Calculate_fO2

June 29, 2022

1 Calculate the fO_2 of a metal-silicate system from compositional data

For experiments that produced coexisting metallic alloy and silicate melt, the experimental fO_2 is calculated below using both Fe-FeO and Si-SiO_2 equilibrium:

$$FeO_{silicate-melt} = Fe_{metal} + \frac{1}{2}O_2$$
$$SiO_{2_{silicate-melt}} = Si_{metal} + O_2$$

where the fO_2 of the experiment can be expressed relative to the fO_2 of the iron-wüstite (IW) buffer or Si-SiO_2 buffer, respectively, as:

$$2log(\alpha_{FeO}/\alpha_{Fe}) = 2log(X_{FeO} \cdot \gamma_{FeO}/X_{Fe} \cdot \gamma_{Fe}) = \Delta IW$$
$$2log(\alpha_{SiO_2}/\alpha_{Si}) = 2log(X_{SiO_2} \cdot \gamma_{SiO_2}/X_{Si} \cdot \gamma_{Si}) = \Delta SiSiO_2$$

where α, X, and γ are the activity, mole fraction, and fugacity coefficient, respectively, of the subscripted component in the silicate melt or metal. "Δ" indicates the number of log units above or below the listed buffer. Experimental fO_2s are calculated using a non-ideal solution model for both metallic and silicate liquid. For each experiment, the activity coefficient for FeO in the silicate, γFeO, is calculated with a parameterization based on Holzheid et al. (1997), where γFeO is taken as a fixed value in the range 1.7–3 dependent only upon MgO content of the silicate melt: where MgO 20 wt%, γFeO is set equal to 1.7; where MgO is >20 wt%, γFeO is calculated as:

$$\gamma_{FeO} = 1.7 + 0.1(MgO_{silicate,wt\%} - 20)$$

with a maximum allowable γFeO value of 3.0. The activity of SiO_2 in the silicate melt is calculated using MELTS in the ENKI python framework (v. 1.1.0). The activity coefficients for Fe and Si in Fe-rich metal, γFe and γSi, are calculated using the ε-approach (Wagner, 1952; Ma, 2001), which considers non-ideal interactions between components within the metal alloy.

1.1 1. Import necessary python libraries

[1]:
```
import fO2calculate as fc # code written for this work
from thermoengine import equilibrate # ENKI MELTS
```

```
/opt/anaconda3/lib/python3.9/site-packages/numdifftools/multicomplex.py:35:
DeprecationWarning: `finfo.machar` is deprecated (NumPy 1.22)
  _TINY = np.finfo(float).machar.tiny
```

1.2 2. Read in your data file

You can create a single sample object or import an entire spreadsheet (xlsx or csv) with multiple samples. Here we import a spreadsheet containing data from this manuscript.

The BatchFile must have compositional information on each sample in rows. By default, the column used as the index column (corresponding to the name of each sample) is titled "Label". If no "Label" column is found, fo2calculate will choose the first column not containing compositional information as the index column. If an xlsx file is imported, the user can specify which sheet to import by passing the **sheet_name** argument. If no sheet name is given, fo2calculate will import the first sheet in the file.

Both silicate melt and metal compositions should be given together for each sample. Columns titled as oxides (e.g., "SiO2") are identified automatically as belonging to the silicate melt composition. Columns titled as elements (e.g., "Si") are identified as belonging to the metal composition. Note that subscripts, spaces, special characters, or other text such as units should not be used in column titles. Extra information about a sample, for example the temperature to use for calculations, can be given here if desired and have no requirements for how they are named. Any columns not used as the index column or as compositional information will be imported but not used by fO2calculate.

[2]:
```
myfile = fc.BatchFile('MercurySmelting_Data/Compositions_for_Python.xlsx',␣
↪sheet_name='All')
```

Next, we display the contents of the BatchFile to ensure they were imported properly.

[3]:
```
myfile.get_data()
```

```
/opt/anaconda3/lib/python3.9/site-packages/fO2calculate/sample_class.py:75:
UserWarning: Element S was passed as part of sample composition. This will be
assumed to be part of the metal composition.
  w.warn("Element " + str(vol) + " was passed as part of sample composition.
This" +
```

[3]:

	Al2O3	CaO	Cr	Cr2O3	Fe	FeO	K2O	MgO	\
Sample A (1)	24.37	4.75	3.251301	0.12	84.633854	0.18	0.00	16.86	
Sample A (2)	24.37	4.75	3.310400	0.12	84.594675	0.18	0.00	16.86	
Sample A (3)	24.37	4.75	3.407496	0.12	84.606133	0.18	0.00	16.86	
Sample A (4)	24.37	4.75	3.729910	0.12	81.714343	0.18	0.00	16.86	
Sample A (5)	24.37	4.75	1.964736	0.12	85.239295	0.18	0.00	16.86	
Sample A (6)	24.37	4.75	2.008275	0.12	85.074175	0.18	0.00	16.86	
Sample A (7)	24.37	4.75	2.332421	0.12	84.301795	0.18	0.00	16.86	
Sample A (8)	24.37	4.75	2.457943	0.12	84.748665	0.18	0.00	16.86	
Sample A (9)	24.37	4.75	1.184930	0.12	89.457160	0.18	0.00	16.86	
Sample A (10)	24.37	4.75	4.852541	0.12	87.680402	0.18	0.00	16.86	
Sample B (1)	17.11	5.92	2.081007	0.06	84.752817	0.19	0.00	12.64	

Sample B (2)	17.11	5.92	2.087576	0.06	84.714868	0.19	0.00	12.64
Sample B (3)	17.11	5.92	2.060495	0.06	84.754365	0.19	0.00	12.64
Sample B (4)	17.11	5.92	2.473356	0.06	85.732958	0.19	0.00	12.64
Sample B (5)	17.11	5.92	1.908705	0.06	86.124015	0.19	0.00	12.64
Sample B (6)	17.11	5.92	1.970343	0.06	86.055251	0.19	0.00	12.64
Sample B (7)	17.11	5.92	2.123377	0.06	84.673443	0.19	0.00	12.64
Sample B (8)	17.11	5.92	1.922690	0.06	84.749346	0.19	0.00	12.64
Sample B (9)	17.11	5.92	2.104097	0.06	84.415584	0.19	0.00	12.64
Sample C (1)	22.50	9.74	1.922119	0.04	84.981576	0.19	0.00	12.36
Sample C (2)	22.50	9.74	1.845537	0.04	86.469408	0.19	0.00	12.36
Sample C (3)	22.50	9.74	1.666332	0.04	86.589038	0.19	0.00	12.36
Sample C (4)	22.50	9.74	1.677718	0.04	86.678722	0.19	0.00	12.36
Sample C (5)	22.50	9.74	3.609384	0.04	86.294365	0.19	0.00	12.36
Sample C (6)	22.50	9.74	1.507437	0.04	91.294799	0.19	0.00	12.36
Sample C (7)	22.50	9.74	2.319852	0.04	90.166290	0.19	0.00	12.36
Sample C (8)	22.50	9.74	1.547005	0.04	91.461722	0.19	0.00	12.36
Sample C (9)	22.50	9.74	2.003189	0.04	90.900937	0.19	0.00	12.36
Sample C (10)	22.50	9.74	1.363272	0.04	89.605052	0.19	0.00	12.36
Sample C (11)	22.50	9.74	1.286432	0.04	89.758794	0.19	0.00	12.36
Sample D (1)	16.94	8.38	1.169355	0.47	87.278226	2.57	0.00	7.87
Sample D (2)	16.94	8.38	0.379565	0.47	89.926139	2.57	0.00	7.87
Sample D (3)	16.94	8.38	6.405586	0.47	74.580045	2.57	0.00	7.87
Sample D (4)	16.94	8.38	9.333607	0.47	65.869186	2.57	0.00	7.87
Sample D (5)	16.94	8.38	8.559014	0.47	76.465238	2.57	0.00	7.87
Sample D (6)	16.94	8.38	1.191810	0.47	90.934094	2.57	0.00	7.87
Sample D (7)	16.94	8.38	1.492843	0.47	91.441718	2.57	0.00	7.87
Sample D (8)	16.94	8.38	1.532176	0.47	91.767109	2.57	0.00	7.87
Sample D (9)	16.94	8.38	0.566426	0.47	97.909372	2.57	0.00	7.87
Sample D (10)	16.94	8.38	0.227767	0.47	98.809401	2.57	0.00	7.87
Sample N (1)	19.37	7.57	0.636557	0.60	90.845711	1.81	0.02	10.06
Sample N (2)	19.37	7.57	0.581277	0.60	90.628187	1.81	0.02	10.06
Sample N (3)	19.37	7.57	0.712323	0.60	90.882263	1.81	0.02	10.06
Sample N (4)	19.37	7.57	1.012397	0.60	91.301653	1.81	0.02	10.06
Sample N (5)	19.37	7.57	1.131571	0.60	91.101739	1.81	0.02	10.06
Sample N (6)	19.37	7.57	1.085720	0.60	91.262537	1.81	0.02	10.06
Sample N (7)	19.37	7.57	0.893591	0.60	90.591619	1.81	0.02	10.06
Sample N (8)	19.37	7.57	1.429163	0.60	96.447804	1.81	0.02	10.06
Sample N (9)	19.37	7.57	1.892089	0.60	96.153446	1.81	0.02	10.06
Sample N (10)	19.37	7.57	1.623075	0.60	96.423033	1.81	0.02	10.06
Sample O (1)	18.12	7.35	1.051248	0.54	87.152532	0.95	0.13	8.12
Sample O (2)	18.12	7.35	0.264308	0.54	88.543255	0.95	0.13	8.12
Sample O (3)	18.12	7.35	0.237505	0.54	89.343247	0.95	0.13	8.12
Sample O (4)	18.12	7.35	1.073327	0.54	93.640285	0.95	0.13	8.12
Sample O (5)	18.12	7.35	0.651532	0.54	87.529268	0.95	0.13	8.12
Sample O (6)	18.12	7.35	0.475998	0.54	98.339072	0.95	0.13	8.12
Sample O (7)	18.12	7.35	0.279706	0.54	99.419869	0.95	0.13	8.12
Sample O (8)	18.12	7.35	0.150572	0.54	99.387673	0.95	0.13	8.12

Sample O (9)	18.12	7.35	0.262732	0.54	99.130962	0.95	0.13	8.12

	MnO	Na2O	P	S	Si	SiO2	Ti	\
Sample A (1)	0.00	0.00	0.190076	0.000000	11.934774	51.11	0.000000	
Sample A (2)	0.00	0.00	0.169508	0.000000	11.855619	51.11	0.069798	
Sample A (3)	0.00	0.00	0.100220	0.000000	11.896172	51.11	0.000000	
Sample A (4)	0.00	0.00	0.363894	0.000000	14.100879	51.11	0.090973	
Sample A (5)	0.00	0.00	0.000000	0.000000	12.654912	51.11	0.141058	
Sample A (6)	0.00	0.00	0.000000	0.000000	12.776264	51.11	0.141286	
Sample A (7)	0.00	0.00	0.081128	0.000000	13.142683	51.11	0.131832	
Sample A (8)	0.00	0.00	0.060441	0.000000	12.581847	51.11	0.151103	
Sample A (9)	0.00	0.00	0.151914	0.000000	9.094592	51.11	0.121531	
Sample A (10)	0.00	0.00	0.167329	0.000000	7.069651	51.11	0.219619	
Sample B (1)	0.12	0.00	0.101513	0.000000	12.973302	63.71	0.091361	
Sample B (2)	0.12	0.00	0.122200	0.000000	12.912424	63.71	0.173116	
Sample B (3)	0.12	0.00	0.121803	0.000000	12.961835	63.71	0.101502	
Sample B (4)	0.12	0.00	0.160869	0.030163	11.381460	63.71	0.211140	
Sample B (5)	0.12	0.00	0.121188	0.000000	11.684508	63.71	0.161584	
Sample B (6)	0.12	0.00	0.253910	0.000000	11.588462	63.71	0.132033	
Sample B (7)	0.12	0.00	0.181141	0.000000	12.740264	63.71	0.281775	
Sample B (8)	0.12	0.00	0.211395	0.000000	12.905174	63.71	0.211395	
Sample B (9)	0.12	0.00	0.302024	0.000000	13.007148	63.71	0.181214	
Sample C (1)	0.00	0.00	0.288816	0.000000	12.707898	54.99	0.099592	
Sample C (2)	0.00	0.00	0.150451	0.000000	11.384152	54.99	0.150451	
Sample C (3)	0.00	0.00	0.130496	0.000000	11.453523	54.99	0.150572	
Sample C (4)	0.00	0.00	0.150693	0.000000	11.352220	54.99	0.140647	
Sample C (5)	0.00	0.00	0.340886	0.000000	9.755364	54.99	0.000000	
Sample C (6)	0.00	0.00	0.499151	0.000000	6.588799	54.99	0.109813	
Sample C (7)	0.00	0.00	0.667214	0.041059	6.682406	54.99	0.112913	
Sample C (8)	0.00	0.00	0.416501	0.000000	6.564855	54.99	0.000000	
Sample C (9)	0.00	0.00	0.448475	0.000000	6.557704	54.99	0.079729	
Sample C (10)	0.00	0.00	0.370890	0.000000	8.660786	54.99	0.000000	
Sample C (11)	0.00	0.00	0.331658	0.000000	8.613065	54.99	0.000000	
Sample D (1)	0.82	0.00	0.201613	0.000000	11.350806	61.28	0.000000	
Sample D (2)	0.82	0.00	0.348789	0.000000	9.345507	61.28	0.000000	
Sample D (3)	0.82	0.00	0.374418	0.000000	18.528638	61.28	0.121433	
Sample D (4)	0.82	0.00	0.123216	0.000000	23.452100	61.28	1.211623	
Sample D (5)	0.82	0.00	0.040420	0.000000	14.834276	61.28	0.090946	
Sample D (6)	0.82	0.00	0.499134	0.000000	7.303657	61.28	0.071305	
Sample D (7)	0.82	0.00	0.449898	0.000000	6.615542	61.28	0.000000	
Sample D (8)	0.82	0.00	0.623085	0.000000	6.016343	61.28	0.061287	
Sample D (9)	0.82	0.00	0.679712	0.041195	0.731205	61.28	0.061792	
Sample D (10)	0.82	0.00	0.693654	0.000000	0.207061	61.28	0.062118	
Sample N (1)	0.31	0.16	0.555724	0.000000	7.972113	58.57	0.000000	
Sample N (2)	0.31	0.16	0.550683	0.000000	8.158270	58.57	0.071385	
Sample N (3)	0.31	0.16	0.478274	0.000000	7.855907	58.57	0.081408	
Sample N (4)	0.31	0.16	0.475207	0.000000	7.210744	58.57	0.000000	

Sample N (5)	0.31	0.16	0.452628	0.000000	7.303775	58.57	0.000000
Sample N (6)	0.31	0.16	0.475649	0.000000	7.186434	58.57	0.000000
Sample N (7)	0.31	0.16	0.523829	0.000000	7.990961	58.57	0.000000
Sample N (8)	0.31	0.16	0.403894	0.000000	1.719138	58.57	0.000000
Sample N (9)	0.31	0.16	0.374259	0.000000	1.517829	58.57	0.062377
Sample N (10)	0.31	0.16	0.310142	0.000000	1.643751	58.57	0.000000
Sample O (1)	0.55	0.66	0.283028	0.000000	11.452542	62.19	0.060649
Sample O (2)	0.55	0.66	0.274474	0.000000	10.846803	62.19	0.071160
Sample O (3)	0.55	0.66	0.413052	0.000000	10.006196	62.19	0.000000
Sample O (4)	0.55	0.66	0.230715	0.000000	5.065704	62.19	0.000000
Sample O (5)	0.55	0.66	0.274865	0.000000	11.473073	62.19	0.071261
Sample O (6)	0.55	0.66	0.060766	0.921612	0.111404	62.19	0.091148
Sample O (7)	0.55	0.66	0.134673	0.000000	0.165752	62.19	0.000000
Sample O (8)	0.55	0.66	0.381450	0.000000	0.080305	62.19	0.000000
Sample O (9)	0.55	0.66	0.383994	0.000000	0.111156	62.19	0.111156

	TiO2	Temp_C	Total WT%	Which metal?	Si-poor/Si-rich
Sample A (1)	2.59	1340.0	99.96		0.0
Sample A (2)	2.59	1340.0	100.29		0.0
Sample A (3)	2.59	1340.0	99.78		0.0
Sample A (4)	2.59	1340.0	98.93		0.0
Sample A (5)	2.59	1340.0	99.25		0.0
Sample A (6)	2.59	1340.0	99.09		0.0
Sample A (7)	2.59	1340.0	98.61		0.0
Sample A (8)	2.59	1340.0	99.27		0.0
Sample A (9)	2.59	1340.0	98.74		0.0
Sample A (10)	2.59	1340.0	95.62		0.0
Sample B (1)	0.24	1290.0	98.51		0.0
Sample B (2)	0.24	1290.0	98.20		0.0
Sample B (3)	0.24	1290.0	98.52		0.0
Sample B (4)	0.24	1290.0	99.46		0.0
Sample B (5)	0.24	1290.0	99.02		0.0
Sample B (6)	0.24	1290.0	98.46		0.0
Sample B (7)	0.24	1290.0	99.37		0.0
Sample B (8)	0.24	1290.0	99.34		0.0
Sample B (9)	0.24	1290.0	99.33		0.0
Sample C (1)	0.20	1245.0	100.41		0.0
Sample C (2)	0.20	1245.0	99.70		0.0
Sample C (3)	0.20	1245.0	99.62		0.0
Sample C (4)	0.20	1245.0	99.54		0.0
Sample C (5)	0.20	1245.0	99.74		0.0
Sample C (6)	0.20	1245.0	100.17		0.0
Sample C (7)	0.20	1245.0	97.42		0.0
Sample C (8)	0.20	1245.0	100.84		0.0
Sample C (9)	0.20	1245.0	100.34		0.0
Sample C (10)	0.20	1245.0	99.76		0.0
Sample C (11)	0.20	1245.0	99.50		0.0

```
Sample D (1)   1.68  1200.0      99.20                      0.0
Sample D (2)   1.68  1200.0      97.48                      0.0
Sample D (3)   1.68  1200.0      98.82                      0.0
Sample D (4)   1.68  1200.0      97.39                      0.0
Sample D (5)   1.68  1200.0      98.96                      0.0
Sample D (6)   1.68  1200.0      98.17                      0.0
Sample D (7)   1.68  1200.0      97.80                      0.0
Sample D (8)   1.68  1200.0      97.90                      0.0
Sample D (9)   1.68  1200.0      97.10                      0.0
Sample D (10)  1.68  1200.0      96.59                      0.0
Sample N (1)   1.49  1245.0      98.97                      0.0
Sample N (2)   1.49  1245.0      98.06                      0.0
Sample N (3)   1.49  1245.0      98.27                      0.0
Sample N (4)   1.49  1245.0      96.80                      0.0
Sample N (5)   1.49  1245.0      97.21                      0.0
Sample N (6)   1.49  1245.0      96.71                      0.0
Sample N (7)   1.49  1245.0      97.36                      0.0
Sample N (8)   1.49  1245.0      96.56                      0.0
Sample N (9)   1.49  1245.0      96.19                      0.0
Sample N (10)  1.49  1245.0      96.73                      0.0
Sample O (1)   1.32  1200.0      98.93                      0.0
Sample O (2)   1.32  1200.0      98.37                      0.0
Sample O (3)   1.32  1200.0      96.84                      0.0
Sample O (4)   1.32  1200.0      99.69                      0.0
Sample O (5)   1.32  1200.0      98.23                      0.0
Sample O (6)   1.32  1200.0      98.74                      0.0
Sample O (7)   1.32  1200.0      96.53                      0.0
Sample O (8)   1.32  1200.0      99.62                      0.0
Sample O (9)   1.32  1200.0      98.96                      0.0
```

1.3 3. Calculate the fO_2 in terms of the iron-wüstite buffer

Here we calculate the ΔIW values for all measurements and display the results.

[4]:
```
dIWs = myfile.calculate_dIW(temperature='Temp_C', pressure=1)
dIWs
```

```
[                    ] 2%  Working on sample Sample A (1)
/opt/anaconda3/lib/python3.9/site-packages/fO2calculate/sample_class.py:75:
UserWarning: Element S was passed as part of sample composition. This will be
assumed to be part of the metal composition.
  w.warn("Element " + str(vol) + " was passed as part of sample composition.
This" +
/opt/anaconda3/lib/python3.9/site-packages/fO2calculate/sample_class.py:75:
UserWarning: Element Cl was passed as part of sample composition. This will be
assumed to be part of the metal composition.
  w.warn("Element " + str(vol) + " was passed as part of sample composition.
```

```
This" +
/opt/anaconda3/lib/python3.9/site-packages/fO2calculate/sample_class.py:75:
UserWarning: Element F was passed as part of sample composition. This will be
assumed to be part of the metal composition.
  w.warn("Element " + str(vol) + " was passed as part of sample composition.
This" +

[====================] 100%  Working on sample Sample O (9)
```

[4]:

	Al2O3	CaO	Cr	Cr2O3	Fe	FeO	K2O	MgO	\
Sample A (1)	24.37	4.75	3.251301	0.12	84.633854	0.18	0.00	16.86	
Sample A (2)	24.37	4.75	3.310400	0.12	84.594675	0.18	0.00	16.86	
Sample A (3)	24.37	4.75	3.407496	0.12	84.606133	0.18	0.00	16.86	
Sample A (4)	24.37	4.75	3.729910	0.12	81.714343	0.18	0.00	16.86	
Sample A (5)	24.37	4.75	1.964736	0.12	85.239295	0.18	0.00	16.86	
Sample A (6)	24.37	4.75	2.008275	0.12	85.074175	0.18	0.00	16.86	
Sample A (7)	24.37	4.75	2.332421	0.12	84.301795	0.18	0.00	16.86	
Sample A (8)	24.37	4.75	2.457943	0.12	84.748665	0.18	0.00	16.86	
Sample A (9)	24.37	4.75	1.184930	0.12	89.457160	0.18	0.00	16.86	
Sample A (10)	24.37	4.75	4.852541	0.12	87.680402	0.18	0.00	16.86	
Sample B (1)	17.11	5.92	2.081007	0.06	84.752817	0.19	0.00	12.64	
Sample B (2)	17.11	5.92	2.087576	0.06	84.714868	0.19	0.00	12.64	
Sample B (3)	17.11	5.92	2.060495	0.06	84.754365	0.19	0.00	12.64	
Sample B (4)	17.11	5.92	2.473356	0.06	85.732958	0.19	0.00	12.64	
Sample B (5)	17.11	5.92	1.908705	0.06	86.124015	0.19	0.00	12.64	
Sample B (6)	17.11	5.92	1.970343	0.06	86.055251	0.19	0.00	12.64	
Sample B (7)	17.11	5.92	2.123377	0.06	84.673443	0.19	0.00	12.64	
Sample B (8)	17.11	5.92	1.922690	0.06	84.749346	0.19	0.00	12.64	
Sample B (9)	17.11	5.92	2.104097	0.06	84.415584	0.19	0.00	12.64	
Sample C (1)	22.50	9.74	1.922119	0.04	84.981576	0.19	0.00	12.36	
Sample C (2)	22.50	9.74	1.845537	0.04	86.469408	0.19	0.00	12.36	
Sample C (3)	22.50	9.74	1.666332	0.04	86.589038	0.19	0.00	12.36	
Sample C (4)	22.50	9.74	1.677718	0.04	86.678722	0.19	0.00	12.36	
Sample C (5)	22.50	9.74	3.609384	0.04	86.294365	0.19	0.00	12.36	
Sample C (6)	22.50	9.74	1.507437	0.04	91.294799	0.19	0.00	12.36	
Sample C (7)	22.50	9.74	2.319852	0.04	90.166290	0.19	0.00	12.36	
Sample C (8)	22.50	9.74	1.547005	0.04	91.461722	0.19	0.00	12.36	
Sample C (9)	22.50	9.74	2.003189	0.04	90.900937	0.19	0.00	12.36	
Sample C (10)	22.50	9.74	1.363272	0.04	89.605052	0.19	0.00	12.36	
Sample C (11)	22.50	9.74	1.286432	0.04	89.758794	0.19	0.00	12.36	
Sample D (1)	16.94	8.38	1.169355	0.47	87.278226	2.57	0.00	7.87	
Sample D (2)	16.94	8.38	0.379565	0.47	89.926139	2.57	0.00	7.87	
Sample D (3)	16.94	8.38	6.405586	0.47	74.580045	2.57	0.00	7.87	
Sample D (4)	16.94	8.38	9.333607	0.47	65.869186	2.57	0.00	7.87	
Sample D (5)	16.94	8.38	8.559014	0.47	76.465238	2.57	0.00	7.87	
Sample D (6)	16.94	8.38	1.191810	0.47	90.934094	2.57	0.00	7.87	
Sample D (7)	16.94	8.38	1.492843	0.47	91.441718	2.57	0.00	7.87	
Sample D (8)	16.94	8.38	1.532176	0.47	91.767109	2.57	0.00	7.87	

Sample D (9)	16.94	8.38	0.566426	0.47	97.909372	2.57	0.00	7.87
Sample D (10)	16.94	8.38	0.227767	0.47	98.809401	2.57	0.00	7.87
Sample N (1)	19.37	7.57	0.636557	0.60	90.845711	1.81	0.02	10.06
Sample N (2)	19.37	7.57	0.581277	0.60	90.628187	1.81	0.02	10.06
Sample N (3)	19.37	7.57	0.712323	0.60	90.882263	1.81	0.02	10.06
Sample N (4)	19.37	7.57	1.012397	0.60	91.301653	1.81	0.02	10.06
Sample N (5)	19.37	7.57	1.131571	0.60	91.101739	1.81	0.02	10.06
Sample N (6)	19.37	7.57	1.085720	0.60	91.262537	1.81	0.02	10.06
Sample N (7)	19.37	7.57	0.893591	0.60	90.591619	1.81	0.02	10.06
Sample N (8)	19.37	7.57	1.429163	0.60	96.447804	1.81	0.02	10.06
Sample N (9)	19.37	7.57	1.892089	0.60	96.153446	1.81	0.02	10.06
Sample N (10)	19.37	7.57	1.623075	0.60	96.423033	1.81	0.02	10.06
Sample O (1)	18.12	7.35	1.051248	0.54	87.152532	0.95	0.13	8.12
Sample O (2)	18.12	7.35	0.264308	0.54	88.543255	0.95	0.13	8.12
Sample O (3)	18.12	7.35	0.237505	0.54	89.343247	0.95	0.13	8.12
Sample O (4)	18.12	7.35	1.073327	0.54	93.640285	0.95	0.13	8.12
Sample O (5)	18.12	7.35	0.651532	0.54	87.529268	0.95	0.13	8.12
Sample O (6)	18.12	7.35	0.475998	0.54	98.339072	0.95	0.13	8.12
Sample O (7)	18.12	7.35	0.279706	0.54	99.419869	0.95	0.13	8.12
Sample O (8)	18.12	7.35	0.150572	0.54	99.387673	0.95	0.13	8.12
Sample O (9)	18.12	7.35	0.262732	0.54	99.130962	0.95	0.13	8.12

	MnO	Na2O	…	Si	SiO2	Ti	TiO2	Temp_C	\
Sample A (1)	0.00	0.00	…	11.934774	51.11	0.000000	2.59	1340.0	
Sample A (2)	0.00	0.00	…	11.855619	51.11	0.069798	2.59	1340.0	
Sample A (3)	0.00	0.00	…	11.896172	51.11	0.000000	2.59	1340.0	
Sample A (4)	0.00	0.00	…	14.100879	51.11	0.090973	2.59	1340.0	
Sample A (5)	0.00	0.00	…	12.654912	51.11	0.141058	2.59	1340.0	
Sample A (6)	0.00	0.00	…	12.776264	51.11	0.141286	2.59	1340.0	
Sample A (7)	0.00	0.00	…	13.142683	51.11	0.131832	2.59	1340.0	
Sample A (8)	0.00	0.00	…	12.581847	51.11	0.151103	2.59	1340.0	
Sample A (9)	0.00	0.00	…	9.094592	51.11	0.121531	2.59	1340.0	
Sample A (10)	0.00	0.00	…	7.069651	51.11	0.219619	2.59	1340.0	
Sample B (1)	0.12	0.00	…	12.973302	63.71	0.091361	0.24	1290.0	
Sample B (2)	0.12	0.00	…	12.912424	63.71	0.173116	0.24	1290.0	
Sample B (3)	0.12	0.00	…	12.961835	63.71	0.101502	0.24	1290.0	
Sample B (4)	0.12	0.00	…	11.381460	63.71	0.211140	0.24	1290.0	
Sample B (5)	0.12	0.00	…	11.684508	63.71	0.161584	0.24	1290.0	
Sample B (6)	0.12	0.00	…	11.588462	63.71	0.132033	0.24	1290.0	
Sample B (7)	0.12	0.00	…	12.740264	63.71	0.281775	0.24	1290.0	
Sample B (8)	0.12	0.00	…	12.905174	63.71	0.211395	0.24	1290.0	
Sample B (9)	0.12	0.00	…	13.007148	63.71	0.181214	0.24	1290.0	
Sample C (1)	0.00	0.00	…	12.707898	54.99	0.099592	0.20	1245.0	
Sample C (2)	0.00	0.00	…	11.384152	54.99	0.150451	0.20	1245.0	
Sample C (3)	0.00	0.00	…	11.453523	54.99	0.150572	0.20	1245.0	
Sample C (4)	0.00	0.00	…	11.352220	54.99	0.140647	0.20	1245.0	
Sample C (5)	0.00	0.00	…	9.755364	54.99	0.000000	0.20	1245.0	

Sample C (6)	0.00	0.00	…	6.588799	54.99	0.109813	0.20	1245.0
Sample C (7)	0.00	0.00	…	6.682406	54.99	0.112913	0.20	1245.0
Sample C (8)	0.00	0.00	…	6.564855	54.99	0.000000	0.20	1245.0
Sample C (9)	0.00	0.00	…	6.557704	54.99	0.079729	0.20	1245.0
Sample C (10)	0.00	0.00	…	8.660786	54.99	0.000000	0.20	1245.0
Sample C (11)	0.00	0.00	…	8.613065	54.99	0.000000	0.20	1245.0
Sample D (1)	0.82	0.00	…	11.350806	61.28	0.000000	1.68	1200.0
Sample D (2)	0.82	0.00	…	9.345507	61.28	0.000000	1.68	1200.0
Sample D (3)	0.82	0.00	…	18.528638	61.28	0.121433	1.68	1200.0
Sample D (4)	0.82	0.00	…	23.452100	61.28	1.211623	1.68	1200.0
Sample D (5)	0.82	0.00	…	14.834276	61.28	0.090946	1.68	1200.0
Sample D (6)	0.82	0.00	…	7.303657	61.28	0.071305	1.68	1200.0
Sample D (7)	0.82	0.00	…	6.615542	61.28	0.000000	1.68	1200.0
Sample D (8)	0.82	0.00	…	6.016343	61.28	0.061287	1.68	1200.0
Sample D (9)	0.82	0.00	…	0.731205	61.28	0.061792	1.68	1200.0
Sample D (10)	0.82	0.00	…	0.207061	61.28	0.062118	1.68	1200.0
Sample N (1)	0.31	0.16	…	7.972113	58.57	0.000000	1.49	1245.0
Sample N (2)	0.31	0.16	…	8.158270	58.57	0.071385	1.49	1245.0
Sample N (3)	0.31	0.16	…	7.855907	58.57	0.081408	1.49	1245.0
Sample N (4)	0.31	0.16	…	7.210744	58.57	0.000000	1.49	1245.0
Sample N (5)	0.31	0.16	…	7.303775	58.57	0.000000	1.49	1245.0
Sample N (6)	0.31	0.16	…	7.186434	58.57	0.000000	1.49	1245.0
Sample N (7)	0.31	0.16	…	7.990961	58.57	0.000000	1.49	1245.0
Sample N (8)	0.31	0.16	…	1.719138	58.57	0.000000	1.49	1245.0
Sample N (9)	0.31	0.16	…	1.517829	58.57	0.062377	1.49	1245.0
Sample N (10)	0.31	0.16	…	1.643751	58.57	0.000000	1.49	1245.0
Sample O (1)	0.55	0.66	…	11.452542	62.19	0.060649	1.32	1200.0
Sample O (2)	0.55	0.66	…	10.846803	62.19	0.071160	1.32	1200.0
Sample O (3)	0.55	0.66	…	10.006196	62.19	0.000000	1.32	1200.0
Sample O (4)	0.55	0.66	…	5.065704	62.19	0.000000	1.32	1200.0
Sample O (5)	0.55	0.66	…	11.473073	62.19	0.071261	1.32	1200.0
Sample O (6)	0.55	0.66	…	0.111404	62.19	0.091148	1.32	1200.0
Sample O (7)	0.55	0.66	…	0.165752	62.19	0.000000	1.32	1200.0
Sample O (8)	0.55	0.66	…	0.080305	62.19	0.000000	1.32	1200.0
Sample O (9)	0.55	0.66	…	0.111156	62.19	0.111156	1.32	1200.0

	Total WT%	Which metal?	Si-poor/Si-rich	dIW_Calculated	\
Sample A (1)	99.96		0.0	-4.592162	
Sample A (2)	100.29		0.0	-4.596586	
Sample A (3)	99.78		0.0	-4.594302	
Sample A (4)	98.93		0.0	-4.420202	
Sample A (5)	99.25		0.0	-4.553620	
Sample A (6)	99.09		0.0	-4.544111	
Sample A (7)	98.61		0.0	-4.512190	
Sample A (8)	99.27		0.0	-4.553184	
Sample A (9)	98.74		0.0	-4.797845	
Sample A (10)	95.62		0.0	-4.869998	

Sample B (1)	98.51	0.0	-4.482770
Sample B (2)	98.20	0.0	-4.486464
Sample B (3)	98.52	0.0	-4.483559
Sample B (4)	99.46	0.0	-5.266961
Sample B (5)	99.02	0.0	-4.579870
Sample B (6)	98.46	0.0	-4.584921
Sample B (7)	99.37	0.0	-4.497481
Sample B (8)	99.34	0.0	-4.487314
Sample B (9)	99.33	0.0	-4.477039
Sample C (1)	100.41	0.0	-4.473737
Sample C (2)	99.70	0.0	-4.574811
Sample C (3)	99.62	0.0	-4.571770
Sample C (4)	99.54	0.0	-4.578928
Sample C (5)	99.74	0.0	-4.667369
Sample C (6)	100.17	0.0	-4.867254
Sample C (7)	97.42	0.0	-5.084461
Sample C (8)	100.84	0.0	-4.870356
Sample C (9)	100.34	0.0	-4.864843
Sample C (10)	99.76	0.0	-4.758048
Sample C (11)	99.50	0.0	-4.762127
Sample D (1)	99.20	0.0	-2.302563
Sample D (2)	97.48	0.0	-2.446861
Sample D (3)	98.82	0.0	-1.599872
Sample D (4)	97.39	0.0	-0.980122
Sample D (5)	98.96	0.0	-1.939408
Sample D (6)	98.17	0.0	-2.557005
Sample D (7)	97.80	0.0	-2.591725
Sample D (8)	97.90	0.0	-2.617922
Sample D (9)	97.10	0.0	-2.812985
Sample D (10)	96.59	0.0	-2.824122
Sample N (1)	98.97	0.0	-2.835666
Sample N (2)	98.06	0.0	-2.824885
Sample N (3)	98.27	0.0	-2.841629
Sample N (4)	96.80	0.0	-2.874537
Sample N (5)	97.21	0.0	-2.868682
Sample N (6)	96.71	0.0	-2.875124
Sample N (7)	97.36	0.0	-2.832418
Sample N (8)	96.56	0.0	-3.089756
Sample N (9)	96.19	0.0	-3.090291
Sample N (10)	96.73	0.0	-3.091327
Sample O (1)	98.93	0.0	-3.157081
Sample O (2)	98.37	0.0	-3.208973
Sample O (3)	96.84	0.0	-3.266472
Sample O (4)	99.69	0.0	-3.534835
Sample O (5)	98.23	0.0	-3.159593
Sample O (6)	98.74	0.0	-3.684015
Sample O (7)	96.53	0.0	-3.696145

Sample O (8)	99.62		0.0	-3.695020
Sample O (9)	98.96		0.0	-3.692244

	logfO2_dIW	Pressure_Modeled
Sample A (1)	-15.509828	1
Sample A (2)	-15.514253	1
Sample A (3)	-15.511969	1
Sample A (4)	-15.337869	1
Sample A (5)	-15.471286	1
Sample A (6)	-15.461778	1
Sample A (7)	-15.429857	1
Sample A (8)	-15.470851	1
Sample A (9)	-15.715512	1
Sample A (10)	-15.787665	1
Sample B (1)	-15.958884	1
Sample B (2)	-15.962577	1
Sample B (3)	-15.959672	1
Sample B (4)	-16.743075	1
Sample B (5)	-16.055984	1
Sample B (6)	-16.061035	1
Sample B (7)	-15.973594	1
Sample B (8)	-15.963428	1
Sample B (9)	-15.953153	1
Sample C (1)	-16.483903	1
Sample C (2)	-16.584978	1
Sample C (3)	-16.581937	1
Sample C (4)	-16.589095	1
Sample C (5)	-16.677536	1
Sample C (6)	-16.877421	1
Sample C (7)	-17.094628	1
Sample C (8)	-16.880523	1
Sample C (9)	-16.875010	1
Sample C (10)	-16.768215	1
Sample C (11)	-16.772294	1
Sample D (1)	-14.879411	1
Sample D (2)	-15.023708	1
Sample D (3)	-14.176720	1
Sample D (4)	-13.556969	1
Sample D (5)	-14.516255	1
Sample D (6)	-15.133852	1
Sample D (7)	-15.168573	1
Sample D (8)	-15.194769	1
Sample D (9)	-15.389833	1
Sample D (10)	-15.400969	1
Sample N (1)	-14.845833	1
Sample N (2)	-14.835051	1
Sample N (3)	-14.851796	1

```
Sample N (4)   -14.884704                1
Sample N (5)   -14.878849                1
Sample N (6)   -14.885291                1
Sample N (7)   -14.842585                1
Sample N (8)   -15.099923                1
Sample N (9)   -15.100458                1
Sample N (10)  -15.101494                1
Sample O (1)   -15.733929                1
Sample O (2)   -15.785821                1
Sample O (3)   -15.843319                1
Sample O (4)   -16.111683                1
Sample O (5)   -15.736440                1
Sample O (6)   -16.260863                1
Sample O (7)   -16.272993                1
Sample O (8)   -16.271867                1
Sample O (9)   -16.269091                1

[59 rows x 22 columns]
```

Here we save the results to an excel file.

[5]:
```
myfile.save_excel(filename='dIW.xlsx', calculations=[dIWs])
```

```
Saved dIW.xlsx
```

1.4 4. Calculate the fO_2 in terms of the silicon-silica buffer

1.4.1 4.1 First, instantiate a MELTS class and calculate the activity of SiO_2 in the melt for each sample

[6]:
```
# -------------- MELTS preamble --------------- #
# instantiate thermoengine equilibrate MELTS instance
melts = equilibrate.MELTSmodel('1.1.0')

# Suppress phases not required in the melts simulation
phases = melts.get_phase_names()
for phase in phases:
    melts.set_phase_inclusion_status({phase: False})
melts.set_phase_inclusion_status({'Fluid': True, 'Liquid': True})
# ---------------------------------------------- #
```

[7]:
```
# extract only silicate compositions from the dataset
silicate_compositions = [myfile.get_sample_composition(samplename=i,␣
 ↪how='silicate') for i in myfile.get_data().index]

# extract the temperature corresponding to each sample
temperatures = [row['Temp_C'] for index, row in myfile.get_data().iterrows()]
```

```
/opt/anaconda3/lib/python3.9/site-packages/fO2calculate/sample_class.py:75:
UserWarning: Element S was passed as part of sample composition. This will be
assumed to be part of the metal composition.
  w.warn("Element " + str(vol) + " was passed as part of sample composition.
This" +
```

[8]:
```
# calculate the silica activity using ENKI MELTS and save those values to a list
aSiO2_list = []
for i, comp in enumerate(silicate_compositions):
    del comp['S']
    melts.set_bulk_composition(comp)
    output = melts.equilibrate_tp(temperatures[i], 0.1, initialize=True)
    (status, temperature, pressureMPa, xmlout) = output[0]
    activities = melts.get_thermo_properties_of_phase_components(xmlout,␣
 ↪phase_name='Liquid', mode='activity')
    aSiO2_list.append(activities['SiO2'])
```

[9]:
```
# add silica activities to our BatchFile
myfile.data['aSiO2'] = aSiO2_list
```

Here we print the BatchFile to ensure the data was calculated and written correctly

[10]:
```
myfile.get_data()
```

[10]:

	Al2O3	CaO	Cr	Cr2O3	Fe	FeO	K2O	MgO	\
Sample A (1)	24.37	4.75	3.251301	0.12	84.633854	0.18	0.00	16.86	
Sample A (2)	24.37	4.75	3.310400	0.12	84.594675	0.18	0.00	16.86	
Sample A (3)	24.37	4.75	3.407496	0.12	84.606133	0.18	0.00	16.86	
Sample A (4)	24.37	4.75	3.729910	0.12	81.714343	0.18	0.00	16.86	
Sample A (5)	24.37	4.75	1.964736	0.12	85.239295	0.18	0.00	16.86	
Sample A (6)	24.37	4.75	2.008275	0.12	85.074175	0.18	0.00	16.86	
Sample A (7)	24.37	4.75	2.332421	0.12	84.301795	0.18	0.00	16.86	
Sample A (8)	24.37	4.75	2.457943	0.12	84.748665	0.18	0.00	16.86	
Sample A (9)	24.37	4.75	1.184930	0.12	89.457160	0.18	0.00	16.86	
Sample A (10)	24.37	4.75	4.852541	0.12	87.680402	0.18	0.00	16.86	
Sample B (1)	17.11	5.92	2.081007	0.06	84.752817	0.19	0.00	12.64	
Sample B (2)	17.11	5.92	2.087576	0.06	84.714868	0.19	0.00	12.64	
Sample B (3)	17.11	5.92	2.060495	0.06	84.754365	0.19	0.00	12.64	
Sample B (4)	17.11	5.92	2.473356	0.06	85.732958	0.19	0.00	12.64	
Sample B (5)	17.11	5.92	1.908705	0.06	86.124015	0.19	0.00	12.64	
Sample B (6)	17.11	5.92	1.970343	0.06	86.055251	0.19	0.00	12.64	
Sample B (7)	17.11	5.92	2.123377	0.06	84.673443	0.19	0.00	12.64	
Sample B (8)	17.11	5.92	1.922690	0.06	84.749346	0.19	0.00	12.64	
Sample B (9)	17.11	5.92	2.104097	0.06	84.415584	0.19	0.00	12.64	
Sample C (1)	22.50	9.74	1.922119	0.04	84.981576	0.19	0.00	12.36	
Sample C (2)	22.50	9.74	1.845537	0.04	86.469408	0.19	0.00	12.36	
Sample C (3)	22.50	9.74	1.666332	0.04	86.589038	0.19	0.00	12.36	
Sample C (4)	22.50	9.74	1.677718	0.04	86.678722	0.19	0.00	12.36	

Sample C (5)	22.50	9.74	3.609384	0.04	86.294365	0.19	0.00	12.36
Sample C (6)	22.50	9.74	1.507437	0.04	91.294799	0.19	0.00	12.36
Sample C (7)	22.50	9.74	2.319852	0.04	90.166290	0.19	0.00	12.36
Sample C (8)	22.50	9.74	1.547005	0.04	91.461722	0.19	0.00	12.36
Sample C (9)	22.50	9.74	2.003189	0.04	90.900937	0.19	0.00	12.36
Sample C (10)	22.50	9.74	1.363272	0.04	89.605052	0.19	0.00	12.36
Sample C (11)	22.50	9.74	1.286432	0.04	89.758794	0.19	0.00	12.36
Sample D (1)	16.94	8.38	1.169355	0.47	87.278226	2.57	0.00	7.87
Sample D (2)	16.94	8.38	0.379565	0.47	89.926139	2.57	0.00	7.87
Sample D (3)	16.94	8.38	6.405586	0.47	74.580045	2.57	0.00	7.87
Sample D (4)	16.94	8.38	9.333607	0.47	65.869186	2.57	0.00	7.87
Sample D (5)	16.94	8.38	8.559014	0.47	76.465238	2.57	0.00	7.87
Sample D (6)	16.94	8.38	1.191810	0.47	90.934094	2.57	0.00	7.87
Sample D (7)	16.94	8.38	1.492843	0.47	91.441718	2.57	0.00	7.87
Sample D (8)	16.94	8.38	1.532176	0.47	91.767109	2.57	0.00	7.87
Sample D (9)	16.94	8.38	0.566426	0.47	97.909372	2.57	0.00	7.87
Sample D (10)	16.94	8.38	0.227767	0.47	98.809401	2.57	0.00	7.87
Sample N (1)	19.37	7.57	0.636557	0.60	90.845711	1.81	0.02	10.06
Sample N (2)	19.37	7.57	0.581277	0.60	90.628187	1.81	0.02	10.06
Sample N (3)	19.37	7.57	0.712323	0.60	90.882263	1.81	0.02	10.06
Sample N (4)	19.37	7.57	1.012397	0.60	91.301653	1.81	0.02	10.06
Sample N (5)	19.37	7.57	1.131571	0.60	91.101739	1.81	0.02	10.06
Sample N (6)	19.37	7.57	1.085720	0.60	91.262537	1.81	0.02	10.06
Sample N (7)	19.37	7.57	0.893591	0.60	90.591619	1.81	0.02	10.06
Sample N (8)	19.37	7.57	1.429163	0.60	96.447804	1.81	0.02	10.06
Sample N (9)	19.37	7.57	1.892089	0.60	96.153446	1.81	0.02	10.06
Sample N (10)	19.37	7.57	1.623075	0.60	96.423033	1.81	0.02	10.06
Sample O (1)	18.12	7.35	1.051248	0.54	87.152532	0.95	0.13	8.12
Sample O (2)	18.12	7.35	0.264308	0.54	88.543255	0.95	0.13	8.12
Sample O (3)	18.12	7.35	0.237505	0.54	89.343247	0.95	0.13	8.12
Sample O (4)	18.12	7.35	1.073327	0.54	93.640285	0.95	0.13	8.12
Sample O (5)	18.12	7.35	0.651532	0.54	87.529268	0.95	0.13	8.12
Sample O (6)	18.12	7.35	0.475998	0.54	98.339072	0.95	0.13	8.12
Sample O (7)	18.12	7.35	0.279706	0.54	99.419869	0.95	0.13	8.12
Sample O (8)	18.12	7.35	0.150572	0.54	99.387673	0.95	0.13	8.12
Sample O (9)	18.12	7.35	0.262732	0.54	99.130962	0.95	0.13	8.12

	MnO	Na2O	P	S	Si	SiO2	Ti	\
Sample A (1)	0.00	0.00	0.190076	0.000000	11.934774	51.11	0.000000	
Sample A (2)	0.00	0.00	0.169508	0.000000	11.855619	51.11	0.069798	
Sample A (3)	0.00	0.00	0.100220	0.000000	11.896172	51.11	0.000000	
Sample A (4)	0.00	0.00	0.363894	0.000000	14.100879	51.11	0.090973	
Sample A (5)	0.00	0.00	0.000000	0.000000	12.654912	51.11	0.141058	
Sample A (6)	0.00	0.00	0.000000	0.000000	12.776264	51.11	0.141286	
Sample A (7)	0.00	0.00	0.081128	0.000000	13.142683	51.11	0.131832	
Sample A (8)	0.00	0.00	0.060441	0.000000	12.581847	51.11	0.151103	
Sample A (9)	0.00	0.00	0.151914	0.000000	9.094592	51.11	0.121531	

Sample A (10)	0.00	0.00	0.167329	0.000000	7.069651	51.11	0.219619
Sample B (1)	0.12	0.00	0.101513	0.000000	12.973302	63.71	0.091361
Sample B (2)	0.12	0.00	0.122200	0.000000	12.912424	63.71	0.173116
Sample B (3)	0.12	0.00	0.121803	0.000000	12.961835	63.71	0.101502
Sample B (4)	0.12	0.00	0.160869	0.030163	11.381460	63.71	0.211140
Sample B (5)	0.12	0.00	0.121188	0.000000	11.684508	63.71	0.161584
Sample B (6)	0.12	0.00	0.253910	0.000000	11.588462	63.71	0.132033
Sample B (7)	0.12	0.00	0.181141	0.000000	12.740264	63.71	0.281775
Sample B (8)	0.12	0.00	0.211395	0.000000	12.905174	63.71	0.211395
Sample B (9)	0.12	0.00	0.302024	0.000000	13.007148	63.71	0.181214
Sample C (1)	0.00	0.00	0.288816	0.000000	12.707898	54.99	0.099592
Sample C (2)	0.00	0.00	0.150451	0.000000	11.384152	54.99	0.150451
Sample C (3)	0.00	0.00	0.130496	0.000000	11.453523	54.99	0.150572
Sample C (4)	0.00	0.00	0.150693	0.000000	11.352220	54.99	0.140647
Sample C (5)	0.00	0.00	0.340886	0.000000	9.755364	54.99	0.000000
Sample C (6)	0.00	0.00	0.499151	0.000000	6.588799	54.99	0.109813
Sample C (7)	0.00	0.00	0.667214	0.041059	6.682406	54.99	0.112913
Sample C (8)	0.00	0.00	0.416501	0.000000	6.564855	54.99	0.000000
Sample C (9)	0.00	0.00	0.448475	0.000000	6.557704	54.99	0.079729
Sample C (10)	0.00	0.00	0.370890	0.000000	8.660786	54.99	0.000000
Sample C (11)	0.00	0.00	0.331658	0.000000	8.613065	54.99	0.000000
Sample D (1)	0.82	0.00	0.201613	0.000000	11.350806	61.28	0.000000
Sample D (2)	0.82	0.00	0.348789	0.000000	9.345507	61.28	0.000000
Sample D (3)	0.82	0.00	0.374418	0.000000	18.528638	61.28	0.121433
Sample D (4)	0.82	0.00	0.123216	0.000000	23.452100	61.28	1.211623
Sample D (5)	0.82	0.00	0.040420	0.000000	14.834276	61.28	0.090946
Sample D (6)	0.82	0.00	0.499134	0.000000	7.303657	61.28	0.071305
Sample D (7)	0.82	0.00	0.449898	0.000000	6.615542	61.28	0.000000
Sample D (8)	0.82	0.00	0.623085	0.000000	6.016343	61.28	0.061287
Sample D (9)	0.82	0.00	0.679712	0.041195	0.731205	61.28	0.061792
Sample D (10)	0.82	0.00	0.693654	0.000000	0.207061	61.28	0.062118
Sample N (1)	0.31	0.16	0.555724	0.000000	7.972113	58.57	0.000000
Sample N (2)	0.31	0.16	0.550683	0.000000	8.158270	58.57	0.071385
Sample N (3)	0.31	0.16	0.478274	0.000000	7.855907	58.57	0.081408
Sample N (4)	0.31	0.16	0.475207	0.000000	7.210744	58.57	0.000000
Sample N (5)	0.31	0.16	0.452628	0.000000	7.303775	58.57	0.000000
Sample N (6)	0.31	0.16	0.475649	0.000000	7.186434	58.57	0.000000
Sample N (7)	0.31	0.16	0.523829	0.000000	7.990961	58.57	0.000000
Sample N (8)	0.31	0.16	0.403894	0.000000	1.719138	58.57	0.000000
Sample N (9)	0.31	0.16	0.374259	0.000000	1.517829	58.57	0.062377
Sample N (10)	0.31	0.16	0.310142	0.000000	1.643751	58.57	0.000000
Sample O (1)	0.55	0.66	0.283028	0.000000	11.452542	62.19	0.060649
Sample O (2)	0.55	0.66	0.274474	0.000000	10.846803	62.19	0.071160
Sample O (3)	0.55	0.66	0.413052	0.000000	10.006196	62.19	0.000000
Sample O (4)	0.55	0.66	0.230715	0.000000	5.065704	62.19	0.000000
Sample O (5)	0.55	0.66	0.274865	0.000000	11.473073	62.19	0.071261
Sample O (6)	0.55	0.66	0.060766	0.921612	0.111404	62.19	0.091148

Sample O (7)	0.55	0.66	0.134673	0.000000	0.165752	62.19	0.000000
Sample O (8)	0.55	0.66	0.381450	0.000000	0.080305	62.19	0.000000
Sample O (9)	0.55	0.66	0.383994	0.000000	0.111156	62.19	0.111156

	TiO2	Temp_C	Total WT%	Which metal?	Si-poor/Si-rich	aSiO2
Sample A (1)	2.59	1340.0	99.96		0.0	0.475599
Sample A (2)	2.59	1340.0	100.29		0.0	0.475599
Sample A (3)	2.59	1340.0	99.78		0.0	0.475599
Sample A (4)	2.59	1340.0	98.93		0.0	0.475599
Sample A (5)	2.59	1340.0	99.25		0.0	0.475599
Sample A (6)	2.59	1340.0	99.09		0.0	0.475599
Sample A (7)	2.59	1340.0	98.61		0.0	0.475599
Sample A (8)	2.59	1340.0	99.27		0.0	0.475599
Sample A (9)	2.59	1340.0	98.74		0.0	0.475599
Sample A (10)	2.59	1340.0	95.62		0.0	0.475599
Sample B (1)	0.24	1290.0	98.51		0.0	0.641694
Sample B (2)	0.24	1290.0	98.20		0.0	0.641694
Sample B (3)	0.24	1290.0	98.52		0.0	0.641694
Sample B (4)	0.24	1290.0	99.46		0.0	0.641694
Sample B (5)	0.24	1290.0	99.02		0.0	0.641694
Sample B (6)	0.24	1290.0	98.46		0.0	0.641694
Sample B (7)	0.24	1290.0	99.37		0.0	0.641694
Sample B (8)	0.24	1290.0	99.34		0.0	0.641694
Sample B (9)	0.24	1290.0	99.33		0.0	0.641694
Sample C (1)	0.20	1245.0	100.41		0.0	0.507057
Sample C (2)	0.20	1245.0	99.70		0.0	0.507057
Sample C (3)	0.20	1245.0	99.62		0.0	0.507057
Sample C (4)	0.20	1245.0	99.54		0.0	0.507057
Sample C (5)	0.20	1245.0	99.74		0.0	0.507057
Sample C (6)	0.20	1245.0	100.17		0.0	0.507057
Sample C (7)	0.20	1245.0	97.42		0.0	0.507057
Sample C (8)	0.20	1245.0	100.84		0.0	0.507057
Sample C (9)	0.20	1245.0	100.34		0.0	0.507057
Sample C (10)	0.20	1245.0	99.76		0.0	0.507057
Sample C (11)	0.20	1245.0	99.50		0.0	0.507057
Sample D (1)	1.68	1200.0	99.20		0.0	0.638417
Sample D (2)	1.68	1200.0	97.48		0.0	0.638417
Sample D (3)	1.68	1200.0	98.82		0.0	0.638417
Sample D (4)	1.68	1200.0	97.39		0.0	0.638417
Sample D (5)	1.68	1200.0	98.96		0.0	0.638417
Sample D (6)	1.68	1200.0	98.17		0.0	0.638417
Sample D (7)	1.68	1200.0	97.80		0.0	0.638417
Sample D (8)	1.68	1200.0	97.90		0.0	0.638417
Sample D (9)	1.68	1200.0	97.10		0.0	0.638417
Sample D (10)	1.68	1200.0	96.59		0.0	0.638417
Sample N (1)	1.49	1245.0	98.97		0.0	0.591802
Sample N (2)	1.49	1245.0	98.06		0.0	0.591802

Sample N (3)	1.49	1245.0	98.27		0.0	0.591802
Sample N (4)	1.49	1245.0	96.80		0.0	0.591802
Sample N (5)	1.49	1245.0	97.21		0.0	0.591802
Sample N (6)	1.49	1245.0	96.71		0.0	0.591802
Sample N (7)	1.49	1245.0	97.36		0.0	0.591802
Sample N (8)	1.49	1245.0	96.56		0.0	0.591802
Sample N (9)	1.49	1245.0	96.19		0.0	0.591802
Sample N (10)	1.49	1245.0	96.73		0.0	0.591802
Sample O (1)	1.32	1200.0	98.93		0.0	0.625018
Sample O (2)	1.32	1200.0	98.37		0.0	0.625018
Sample O (3)	1.32	1200.0	96.84		0.0	0.625018
Sample O (4)	1.32	1200.0	99.69		0.0	0.625018
Sample O (5)	1.32	1200.0	98.23		0.0	0.625018
Sample O (6)	1.32	1200.0	98.74		0.0	0.625018
Sample O (7)	1.32	1200.0	96.53		0.0	0.625018
Sample O (8)	1.32	1200.0	99.62		0.0	0.625018
Sample O (9)	1.32	1200.0	98.96		0.0	0.625018

1.4.2 4.2 Next, use the fO2calculate module to calculate $\Delta SiSiO_2$ for all samples

Here we calculate $\Delta SiSiO_2$ for all measurements and print the results.

[11]:
```
dSiSiO2s = myfile.calculate_dSiSiO2(temperature='Temp_C', aSiO2='aSiO2',␣
↪pressure=1)
dSiSiO2s
```

```
[                    ] 3%  Working on sample Sample A (2)
```

```
/opt/anaconda3/lib/python3.9/site-packages/fO2calculate/sample_class.py:75:
UserWarning: Element S was passed as part of sample composition. This will be
assumed to be part of the metal composition.
  w.warn("Element " + str(vol) + " was passed as part of sample composition.
This" +
/opt/anaconda3/lib/python3.9/site-packages/fO2calculate/sample_class.py:75:
UserWarning: Element Cl was passed as part of sample composition. This will be
assumed to be part of the metal composition.
  w.warn("Element " + str(vol) + " was passed as part of sample composition.
This" +
/opt/anaconda3/lib/python3.9/site-packages/fO2calculate/sample_class.py:75:
UserWarning: Element F was passed as part of sample composition. This will be
assumed to be part of the metal composition.
  w.warn("Element " + str(vol) + " was passed as part of sample composition.
This" +
```

```
[====================] 100%  Working on sample Sample O (9)
```

[11]:

	Al2O3	CaO	Cr	Cr2O3	Fe	FeO	K2O	MgO	\
Sample A (1)	24.37	4.75	3.251301	0.12	84.633854	0.18	0.00	16.86	

Sample A (2)	24.37	4.75	3.310400	0.12	84.594675	0.18	0.00	16.86
Sample A (3)	24.37	4.75	3.407496	0.12	84.606133	0.18	0.00	16.86
Sample A (4)	24.37	4.75	3.729910	0.12	81.714343	0.18	0.00	16.86
Sample A (5)	24.37	4.75	1.964736	0.12	85.239295	0.18	0.00	16.86
Sample A (6)	24.37	4.75	2.008275	0.12	85.074175	0.18	0.00	16.86
Sample A (7)	24.37	4.75	2.332421	0.12	84.301795	0.18	0.00	16.86
Sample A (8)	24.37	4.75	2.457943	0.12	84.748665	0.18	0.00	16.86
Sample A (9)	24.37	4.75	1.184930	0.12	89.457160	0.18	0.00	16.86
Sample A (10)	24.37	4.75	4.852541	0.12	87.680402	0.18	0.00	16.86
Sample B (1)	17.11	5.92	2.081007	0.06	84.752817	0.19	0.00	12.64
Sample B (2)	17.11	5.92	2.087576	0.06	84.714868	0.19	0.00	12.64
Sample B (3)	17.11	5.92	2.060495	0.06	84.754365	0.19	0.00	12.64
Sample B (4)	17.11	5.92	2.473356	0.06	85.732958	0.19	0.00	12.64
Sample B (5)	17.11	5.92	1.908705	0.06	86.124015	0.19	0.00	12.64
Sample B (6)	17.11	5.92	1.970343	0.06	86.055251	0.19	0.00	12.64
Sample B (7)	17.11	5.92	2.123377	0.06	84.673443	0.19	0.00	12.64
Sample B (8)	17.11	5.92	1.922690	0.06	84.749346	0.19	0.00	12.64
Sample B (9)	17.11	5.92	2.104097	0.06	84.415584	0.19	0.00	12.64
Sample C (1)	22.50	9.74	1.922119	0.04	84.981576	0.19	0.00	12.36
Sample C (2)	22.50	9.74	1.845537	0.04	86.469408	0.19	0.00	12.36
Sample C (3)	22.50	9.74	1.666332	0.04	86.589038	0.19	0.00	12.36
Sample C (4)	22.50	9.74	1.677718	0.04	86.678722	0.19	0.00	12.36
Sample C (5)	22.50	9.74	3.609384	0.04	86.294365	0.19	0.00	12.36
Sample C (6)	22.50	9.74	1.507437	0.04	91.294799	0.19	0.00	12.36
Sample C (7)	22.50	9.74	2.319852	0.04	90.166290	0.19	0.00	12.36
Sample C (8)	22.50	9.74	1.547005	0.04	91.461722	0.19	0.00	12.36
Sample C (9)	22.50	9.74	2.003189	0.04	90.900937	0.19	0.00	12.36
Sample C (10)	22.50	9.74	1.363272	0.04	89.605052	0.19	0.00	12.36
Sample C (11)	22.50	9.74	1.286432	0.04	89.758794	0.19	0.00	12.36
Sample D (1)	16.94	8.38	1.169355	0.47	87.278226	2.57	0.00	7.87
Sample D (2)	16.94	8.38	0.379565	0.47	89.926139	2.57	0.00	7.87
Sample D (3)	16.94	8.38	6.405586	0.47	74.580045	2.57	0.00	7.87
Sample D (4)	16.94	8.38	9.333607	0.47	65.869186	2.57	0.00	7.87
Sample D (5)	16.94	8.38	8.559014	0.47	76.465238	2.57	0.00	7.87
Sample D (6)	16.94	8.38	1.191810	0.47	90.934094	2.57	0.00	7.87
Sample D (7)	16.94	8.38	1.492843	0.47	91.441718	2.57	0.00	7.87
Sample D (8)	16.94	8.38	1.532176	0.47	91.767109	2.57	0.00	7.87
Sample D (9)	16.94	8.38	0.566426	0.47	97.909372	2.57	0.00	7.87
Sample D (10)	16.94	8.38	0.227767	0.47	98.809401	2.57	0.00	7.87
Sample N (1)	19.37	7.57	0.636557	0.60	90.845711	1.81	0.02	10.06
Sample N (2)	19.37	7.57	0.581277	0.60	90.628187	1.81	0.02	10.06
Sample N (3)	19.37	7.57	0.712323	0.60	90.882263	1.81	0.02	10.06
Sample N (4)	19.37	7.57	1.012397	0.60	91.301653	1.81	0.02	10.06
Sample N (5)	19.37	7.57	1.131571	0.60	91.101739	1.81	0.02	10.06
Sample N (6)	19.37	7.57	1.085720	0.60	91.262537	1.81	0.02	10.06
Sample N (7)	19.37	7.57	0.893591	0.60	90.591619	1.81	0.02	10.06
Sample N (8)	19.37	7.57	1.429163	0.60	96.447804	1.81	0.02	10.06

Sample N (9)	19.37	7.57	1.892089	0.60	96.153446	1.81	0.02	10.06
Sample N (10)	19.37	7.57	1.623075	0.60	96.423033	1.81	0.02	10.06
Sample O (1)	18.12	7.35	1.051248	0.54	87.152532	0.95	0.13	8.12
Sample O (2)	18.12	7.35	0.264308	0.54	88.543255	0.95	0.13	8.12
Sample O (3)	18.12	7.35	0.237505	0.54	89.343247	0.95	0.13	8.12
Sample O (4)	18.12	7.35	1.073327	0.54	93.640285	0.95	0.13	8.12
Sample O (5)	18.12	7.35	0.651532	0.54	87.529268	0.95	0.13	8.12
Sample O (6)	18.12	7.35	0.475998	0.54	98.339072	0.95	0.13	8.12
Sample O (7)	18.12	7.35	0.279706	0.54	99.419869	0.95	0.13	8.12
Sample O (8)	18.12	7.35	0.150572	0.54	99.387673	0.95	0.13	8.12
Sample O (9)	18.12	7.35	0.262732	0.54	99.130962	0.95	0.13	8.12

	MnO	Na2O	…	Ti	TiO2	Temp_C	Total WT%	\
Sample A (1)	0.00	0.00	…	0.000000	2.59	1340.0	99.96	
Sample A (2)	0.00	0.00	…	0.069798	2.59	1340.0	100.29	
Sample A (3)	0.00	0.00	…	0.000000	2.59	1340.0	99.78	
Sample A (4)	0.00	0.00	…	0.090973	2.59	1340.0	98.93	
Sample A (5)	0.00	0.00	…	0.141058	2.59	1340.0	99.25	
Sample A (6)	0.00	0.00	…	0.141286	2.59	1340.0	99.09	
Sample A (7)	0.00	0.00	…	0.131832	2.59	1340.0	98.61	
Sample A (8)	0.00	0.00	…	0.151103	2.59	1340.0	99.27	
Sample A (9)	0.00	0.00	…	0.121531	2.59	1340.0	98.74	
Sample A (10)	0.00	0.00	…	0.219619	2.59	1340.0	95.62	
Sample B (1)	0.12	0.00	…	0.091361	0.24	1290.0	98.51	
Sample B (2)	0.12	0.00	…	0.173116	0.24	1290.0	98.20	
Sample B (3)	0.12	0.00	…	0.101502	0.24	1290.0	98.52	
Sample B (4)	0.12	0.00	…	0.211140	0.24	1290.0	99.46	
Sample B (5)	0.12	0.00	…	0.161584	0.24	1290.0	99.02	
Sample B (6)	0.12	0.00	…	0.132033	0.24	1290.0	98.46	
Sample B (7)	0.12	0.00	…	0.281775	0.24	1290.0	99.37	
Sample B (8)	0.12	0.00	…	0.211395	0.24	1290.0	99.34	
Sample B (9)	0.12	0.00	…	0.181214	0.24	1290.0	99.33	
Sample C (1)	0.00	0.00	…	0.099592	0.20	1245.0	100.41	
Sample C (2)	0.00	0.00	…	0.150451	0.20	1245.0	99.70	
Sample C (3)	0.00	0.00	…	0.150572	0.20	1245.0	99.62	
Sample C (4)	0.00	0.00	…	0.140647	0.20	1245.0	99.54	
Sample C (5)	0.00	0.00	…	0.000000	0.20	1245.0	99.74	
Sample C (6)	0.00	0.00	…	0.109813	0.20	1245.0	100.17	
Sample C (7)	0.00	0.00	…	0.112913	0.20	1245.0	97.42	
Sample C (8)	0.00	0.00	…	0.000000	0.20	1245.0	100.84	
Sample C (9)	0.00	0.00	…	0.079729	0.20	1245.0	100.34	
Sample C (10)	0.00	0.00	…	0.000000	0.20	1245.0	99.76	
Sample C (11)	0.00	0.00	…	0.000000	0.20	1245.0	99.50	
Sample D (1)	0.82	0.00	…	0.000000	1.68	1200.0	99.20	
Sample D (2)	0.82	0.00	…	0.000000	1.68	1200.0	97.48	
Sample D (3)	0.82	0.00	…	0.121433	1.68	1200.0	98.82	
Sample D (4)	0.82	0.00	…	1.211623	1.68	1200.0	97.39	

Sample D (5)	0.82	0.00	…	0.090946	1.68	1200.0	98.96
Sample D (6)	0.82	0.00	…	0.071305	1.68	1200.0	98.17
Sample D (7)	0.82	0.00	…	0.000000	1.68	1200.0	97.80
Sample D (8)	0.82	0.00	…	0.061287	1.68	1200.0	97.90
Sample D (9)	0.82	0.00	…	0.061792	1.68	1200.0	97.10
Sample D (10)	0.82	0.00	…	0.062118	1.68	1200.0	96.59
Sample N (1)	0.31	0.16	…	0.000000	1.49	1245.0	98.97
Sample N (2)	0.31	0.16	…	0.071385	1.49	1245.0	98.06
Sample N (3)	0.31	0.16	…	0.081408	1.49	1245.0	98.27
Sample N (4)	0.31	0.16	…	0.000000	1.49	1245.0	96.80
Sample N (5)	0.31	0.16	…	0.000000	1.49	1245.0	97.21
Sample N (6)	0.31	0.16	…	0.000000	1.49	1245.0	96.71
Sample N (7)	0.31	0.16	…	0.000000	1.49	1245.0	97.36
Sample N (8)	0.31	0.16	…	0.000000	1.49	1245.0	96.56
Sample N (9)	0.31	0.16	…	0.062377	1.49	1245.0	96.19
Sample N (10)	0.31	0.16	…	0.000000	1.49	1245.0	96.73
Sample O (1)	0.55	0.66	…	0.060649	1.32	1200.0	98.93
Sample O (2)	0.55	0.66	…	0.071160	1.32	1200.0	98.37
Sample O (3)	0.55	0.66	…	0.000000	1.32	1200.0	96.84
Sample O (4)	0.55	0.66	…	0.000000	1.32	1200.0	99.69
Sample O (5)	0.55	0.66	…	0.071261	1.32	1200.0	98.23
Sample O (6)	0.55	0.66	…	0.091148	1.32	1200.0	98.74
Sample O (7)	0.55	0.66	…	0.000000	1.32	1200.0	96.53
Sample O (8)	0.55	0.66	…	0.000000	1.32	1200.0	99.62
Sample O (9)	0.55	0.66	…	0.111156	1.32	1200.0	98.96

	Which metal?	Si-poor/Si-rich	aSiO2	dSiSiO2_Calculated	\
Sample A (1)		0.0	0.475599	4.754054	
Sample A (2)		0.0	0.475599	4.774649	
Sample A (3)		0.0	0.475599	4.762356	
Sample A (4)		0.0	0.475599	4.209257	
Sample A (5)		0.0	0.475599	4.558737	
Sample A (6)		0.0	0.475599	4.527638	
Sample A (7)		0.0	0.475599	4.436766	
Sample A (8)		0.0	0.475599	4.580415	
Sample A (9)		0.0	0.475599	5.542834	
Sample A (10)		0.0	0.475599	6.184085	
Sample B (1)		0.0	0.641694	4.862894	
Sample B (2)		0.0	0.641694	4.880181	
Sample B (3)		0.0	0.641694	4.866443	
Sample B (4)		0.0	0.641694	4.615264	
Sample B (5)		0.0	0.641694	5.207319	
Sample B (6)		0.0	0.641694	5.236944	
Sample B (7)		0.0	0.641694	4.927271	
Sample B (8)		0.0	0.641694	4.883944	
Sample B (9)		0.0	0.641694	4.860407	
Sample C (1)		0.0	0.507057	4.851824	

Sample C (2)		0.0	0.507057	5.212921
Sample C (3)		0.0	0.507057	5.192107
Sample C (4)		0.0	0.507057	5.221489
Sample C (5)		0.0	0.507057	5.694866
Sample C (6)		0.0	0.507057	6.725378
Sample C (7)		0.0	0.507057	6.456803
Sample C (8)		0.0	0.507057	6.731776
Sample C (9)		0.0	0.507057	6.736020
Sample C (10)		0.0	0.507057	6.028252
Sample C (11)		0.0	0.507057	6.042083
Sample D (1)		0.0	0.638417	5.556462
Sample D (2)		0.0	0.638417	6.161110
Sample D (3)		0.0	0.638417	3.722537
Sample D (4)		0.0	0.638417	2.644365
Sample D (5)		0.0	0.638417	4.622666
Sample D (6)		0.0	0.638417	6.838610
Sample D (7)		0.0	0.638417	7.082084
Sample D (8)		0.0	0.638417	7.307482
Sample D (9)		0.0	0.638417	10.428553
Sample D (10)		0.0	0.638417	11.670534
Sample N (1)		0.0	0.591802	6.386975
Sample N (2)		0.0	0.591802	6.325846
Sample N (3)		0.0	0.591802	6.424065
Sample N (4)		0.0	0.591802	6.640711
Sample N (5)		0.0	0.591802	6.608463
Sample N (6)		0.0	0.591802	6.649436
Sample N (7)		0.0	0.591802	6.380368
Sample N (8)		0.0	0.591802	9.170339
Sample N (9)		0.0	0.591802	9.328502
Sample N (10)		0.0	0.591802	9.227114
Sample O (1)		0.0	0.625018	5.510878
Sample O (2)		0.0	0.625018	5.685191
Sample O (3)		0.0	0.625018	5.939900
Sample O (4)		0.0	0.625018	7.655500
Sample O (5)		0.0	0.625018	5.503829
Sample O (6)		0.0	0.625018	12.056631
Sample O (7)		0.0	0.625018	11.852068
Sample O (8)		0.0	0.625018	12.505685
Sample O (9)		0.0	0.625018	12.215443

	logfO2_dSiSiO2	dIW_SiSiO2	Pressure_Modeled
Sample A (1)	-15.410849	-4.493183	1
Sample A (2)	-15.390255	-4.472588	1
Sample A (3)	-15.402547	-4.484881	1
Sample A (4)	-15.955646	-5.037979	1
Sample A (5)	-15.606167	-4.688500	1
Sample A (6)	-15.637265	-4.719599	1

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Sample A (7)       -15.728137   -4.810470              1
Sample A (8)       -15.584489   -4.666822              1
Sample A (9)       -14.622069   -3.704402              1
Sample A (10)      -13.980818   -3.063151              1
Sample B (1)       -16.238545   -4.762431              1
Sample B (2)       -16.221257   -4.745144              1
Sample B (3)       -16.234995   -4.758881              1
Sample B (4)       -16.486174   -5.010061              1
Sample B (5)       -15.894120   -4.418006              1
Sample B (6)       -15.864495   -4.388381              1
Sample B (7)       -16.174168   -4.698054              1
Sample B (8)       -16.217495   -4.741381              1
Sample B (9)       -16.241032   -4.764918              1
Sample C (1)       -17.145452   -5.135285              1
Sample C (2)       -16.784355   -4.774188              1
Sample C (3)       -16.805170   -4.795003              1
Sample C (4)       -16.775788   -4.765621              1
Sample C (5)       -16.302410   -4.292244              1
Sample C (6)       -15.271899   -3.261732              1
Sample C (7)       -15.540473   -3.530307              1
Sample C (8)       -15.265501   -3.255334              1
Sample C (9)       -15.261257   -3.251090              1
Sample C (10)      -15.969024   -3.958857              1
Sample C (11)      -15.955193   -3.945026              1
Sample D (1)       -17.391596   -4.814749              1
Sample D (2)       -16.786948   -4.210101              1
Sample D (3)       -19.225521   -6.648674              1
Sample D (4)       -20.303694   -7.726846              1
Sample D (5)       -18.325392   -5.748545              1
Sample D (6)       -16.109448   -3.532601              1
Sample D (7)       -15.865974   -3.289127              1
Sample D (8)       -15.640576   -3.063729              1
Sample D (9)       -12.519505    0.057342              1
Sample D (10)      -11.277524    1.299323              1
Sample N (1)       -15.610301   -3.600134              1
Sample N (2)       -15.671431   -3.661264              1
Sample N (3)       -15.573212   -3.563045              1
Sample N (4)       -15.356565   -3.346399              1
Sample N (5)       -15.388813   -3.378647              1
Sample N (6)       -15.347841   -3.337674              1
Sample N (7)       -15.616908   -3.606742              1
Sample N (8)       -12.826938   -0.816771              1
Sample N (9)       -12.668775   -0.658608              1
Sample N (10)      -12.770163   -0.759996              1
Sample O (1)       -17.437181   -4.860333              1
Sample O (2)       -17.262868   -4.686020              1
Sample O (3)       -17.008158   -4.431311              1
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Sample O (4)       -15.292559   -2.715711                1
Sample O (5)       -17.444229   -4.867382                1
Sample O (6)       -10.891427    1.685420                1
Sample O (7)       -11.095990    1.480857                1
Sample O (8)       -10.442373    2.134474                1
Sample O (9)       -10.732616    1.844232                1

[59 rows x 24 columns]
```

Finally, we save all $\Delta SiSiO_2$ values to an excel spreadsheet.

[12]:
```
myfile.save_excel(filename='dSiSiO2.xlsx', calculations=[dSiSiO2s])
```

```
Saved dSiSiO2.xlsx
```