

# CerroNegro\_isobar\_comparison

November 16, 2020

```
[1]: import sys
      sys.path.append('../..')

      import VESIcal as v
      import numpy as np
      import scipy
      import pandas as pd
      import matplotlib.pyplot as plt
```

```
[2]: #Import the data
      basalts = v.ExcelFile("../..\\Datasets\\cerro_negro.xlsx")

      #Calculate the average composition of the entire dataset
      columns = list(basalts.data)
      avg_vals = []
      for col in columns:
          try:
              avg_vals.append(basalts.data[col].mean())
          except:
              avg_vals.append("AVG")

      avg_dict = dict(zip(columns, avg_vals))
      avg_dict = v.get_oxides(avg_dict)
```

```
[3]: #Calculate isobars for all samples at 3,000 bars
      isobar_list = []
      for index, row in basalts.data.iterrows():
          isobar_list.append(v.calculate_isobars_and_isopleths(sample=basalts.
      ↪get_sample_oxide_comp(samplename=row.name), temperature=1200,
      ↪pressure_list=[3000], isopleth_list=[0.5], print_status=True).result[0])
```

Calculating isobar at 3000 bars  
Calculating isobar control point at XH2Ofluid = 0  
Calculating isobar control point at XH2Ofluid = 0.25  
Calculating isopleth at XH2Ofluid = 0.5  
Calculating isobar control point at XH2Ofluid = 0.75  
Calculating isobar control point at XH2Ofluid = 1  
Done!



```
Calculating isobar at 3000 bars
Calculating isobar control point at XH2Ofluid = 0
Calculating isobar control point at XH2Ofluid = 0.25
Calculating isopleth at XH2Ofluid = 0.5
Calculating isobar control point at XH2Ofluid = 0.75
Calculating isobar control point at XH2Ofluid = 1
Done!
```

```
Calculating isobar at 3000 bars
Calculating isobar control point at XH2Ofluid = 0
Calculating isobar control point at XH2Ofluid = 0.25
Calculating isopleth at XH2Ofluid = 0.5
Calculating isobar control point at XH2Ofluid = 0.75
Calculating isobar control point at XH2Ofluid = 1
Done!
```

```
Calculating isobar at 3000 bars
Calculating isobar control point at XH2Ofluid = 0
Calculating isobar control point at XH2Ofluid = 0.25
Calculating isopleth at XH2Ofluid = 0.5
Calculating isobar control point at XH2Ofluid = 0.75
Calculating isobar control point at XH2Ofluid = 1
Done!
```

```
Calculating isobar at 3000 bars
Calculating isobar control point at XH2Ofluid = 0
Calculating isobar control point at XH2Ofluid = 0.25
Calculating isopleth at XH2Ofluid = 0.5
Calculating isobar control point at XH2Ofluid = 0.75
Calculating isobar control point at XH2Ofluid = 1
Done!
```

```
Calculating isobar at 3000 bars
Calculating isobar control point at XH2Ofluid = 0
Calculating isobar control point at XH2Ofluid = 0.25
Calculating isopleth at XH2Ofluid = 0.5
Calculating isobar control point at XH2Ofluid = 0.75
Calculating isobar control point at XH2Ofluid = 1
Done!
```

```
Calculating isobar at 3000 bars
Calculating isobar control point at XH2Ofluid = 0
Calculating isobar control point at XH2Ofluid = 0.25
Calculating isopleth at XH2Ofluid = 0.5
Calculating isobar control point at XH2Ofluid = 0.75
Calculating isobar control point at XH2Ofluid = 1
Done!
```

3



```

Calculating isobar control point at XH2Ofluid = 0.75
Calculating isobar control point at XH2Ofluid = 1
Done!
Calculating isobar at 3000 bars
Calculating isobar control point at XH2Ofluid = 0
Calculating isobar control point at XH2Ofluid = 0.25
Calculating isopleth at XH2Ofluid = 0.5
Calculating isobar control point at XH2Ofluid = 0.75
Calculating isobar control point at XH2Ofluid = 1
Done!
Calculating isobar at 3000 bars
Calculating isobar control point at XH2Ofluid = 0
Calculating isobar control point at XH2Ofluid = 0.25
Calculating isopleth at XH2Ofluid = 0.5
Calculating isobar control point at XH2Ofluid = 0.75
Calculating isobar control point at XH2Ofluid = 1
Done!

```

```

[4]: #Calculate isobar at 3,000 bars for "Average Sample"
avg_isobar = v.calculate_isobars_and_isopleths(sample=avg_dict,
↪temperature=1200, pressure_list=[3000], isopleth_list=[0.5],
↪print_status=True).result[0]

```

```

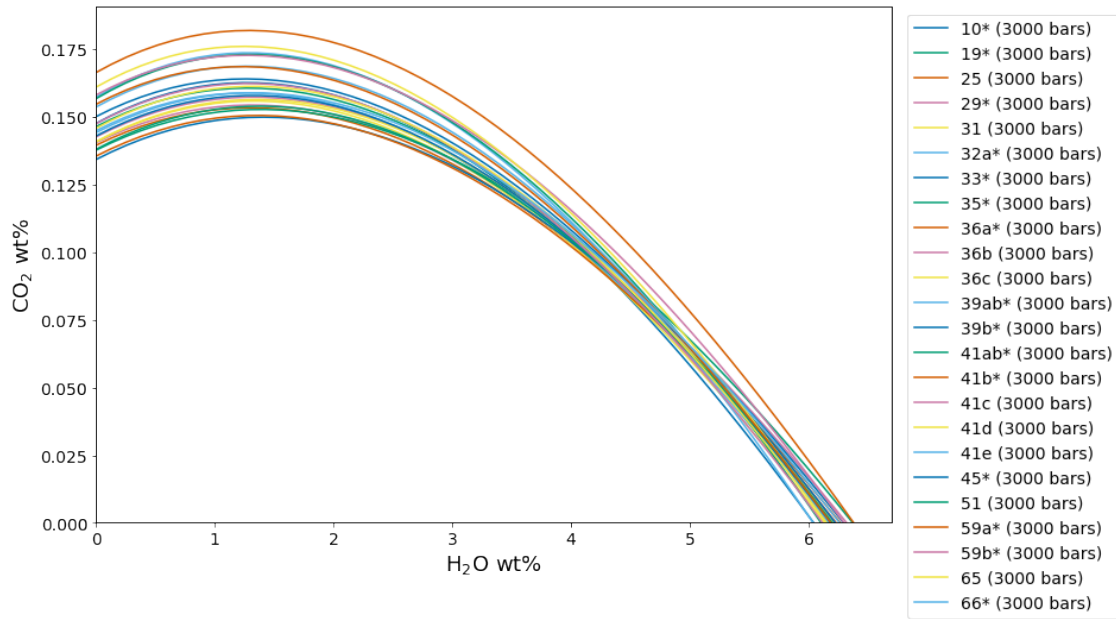
Calculating isobar at 3000 bars
Calculating isobar control point at XH2Ofluid = 0
Calculating isobar control point at XH2Ofluid = 0.25
Calculating isopleth at XH2Ofluid = 0.5
Calculating isobar control point at XH2Ofluid = 0.75
Calculating isobar control point at XH2Ofluid = 1
Done!

```

```

[5]: #Plot all isobars from dataset
v.plot(isobars=[isobar for isobar in isobar_list], isobar_labels=[row.name for
↪index, row in basalts.data.iterrows()], save_fig="cerro_negro_all_isobars.
↪pdf")

```



```
[6]: #calculate area under each curve for dataset and "Average Sample"
areas = []
samples = [row.name for index, row in basalts.data.iterrows()]
for isobar in isobar_list:
    x_vals = np.array([row["H2O_liq"] for index, row in isobar.iterrows()])
    y_vals = np.array([row["CO2_liq"] for index, row in isobar.iterrows()])
    area_under_the_curve = scipy.integrate.simps(y_vals, x_vals)
    areas.append(area_under_the_curve)

average_area = scipy.integrate.simps(avg_isobar['CO2_liq'],
    ↪ avg_isobar['H2O_liq'])
```

```
[7]: #Get maximum and minimum areas from dataset, with corresponding sample names
area_dict = dict(zip(samples, areas))
max_sample = max(area_dict, key=area_dict.get)
min_sample = min(area_dict, key=area_dict.get)
print("ISM values for entire dataset: \n" + str(area_dict) + "\n")
print("'Average Sample' ISM = " + str(average_area))
```

ISM values for entire dataset:

```
{'10*': 0.7022828487672577, '19*': 0.7099145381819657, '25': 0.6857318394996039,
'29*': 0.6959251856306994, '31': 0.6857689022034541, '32a*': 0.6981011318157478,
'33*': 0.6794449586465339, '35*': 0.6983521150777845, '36a*':
0.6737989655978469, '36b': 0.700302346052726, '36c': 0.6967336243009435,
'39ab*': 0.7498555237770486, '39b*': 0.7254222567296, '41ab*':
0.7551972181770662, '41b*': 0.8234964405556267, '41c': 0.7722060723325022,
'41d': 0.7707791453257323, '41e': 0.741450834665261, '45*': 0.698941172320567,
```

'51': 0.6872170715015408, '59a\*': 0.7393347437150143, '59b\*':  
0.7091201176739889, '65': 0.7108222436244777, '66\*': 0.710577511593821}

'Average Sample' ISM = 0.7160100984580687

```
[9]: #Now, calculate isobars for the max and min samples at multiple pressures
max_isobars, max_isopleths = v.calculate_isobars_and_isopleths(sample=basalts.
    ↳get_sample_oxide_comp(max_sample), temperature=1200, pressure_list=[500,
    ↳1000, 2000, 3000, 4000], isopleth_list=[0.5], print_status=True).result
min_isobars, min_isopleths = v.calculate_isobars_and_isopleths(sample=basalts.
    ↳get_sample_oxide_comp(min_sample), temperature=1200, pressure_list=[500,
    ↳1000, 2000, 3000, 4000], isopleth_list=[0.5], print_status=True).result

#Calculate isobars for the average composition
avg_isobars, avg_isopleths = v.calculate_isobars_and_isopleths(sample=avg_dict,
    ↳temperature=1200, pressure_list=[500, 1000, 2000, 3000, 4000],
    ↳isopleth_list=[0.5], print_status=True).result
```

Calculating isobar at 500 bars  
Calculating isobar control point at XH2Ofluid = 0  
Calculating isobar control point at XH2Ofluid = 0.25  
Calculating isopleth at XH2Ofluid = 0.5  
Calculating isobar control point at XH2Ofluid = 0.75  
Calculating isobar control point at XH2Ofluid = 1  
Calculating isobar at 1000 bars  
Calculating isobar control point at XH2Ofluid = 0  
Calculating isobar control point at XH2Ofluid = 0.25  
Calculating isopleth at XH2Ofluid = 0.5  
Calculating isobar control point at XH2Ofluid = 0.75  
Calculating isobar control point at XH2Ofluid = 1  
Calculating isobar at 2000 bars  
Calculating isobar control point at XH2Ofluid = 0  
Calculating isobar control point at XH2Ofluid = 0.25  
Calculating isopleth at XH2Ofluid = 0.5  
Calculating isobar control point at XH2Ofluid = 0.75  
Calculating isobar control point at XH2Ofluid = 1  
Calculating isobar at 3000 bars  
Calculating isobar control point at XH2Ofluid = 0  
Calculating isobar control point at XH2Ofluid = 0.25  
Calculating isopleth at XH2Ofluid = 0.5  
Calculating isobar control point at XH2Ofluid = 0.75  
Calculating isobar control point at XH2Ofluid = 1  
Calculating isobar at 4000 bars  
Calculating isobar control point at XH2Ofluid = 0  
Calculating isobar control point at XH2Ofluid = 0.25  
Calculating isopleth at XH2Ofluid = 0.5  
Calculating isobar control point at XH2Ofluid = 0.75  
Calculating isobar control point at XH2Ofluid = 1





```

Calculating isobar control point at XH2Ofluid = 0.75
Calculating isobar control point at XH2Ofluid = 1
Calculating isobar at 3000 bars
Calculating isobar control point at XH2Ofluid = 0
Calculating isobar control point at XH2Ofluid = 0.25
Calculating isopleth at XH2Ofluid = 0.5
Calculating isobar control point at XH2Ofluid = 0.75
Calculating isobar control point at XH2Ofluid = 1
Calculating isobar at 4000 bars
Calculating isobar control point at XH2Ofluid = 0
Calculating isobar control point at XH2Ofluid = 0.25
Calculating isopleth at XH2Ofluid = 0.5
Calculating isobar control point at XH2Ofluid = 0.75
Calculating isobar control point at XH2Ofluid = 1
Done!

```

```

[10]: #Make dataset with all data except for max and min values
other_data = basalts.data.drop([max_sample, min_sample])

```

```

[11]: #set up what to pass to v.plot
isobars = [max_isobars,
           min_isobars,
           avg_isobars]

isobar_labels = ["Max",
                 "Min",
                 "Avg"]

custom_H2O=[basalts.get_sample_oxide_comp(max_sample)["H2O"],
            basalts.get_sample_oxide_comp(min_sample)["H2O"],
            avg_dict["H2O"],
            other_data["H2O"]]

custom_CO2=[basalts.get_sample_oxide_comp(max_sample)["CO2"],
            basalts.get_sample_oxide_comp(min_sample)["CO2"],
            avg_dict["CO2"],
            other_data["CO2"]]

custom_labels = [str(max_sample) + " (max)",
                 str(min_sample) + " (min)",
                 "Average Sample",
                 "Cerro Negro MI"]

custom_colors = [v.color_list[0],
                 v.color_list[1],
                 v.color_list[2],
                 'silver']

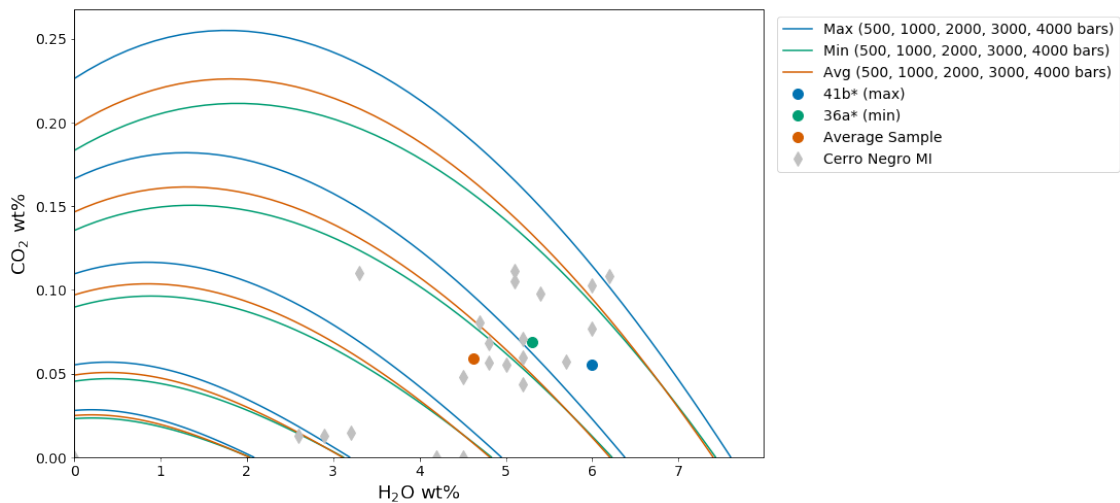
```

```

custom_symbols = ['o',
                  'o',
                  'o',
                  'd']

v.plot(isobars=isobars, isobar_labels=isobar_labels,
       custom_H2O=custom_H2O,
       custom_CO2=custom_CO2,
       custom_labels=custom_labels,
       custom_colors=custom_colors,
       custom_symbols=custom_symbols,
       save_fig='isobar_comparison_figure.pdf')

```



```

[12]: pressure_vals = [500, 1000, 2000, 3000, 4000]

max_IMS_dict = {}
min_IMS_dict = {}
avg_IMS_dict = {}

IMS_dicts = [max_IMS_dict,
             min_IMS_dict,
             avg_IMS_dict]

for i in range(len(isobars)):
    IMS_dicts[i].update({"Pressure": pressure_vals})
    IMS_list = []
    for pressure in pressure_vals:

```

```

        IMS_list.append(scipy.integrate.simps(isobars[i].
↪loc[isobars[i]['Pressure']==pressure]["CO2_liq"], isobars[i].
↪loc[isobars[i]['Pressure']==pressure]["H2O_liq"]))
        IMS_dicts[i].update({"IMS": IMS_list})

labels = ["Maximum, Minimum, Average"]

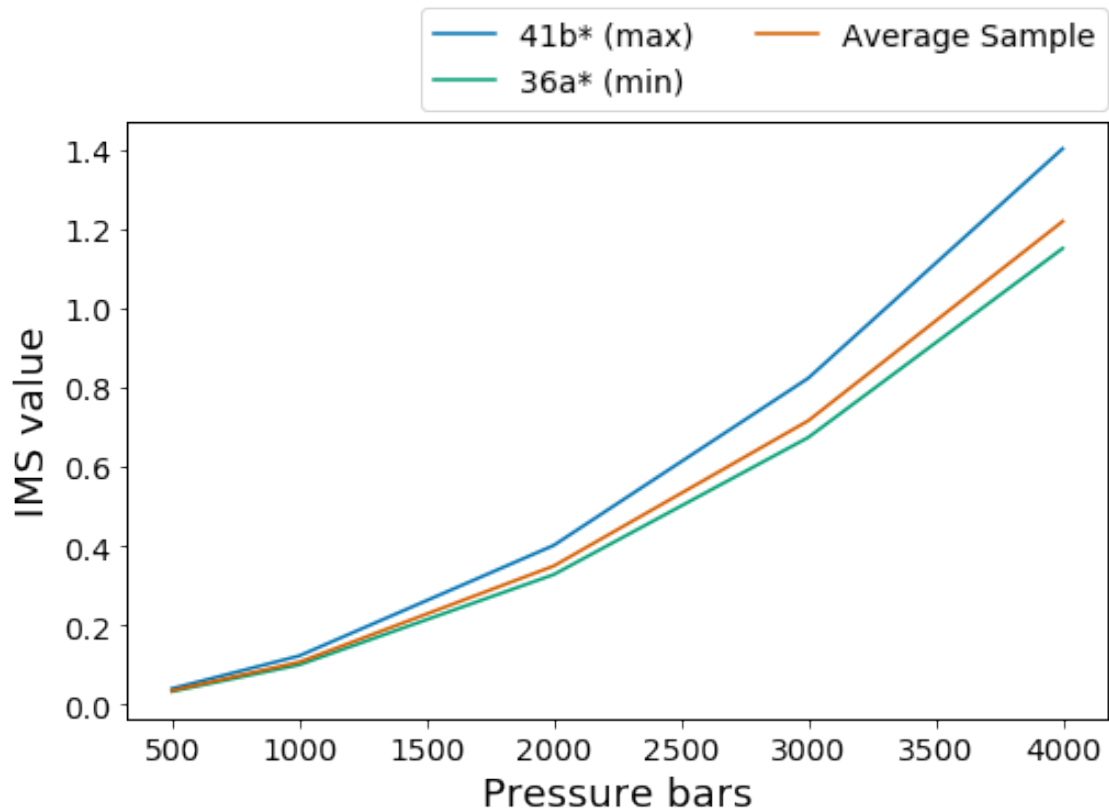
fig, ax = plt.subplots(1, figsize = (8,5))

for i in range(len(IMS_dicts)):
    ax.plot(IMS_dicts[i]["Pressure"], IMS_dicts[i]["IMS"],
↪label=custom_labels[i])
    ax.set_xlabel("Pressure bars")
    ax.set_ylabel("IMS value")

ax.legend(bbox_to_anchor=(0., 1.02, 1., .102), loc='lower right',
          ncol=2, borderaxespad=0.)

fig.savefig('IMS_plot.pdf')

```



```
[13]: max_IMS_dict
```

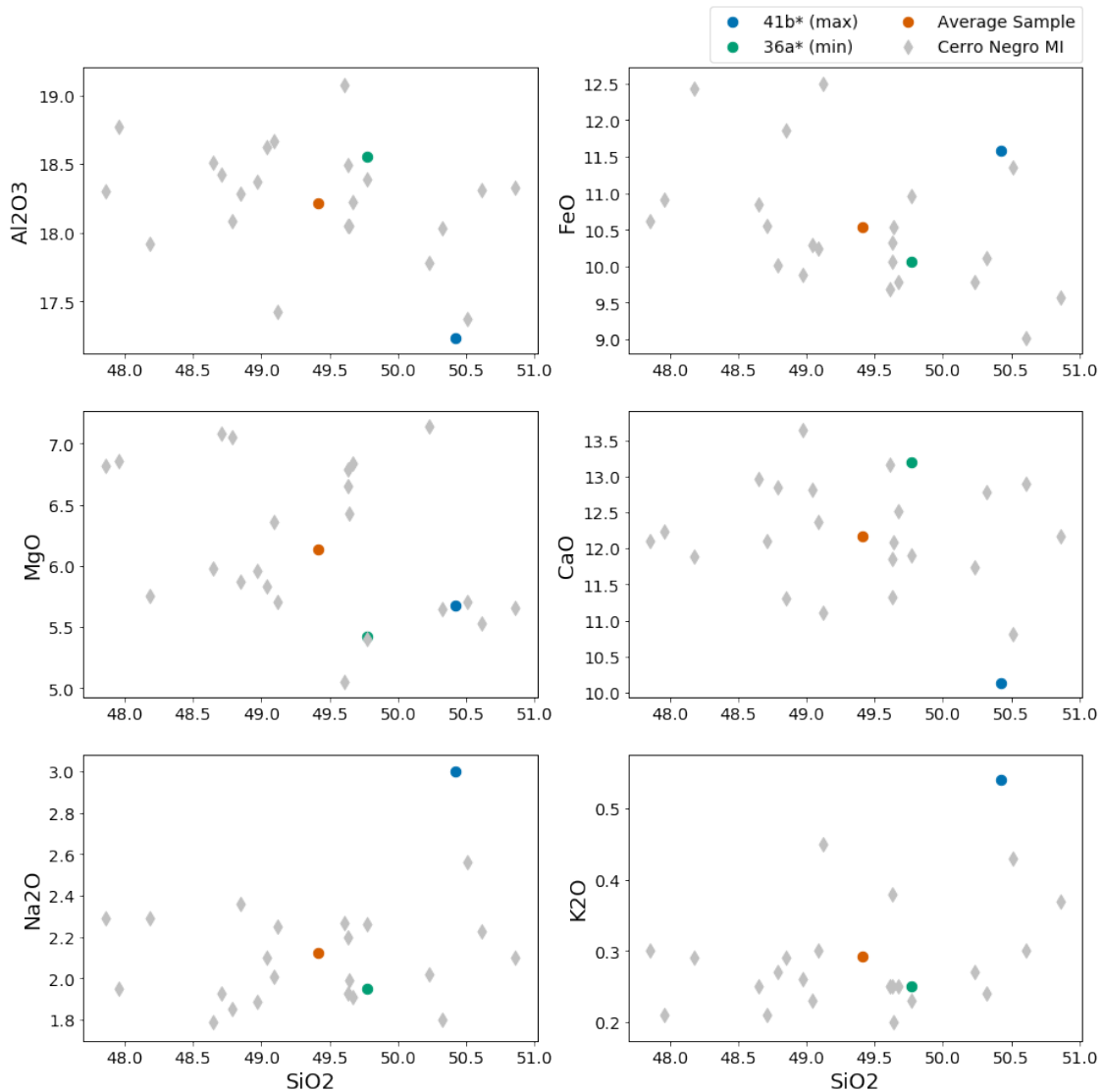
```
[13]: {'Pressure': [500, 1000, 2000, 3000, 4000],  
      'IMS': [0.03964674030557643,  
             0.12230513548704117,  
             0.4013125282055653,  
             0.8234964405556267,  
             1.4033476847858979]}
```

```
[14]: other_oxides = ["Al2O3", "FeO", "MgO", "CaO", "Na2O", "K2O"]  
my_samples = [basalts.get_sample_oxide_comp(max_sample),  
              basalts.get_sample_oxide_comp(min_sample),  
              avg_dict,  
              other_data]  
  
fig, axs = plt.subplots(3,2, figsize = (15,15))  
print(len(axs))  
  
for j in range(len(my_samples)):  
    axs[0][0].scatter(my_samples[j]["SiO2"], my_samples[j]["Al2O3"],  
→marker=custom_symbols[j], s=70, color=custom_colors[j],  
→label=custom_labels[j])  
    axs[0][0].set_ylabel("Al2O3")  
    axs[0][1].scatter(my_samples[j]["SiO2"], my_samples[j]["FeO"],  
→marker=custom_symbols[j], s=70, color=custom_colors[j],  
→label=custom_labels[j])  
    axs[0][1].set_ylabel("FeO")  
    axs[1][0].scatter(my_samples[j]["SiO2"], my_samples[j]["MgO"],  
→marker=custom_symbols[j], s=70, color=custom_colors[j],  
→label=custom_labels[j])  
    axs[1][0].set_ylabel("MgO")  
    axs[1][1].scatter(my_samples[j]["SiO2"], my_samples[j]["CaO"],  
→marker=custom_symbols[j], s=70, color=custom_colors[j],  
→label=custom_labels[j])  
    axs[1][1].set_ylabel("CaO")  
    axs[2][0].scatter(my_samples[j]["SiO2"], my_samples[j]["Na2O"],  
→marker=custom_symbols[j], s=70, color=custom_colors[j],  
→label=custom_labels[j])  
    axs[2][0].set_ylabel("Na2O")  
    axs[2][0].set_xlabel("SiO2")  
    axs[2][1].scatter(my_samples[j]["SiO2"], my_samples[j]["K2O"],  
→marker=custom_symbols[j], s=70, color=custom_colors[j],  
→label=custom_labels[j])  
    axs[2][1].set_ylabel("K2O")  
    axs[2][1].set_xlabel("SiO2")  
  
axs[0][1].legend(bbox_to_anchor=(0., 1.02, 1., .102), loc='lower right',
```

```
ncol=2, borderaxespad=0.)

fig.savefig('cerro_negro_dataset.pdf')
```

3



## 1 Alternative plots

```
[15]: #Calculate Saturation Pressure for all samples
other_file = v.ExcelFile(filename=None, dataframe=other_data)
satP_other = other_file.calculate_saturation_pressure(temperature=1200)
```

```

satP_max = v.calculate_saturation_pressure(sample=basalts.
↳get_sample_oxide_comp(max_sample), temperature=1200, verbose=True).result
satP_min = v.calculate_saturation_pressure(sample=basalts.
↳get_sample_oxide_comp(min_sample), temperature=1200, verbose=True).result
satP_avg = v.calculate_saturation_pressure(sample=avg_dict, temperature=1200,
↳verbose=True).result

```

```

Calculating sample 10*
Calculating sample 19*
Calculating sample 25
Calculating sample 29*
Calculating sample 31
Calculating sample 32a*
Calculating sample 33*
Calculating sample 35*
Calculating sample 36b
Calculating sample 36c
Calculating sample 39ab*
Calculating sample 39b*
Calculating sample 41ab*
Calculating sample 41c
Calculating sample 41d
Calculating sample 41e
Calculating sample 45*
Calculating sample 51
Calculating sample 59a*
Calculating sample 59b*
Calculating sample 65
Calculating sample 66*
Done!

```

```

[16]: #Create alternative plots using Matplotlib
single_data = [satP_max,
               satP_min,
               satP_avg]

single_samples = [basalts.get_sample_oxide_comp(max_sample),
                  basalts.get_sample_oxide_comp(min_sample),
                  avg_dict]

fig, axs = plt.subplots(3, figsize = (8,15))
axs[0].scatter(satP_other["SaturationP_bars_VESIcal"], satP_other["H2O"],
↳marker=custom_symbols[3], s=70, color=custom_colors[3],
↳label=custom_labels[3])
axs[1].scatter(satP_other["SaturationP_bars_VESIcal"], satP_other["CO2"],
↳marker=custom_symbols[3], s=70, color=custom_colors[3],
↳label=custom_labels[3])

```

```

axs[2].scatter(satP_other["SaturationP_bars_VESIcal"],  

    ↳satP_other["XH20_fl_VESIcal"], marker=custom_symbols[3], s=70,  

    ↳color=custom_colors[3], label=custom_labels[3])

for j in range(len(single_data)):
    axs[0].scatter(single_data[j]["SaturationP_bars"],  

    ↳single_samples[j]["H2O"], marker=custom_symbols[j], s=70,  

    ↳color=custom_colors[j], label=custom_labels[j])
    axs[0].set_ylabel("Dissolved H$_2$O wt%")
    axs[0].set_ylim(0)
    axs[0].set_xlim(0)
    axs[1].scatter(single_data[j]["SaturationP_bars"],  

    ↳single_samples[j]["CO2"], marker=custom_symbols[j], s=70,  

    ↳color=custom_colors[j], label=custom_labels[j])
    axs[1].set_ylabel("Dissolved CO$_2$ wt%")
    axs[1].set_ylim(0)
    axs[1].set_xlim(0)
    axs[2].scatter(single_data[j]["SaturationP_bars"],  

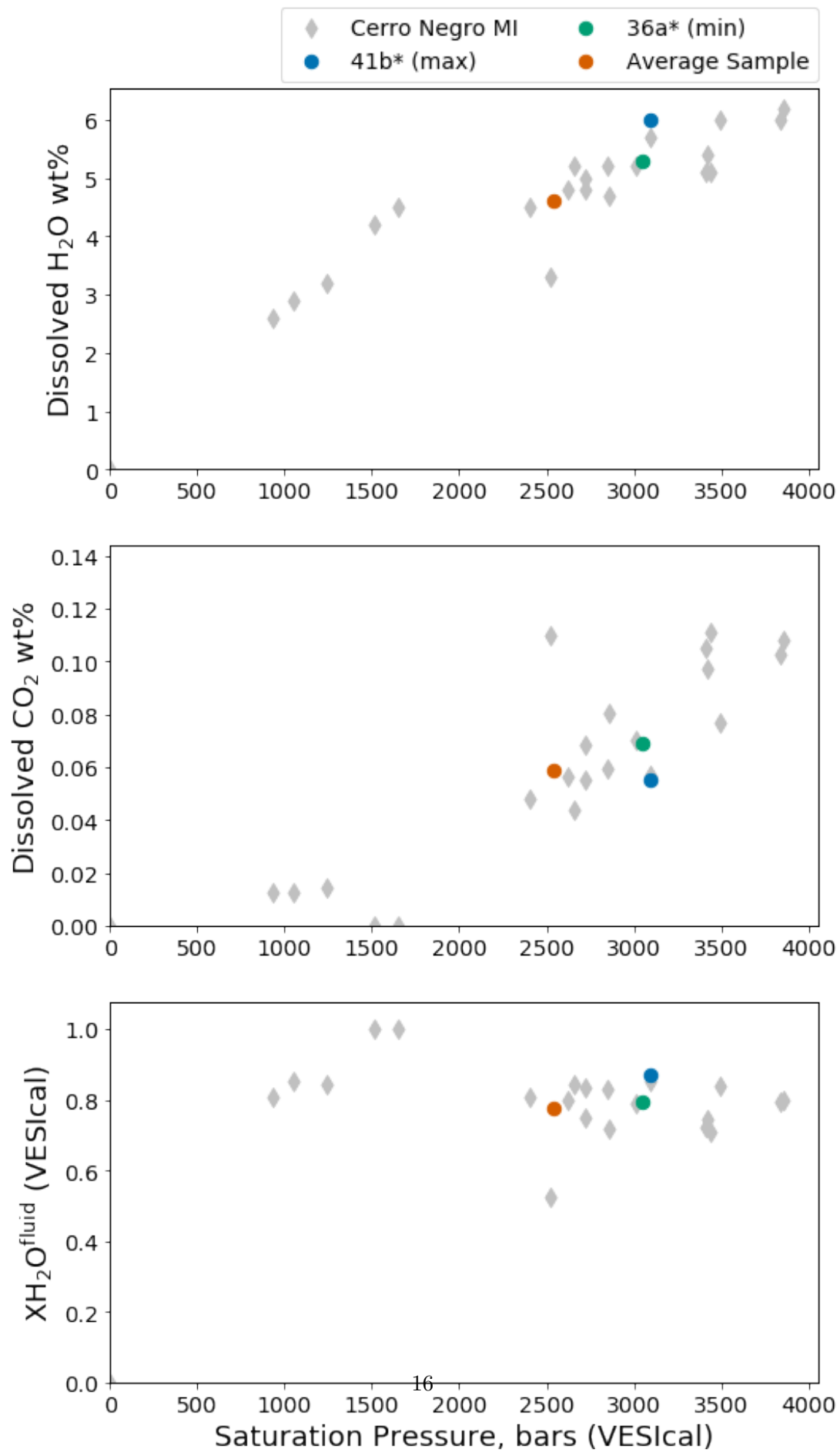
    ↳single_data[j]["XH20_fl"], marker=custom_symbols[j], s=70,  

    ↳color=custom_colors[j], label=custom_labels[j])
    axs[2].set_ylabel("XH$_2$O$^{fluid}$ (VESIcal)")
    axs[2].set_ylim(0)
    axs[2].set_xlabel("Saturation Pressure, bars (VESIcal)")
    axs[2].set_xlim(0)

axs[0].legend(bbox_to_anchor=(0., 1.02, 1., .102), loc='lower right',
    ncol=2, borderaxespad=0.)

fig.savefig('alternate_plots.pdf')

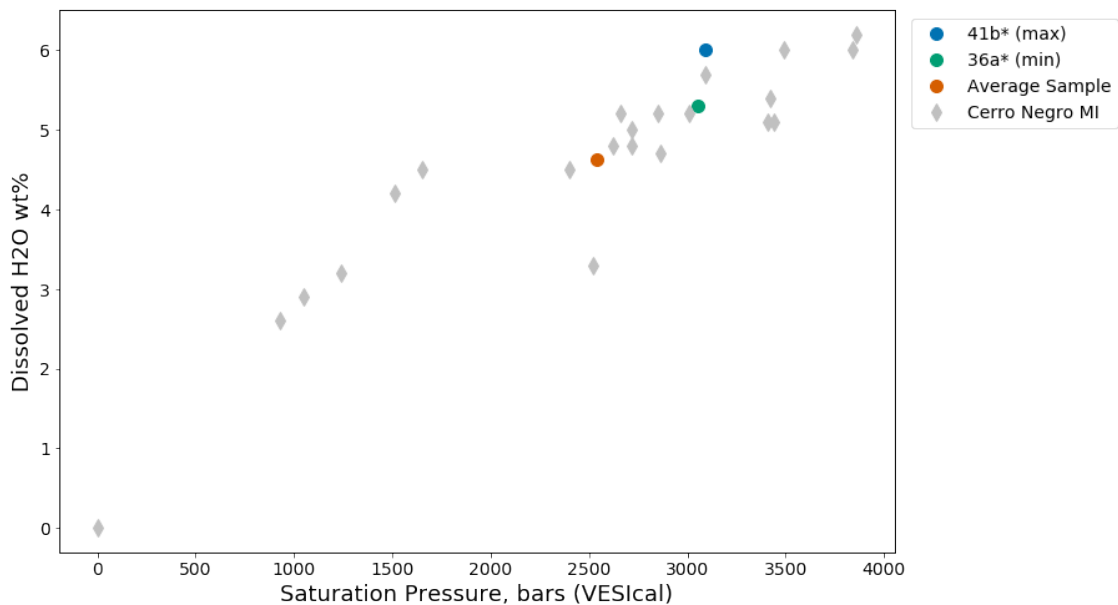
```





```
[17]: #Create alternative plots using VESIcal's scatterplot() function
single_samples = [basalts.get_sample_oxide_comp(max_sample),
                  basalts.get_sample_oxide_comp(min_sample),
                  avg_dict]

v.scatterplot(custom_x=[satP_max['SaturationP_bars'],
                        satP_min['SaturationP_bars'],
                        satP_avg['SaturationP_bars'],
                        satP_other['SaturationP_bars_VESIcal']],
             custom_y=[single_samples[0]['H2O'],
                       single_samples[1]['H2O'],
                       single_samples[2]['H2O'],
                       satP_other['H2O']],
             custom_symbols=custom_symbols,
             custom_colors=custom_colors,
             custom_labels=custom_labels,
             xlabel="Saturation Pressure, bars (VESIcal)",
             ylabel="Dissolved H2O wt%")
```



## 2 Calculate saturation pressures for each composition

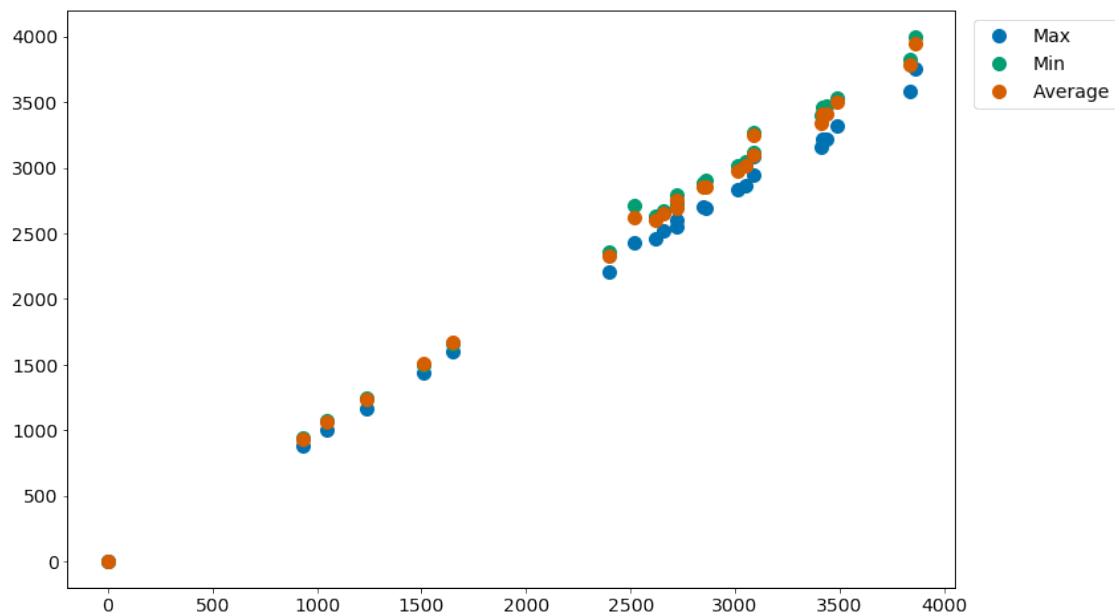
Here we calculate the saturation pressures of each melt inclusion using: a) the composition of the melt inclusion; b) the composition of the “minimum” melt inclusion (36a); c) the composition of the “maximum” melt inclusion (41b); and d) the composition of the “average” melt inclusion as

calculated above.

```
[19]: satP_data_orig = v.ExcelFile('cerro_negro_satP_compare.xlsx')
      satP_data_min = v.ExcelFile('cerro_negro_satP_compare.xlsx', sheet_name='min')
      satP_data_max = v.ExcelFile('cerro_negro_satP_compare.xlsx', sheet_name='max')
      satP_data_avg = v.ExcelFile('cerro_negro_satP_compare.xlsx', sheet_name='avg')
```

```
[20]: satP_orig = satP_data_orig.calculate_saturation_pressure(temperature=1200,
      ↪print_status=False)
      satP_min = satP_data_min.calculate_saturation_pressure(temperature=1200,
      ↪print_status=False)
      satP_max = satP_data_max.calculate_saturation_pressure(temperature=1200,
      ↪print_status=False)
      satP_avg = satP_data_avg.calculate_saturation_pressure(temperature=1200,
      ↪print_status=False)
```

```
[21]: v.scatterplot(custom_x=[satP_orig["SaturationP_bars_VESIcal"],
      ↪satP_orig["SaturationP_bars_VESIcal"],
      ↪satP_orig["SaturationP_bars_VESIcal"]],
      custom_y=[satP_max["SaturationP_bars_VESIcal"],
      ↪satP_min["SaturationP_bars_VESIcal"], satP_avg["SaturationP_bars_VESIcal"]],
      custom_labels=["Max", "Min", "Average"])
```



```
[28]: f = 100*(satP_min["SaturationP_bars_VESIcal"] -
      ↪satP_max["SaturationP_bars_VESIcal"])/satP_max["SaturationP_bars_VESIcal"]
      fmean = f.dropna().mean()
      print(fmean)
```

```
print(satP_min["SaturationP_bars_VESIcal"])
print(satP_max["SaturationP_bars_VESIcal"])
print(satP_avg["SaturationP_bars_VESIcal"])
```

6.785437703427779

10*	2360
19*	3470
25	2670
29*	2900
31	3400
32a*	3820
33*	3460
35*	2790
36a*	3050
36b	940
36c	1240
39ab*	2720
39b*	3120
41ab*	2880
41b*	3270
41c	4000
41d	2710
41e	3530
45*	1500
51	3020
59a*	1070
59b*	0
65	2630
66*	1660

Name: SaturationP\_bars\_VESIcal, dtype: int64

10*	2210
19*	3220
25	2520
29*	2690
31	3160
32a*	3580
33*	3220
35*	2600
36a*	2860
36b	880
36c	1160
39ab*	2550
39b*	2940
41ab*	2700
41b*	3090
41c	3750

41d	2430
41e	3320
45*	1440
51	2830
59a*	1000
59b*	0
65	2460
66*	1600

Name: SaturationP\_bars\_VESIcal, dtype: int64

10*	2330
19*	3410
25	2650
29*	2850
31	3340
32a*	3780
33*	3410
35*	2750
36a*	3020
36b	930
36c	1230
39ab*	2690
39b*	3100
41ab*	2850
41b*	3250
41c	3950
41d	2620
41e	3500
45*	1510
51	2980
59a*	1060
59b*	0
65	2600
66*	1670

Name: SaturationP\_bars\_VESIcal, dtype: int64

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