-Nickle-Oxide buffer as defined by Huebner and Sato (1970), listed as 'd NNO' (in column AI). The Fe-Mg partition coefficient value of olivine and pyroxene is shown in column AL.

⊟	E 5 - 6 - 5														- e ×												
File	Ho	me I	nsert	Page Layou	t Forr	nulas	Data I	Review	View	Acrobat	© ⊺ell i	me what yi	ou want to	do													Sign in 🔉 Share
	💑 Cut		Verda	na	- 10 -	A A	\equiv	- 87 -	📴 Wi	ap Text	Ger	neral		1 💽		🕑 N	ormal 2	No	ormal 2.2 Normal	8	ad	Good	- 3	÷ 1	🗙 👕 🛛 🗙 AutoSu	" * 🗛 🗩 .	
Paste	Cop	у т	8 3	n . Io								- 94 +	6.0 .00	Conditi	onal Form	nat as N	eutral	Ca	culation Check Ce		xplanatory	Input	- Is	nsert Dek	ete Format	Sort & Find &	
-	💖 Forn	nat Painte	r 🖬 -	<u>a</u> . .		· 📥 ·			- <u></u> m	age or cen		. 70 ,	.00 -0.0	Formatt	ing ∗ Tal	ole -					,,		Ŧ		🗸 🕐 Clear 🗸	Filter * Select *	
	Clipboar	d	G.	For	it	6		Alig	nment		rg.	Numbe	r n						Styles					Cel	ls	Editing	^
AN1		¥ 1	× v	fx																			_	-		-	~
-	M	N	0		0	P	e	T 1		N I	w	×	v I	7	44	AB	40	40		AF	46		41				
1				Orthe	pyrox	ene						~		Olivine	~		~	~	~	Resul	ts		~		~ ^		
2	5iO2	TiO2	AI203	Cr203	FeO	MnO	MgO	CaO	Na2O	SiO2	TiO2	AI203	Cr203	FeO	MnO	MgO	CaO	P205	Temperature Celcius	log fO2	d QFM	d IW d NNO	P bars)	T (ke	in) KD Ol-Pyx		
4	50.55	0.36	3.72	0.31	18.88	0.56	22.65	1.39	0.04	35.27	0.02	0.05	0.26	32,828	0.68	27.995	0.17	0.0	1019.0183	-13.223	-3.7629	0.45957 -4.02139	0000		1.40636083		
5	50.55	0.36	3.72	0.31	18.88	0.56	22.65	1.39	0.04	35.72	0.02	0.05	0.26	33.458	0.68	28.984	0.17	0.0	1039.96774	-13.438	-3.8988	0.29089 -4.1631	.0000		1.38441763		
6	50.55	0.36	3.72	0.31	18.88	0.56	22.65	1.39	0.04	35.27	0.03	0.12	0.16	32.828	0.64	27.995	0.29	0.0	1015.60393	-13.709	-3.8241	0.40386 -4.08159	0000		1.40636083		
7	52.76	0.32	1.10	0.43	18.34	0.60	20.97	4.83	0.11	36.22	0.03	0.01	0.01	33.320	0.68	29.430	0.16	0.0	1009.76699	-12.698	-2.7282	1.5091 -2.98406	0000		1.29424933		
9	51.89	0.38	1.15	0.40	17.94	0.63	20.46	5.79	0.15	36.26	0.04	0.02	0.00	32.417	0.65	29.406	0.15	0.0	1275.48410	-10.933	-3.7324	0.14939 -4.05154	0000		1.25739283		
10	51.90	0.38	1.28	0.46	17.68	0.62	19.95	6.48	0.15	36.12	0.04	0.12	0.06	32.291	0.64	29.281	0.21	0.0	1286.58959	-9.6928	-3.0429	0.82666 -3.36422	0000		1.24492648		
11	52.77	0.29	0.93	0.28	18.30	0.65	20.84	4.77	0.10	36.38	0.01	0.03	0.01	29.589	0.62	32.513	0.14	0.0	1216.63509	-10.274	-2.9015	1.04813 -3.20853	0000		1.03634707		
12	52.31	0.35	1.86	1.22	10.35	0.40	17.07	16.29	0.23	36.38	0.01	0.03	0.01	29.589	0.62	32.513	0.14	0.0	1222.95337	-10.544	-3.2399	0.70219 -3.54828	0000		1.5010634		
14	51.38	0.27	1.59	0.66	11.16	0.44	16.99	15.47	0.20	35.86	0.05	0.02	0.30	32.500	0.64	29.550	0.13	0.0	924.188340	-13.334	-2.0278	2.3577 -2.25719	0000		1.67339989		
15	51.43	0.31	1.59	0.75	11.60	0.45	17.55	14.69	0.19	35.97	0.08	0.03	0.63	31.675	0.62	30.244	0.19	0.0	900.024286	-13.706	-1.9867	2.44446 -2.20802	0000		1.5849452		
16	52.43	0.25	0.84	0.47	18.71	0.62	21.57	4.33	0.09	35.98	0.03	0.01	0.06	32.914	0.67	29.572	0.15	0.0	935.276445	-13.447	-2.3241	2.04095 -2.5572	0000		1.28326169		
17	52.83	0.23	0.73	0.29	18.91	0.65	21.26	4.19	0.10	35.95	0.01	0.05	0.04	33.067	0.65	28.705	0.21	0.0	957.531379	-13.139	-2.3757	1.9496 -2.61584	0000		1.2947977		
19	52.50	0.25	1.27	0.42	17.17	0.59	20.93	6.19	0.09	35.89	0.04	0.11	0.31	32.532	0.66	29.156	0.15	0.0	1122.10062	-10.723	-2.259	1.81152 -2.54451	0000		1.36033453		
20	52.85	0.32	0.79	0.41	18.85	0.67	21.07	4.94	0.09	35.89	0.02	0.03	0.11	32.990	0.62	29.089	0.19	0.0	1133.78363	-10.408	-2.0869	1.9678 -2.37523	0000		1.26763944		
21	52.50	0.25	1.27	0.42	17.17	0.59	20.93	6.19	0.09	35.89	0.04	0.11	0.31	32.532	0.66	29.156	0.15	0.0	1126.10742	-10.759	-2.3446	1.72039 -2.63116	.0000		1.36033453		
22	51.98	0.29	0.60	0.22	19.14	0.67	20.88	4.03	0.07	35.61	0.04	0.11	0.01	33.662	0.67	28.012	0.24	0.0	986.970967	-12.57	-2.2623	2.01252 -2.51145	0000		1.31074487		
24	52.35	0.49	0.65	0.24	18.64	0.64	20.31	5.44	0.12	36.05	0.01	0.02	0.00	33,800	0.70	28.917	0.24	0.0	969.071955	-12.647	-2.0642	2.24105 -2.30791	0000		1.27293354		
25	51.83	0.39	0.54	0.17	19.42	0.66	20.92	4.48	0.06	36.00	0.05	0.04	0.07	33.529	0.63	29.018	0.19	0.0	985.312806	-12.522	-2.1892	2.08842 -2.43783	.0000		1.24503182		
26	51.98	0.29	0.60	0.22	19.14	0.67	20.88	4.03	0.07	35.61	0.04	0.11	0.01	33.662	0.67	28.012	0.24	0.0	1000.27567	-12.436	-2.3273	1.92546 -2.58039	0000		1.31074487		
27	51.92	0.47	0.60	0.21	19.39	0.66	20.64	4.33	0.10	35.99	0.01	0.02	0.00	34.134	0.66	28.599	0.19	0.0	966.898494	-12.723	-2.1071	2.2019 -2.35014	0000		1.27070946		
28	52.35	0.49	0.65	0.24	18.64	0.64	20.31	5.44	0.12	36.00	0.01	0.08	0.01	33.800	0.70	20.917	0.24	0.0	951.152495	-12.891	-2.0258	2.51072 -2.26598	0000		1.2/293354		
30	52.63	0.35	0.72	0.23	18.88	0.63	20.82	4.48	0.00	35.86	0.03	0.10	0.03	33.323	0.63	28.515	0.19	0.0	834.960018	-14.615	-1.6946	2.86962 -1.89221	0000		1.28913406		
31	51.80	0.31	0.54	0.20	19.35	0.63	20.92	3.88	0.08	35.86	0.04	0.10	0.03	33.323	0.67	28.515	0.20	0.0	830.18264	-14.728	-1.7137	2.86095 -1.90943	0000		1.26314958		
32	51.98	0.29	0.60	0.22	19.14	0.67	20.88	4.03	0.07	35.86	0.04	0.10	0.03	33.323	0.67	28.515	0.20	0.0	829.790547	-14.785	-1.7636	2.81187 -1.95921	0000		1.27465087		
33	51.80	0.31	0.54	0.20	19.35	0.63	20.92	3.88	0.08	35.86	0.04	0.10	0.03	33.323	0.67	28.515	0.20	0.0	827.132301	-14.818	-1.7437	2.83766 -1.93821	0000		1.26314958		
35	52.38	0.29	0.60	0.22	18.84	0.67	20.88	4.03	0.07	35,80	0.04	0.10	0.03	33,262	0.67	28.934	0.20	0.0	866 10423	-13 778	-1.0885	3.04898 -1.65895	0000		1.27405087		
36	52.16	0.50	0.56	0.21	19.68	0.71	20.64	4.43	0.09	35.99	0.03	0.08	0.01	33.656	0.69	28.658	0.16	0.0	874.532350	-13.641	-1.4677	3.01385 -1.68	0000		1.23187479		
37	52.79	0.29	0.67	0.30	19.06	0.63	21.18	4.29	0.09	36.12	0.05	0.05	0.13	33.564	0.68	28.731	0.15	0.0	824.006465	-14.921	-1.7843	2.80388 -1.97764	0000		1.29773252		
38	51.98	0.32	0.82	0.33	18.68	0.64	20.12	5.11	0.12	36.19	0.04	0.03	0.04	33.73	0.68	29.13	0.14	0.0	1004.17506	-11.941	-1.8893	2.35713 -2.14348	.0000		1.24719812		
40																											
41																							1				
42																											
43			_																1								
		Shee	t1	÷																							Þ
Ready																											+ 90%
-	Ħ	0		8	23	Ai 🛛		1																		^묘ᡧ	14:31 03/05/2023 😼