Calculating μ-μ diagrams tutorial

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In this tutorial I outline the construction of μ-μ diagrams. Such calculations are a fairly recent facility in THERMOCALC, so can only be done with version 3.25 and later. This tutorial was calculated with tc333i on a mac.

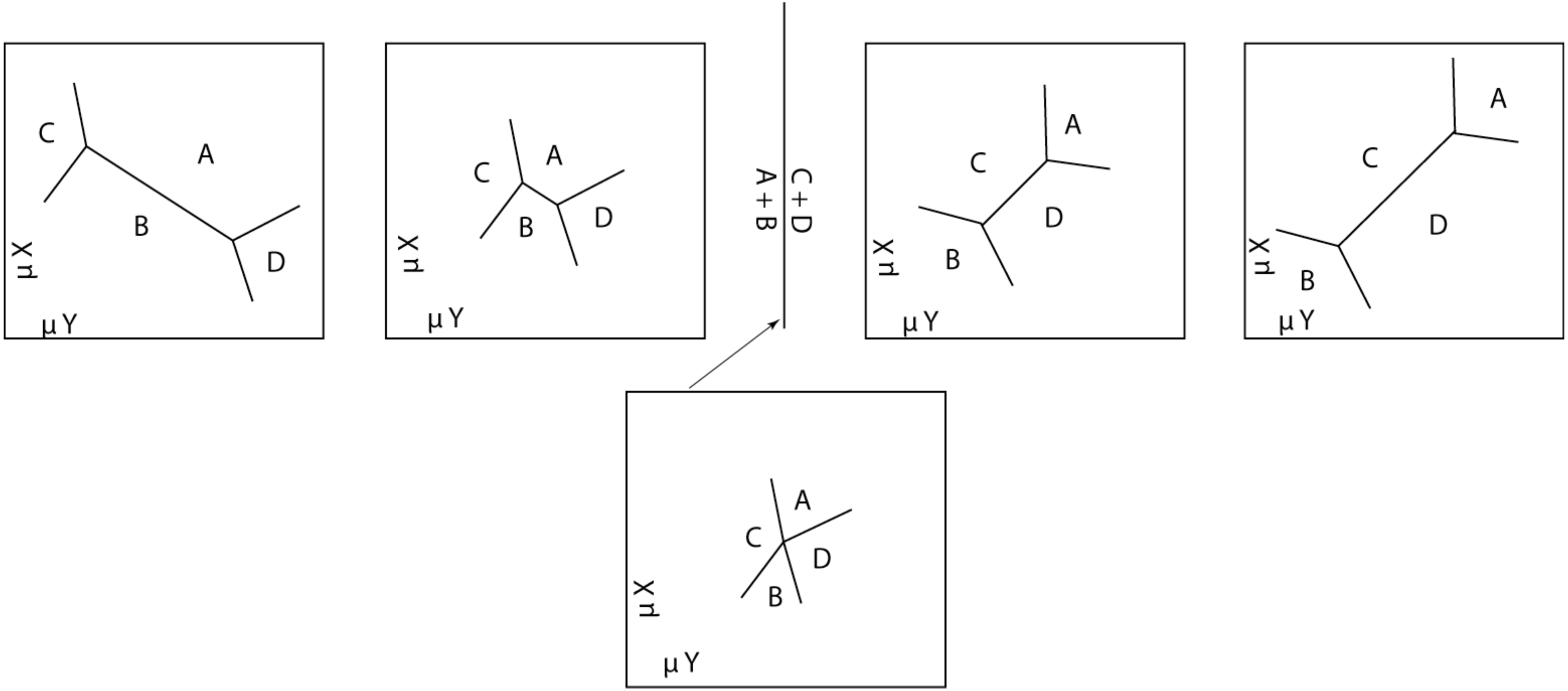
Before doing this tute you should read:

White, R.W., Powell, R. & Baldwin J.A., 2008. Calculated phase equilibria involving chemical potentials to investigate the textural evolution of metamorphic rocks. *Journal of Metamorphic Geology*, **26**, 181–198.

Which outlines many aspects of the approach. I also recommend reading:

White, R.W. & Powell, R. 2010/2011. On the interpretation of retrograde reaction textures in granulite facies rocks. *Journal of Metamorphic Geology*, **29**, xxx–xxx. (see JMG website)

Before embarking on calculating μ-μ diagrams I will go over some of the basic topological features. There are some complications regarding real and effective variances in these diagrams. Firstly, setting a component as a μ value effectively removes that component from consideration in the phase rule such that the variance is reduced by one. At fixed P-T, divariant assemblages occur as points on μ-μ diagrams, trivariant assemblages as lines and quadrivariant assemblages as fields. A good way of seeing why this is so is to consider that the values of the chemical potentials are a consequence of the compositions of the minerals in an assemblage, and for a divariant assemblage at fixed P-T these compositions and hence the chemical potentials are fixed. For a trivariant assemblage we can change the composition of one of the phases and the other is dependent giving one effective degree of freedom. The relationship between the divariant points and any univariant equilibria are also important. For a univariant reaction A + B = C + D, there are two stable divariant assemblages either side of the reaction (A-B-C & A-B-D on the low T side and A-C-D & B-C-D on the high T side). Approaching the reaction from lower T, the divariant points on a μ-μ diagram converge, and meet at the univariant. Above this, the μ-μ diagram inverts. Below is a sketch of this:



In the first exercise I will go through construction of a simple μMgO–μSiO2 diagram in the very simple MAS system at high T conditions, taken from White *et al*., 2008. In these diagrams one chemical potential has to be left as a passive variable, in this case it is μAl2O3.
In your THERMOCALC folder you will need the following files:

tc-mu1
tc-MASp#
dr-mu1 (in whatever folder you have drawpd)

In your tc-prefs file use the scripts;

```
calcmode 1
scriptfile mu1
```

so THERMOCALC automatically uses this script file and knows you are doing phase diagram calculations.

There are two important scripts for μ-μ diagrams being:

```
calcmu         &          setmu
```

This exercise involves sapphirine so you need to use the tc-ds55s dataset. In you tc-prefs file you need the script:

```
dataset 55s
```

To work out which divariant assemblages are stable at the chosen conditions requires knowledge of the underlying univariant relationships in MAS. The calculations here will be done at 9kbar and at various temperatures between 1000 and 1050°C. At these conditions the only MAS reaction to be considered (from Kelsey *et al.*, 2004 *JMG*, **22**, 559-578) is:

opx + sill = sa + q,

which occurs at 1030°C. So at T below this the divariant assemblages opx-sill-sa and opx-sill-q are stable. In addition, the quartz-absent divariant assemblage sa-sill-cor is also stable from the quartz-absent reaction opx + cor = sa + sill that occurs at lower T. The first diagram I'll draw at 1020°C with the stable divariant points being opx-sill-q, opx-sill-sa & sa-sill-cor. To do this the following scripts are set as follows:

```
calctatp yes

setdefTwindow no 600.001 1300.001
setdefPwindow no 3  16

setTwindow yes 1020 1020
setPwindow yes 9 9

calcmu yes
setmu no
```

Run thermocalc for the assemblage opx-sill-q to get:

```
which phases : opx sill q
no phases in excess (from script)
variance of required equilibrium (2?) :

specification of PT window:
at fixed P = 9.0 kbar and T = 1020?C (from script)
```

```
<===================================================>
phases : opx, sill, q

-------------------------------------------------------------------
 P(kbar)     T(?C)   y(opx)
    9.00    1020.0   0.1851

  mu       SiO2    Al2O3      MgO
        -997.47 -1813.06  -699.63
```

Note how the μ's are always negative, so the smaller the absolute value the higher the μ. Running the other two points gives

```
<===================================================>
phases : sa, opx, sill

-------------------------------------------------------------------
 P(kbar)     T(?C)    y(sa)   y(opx)
    9.00    1020.0   0.2480   0.1860

  mu       SiO2    Al2O3      MgO
        -997.53 -1813.00  -699.57
```

and

```
<===================================================>
phases : sa, sill, cor

-------------------------------------------------------------------
 P(kbar)     T(?C)    y(sa)
    9.00    1020.0   0.2864

  mu       SiO2    Al2O3      MgO
        -998.82 -1811.71  -700.45
```

With the tc-mu1-dr data being

```
% ------------------------------
d<k>   opx sill q   divariant

        %        SiO2       Al2O3         MgO
9.000 1020.00
             -997.4706  -1813.0616   -699.6306

% ------------------------------
d<k>   sa opx sill   divariant

        %        SiO2       Al2O3         MgO
9.000 1020.00
             -997.5341  -1812.9983   -699.5737

% ------------------------------
d<k>   sa sill cor   divariant

        %        SiO2       Al2O3         MgO
9.000 1020.00
        -998.8209  -1811.7113   -700.4471
```

copy and paste the tc-dr data into the dr-mu1 datafile. You will have to manually change the existing "d<k>" names to i1, i2 etc
Note also that each line or block of data has 5 variables (ie P, T and 3 μ's) and that x & y are variables 3 (SiO2) and 5 (MgO) respectively. Thus, the initial info in the drawpd file should look like:

```
5    % no of variables in each line of data,
     % in this case, P, T

5    % 6 (KFMASH) - 3 (+q+mu+H2O)

3 5  % which columns to be x,y in phase diagram
```

The other important information regarding the x & y axes (window & ticks) should be set as

```
window -1000 -997 -701 -699

bigticks 0.5 -1000 0.5 -701

smallticks 0.1 0.1
```

running drawpd gives the wholly unimpressive diagram with just 3 points. To calculate lines we need to set one of the μ's that we use as an axis. Here I will set μMgO, and calculate the sa-sill line. We want to set μMgO to a series of different values that define a line. To do this we use the "setmu" script as below

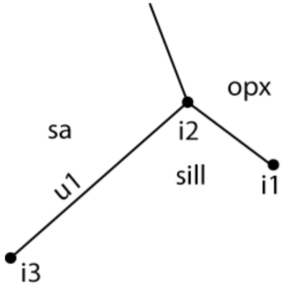
```
setmu MgO
```

so that we are prompted for a μMgO range and μMgO increments. Although this line is nominally trivariant, by setting μMgO we make it a series of divariant points that define a line. So running THERMOCALC with this script set and the sa-sill line, the input/output looks like (μ range and increments highlighted:

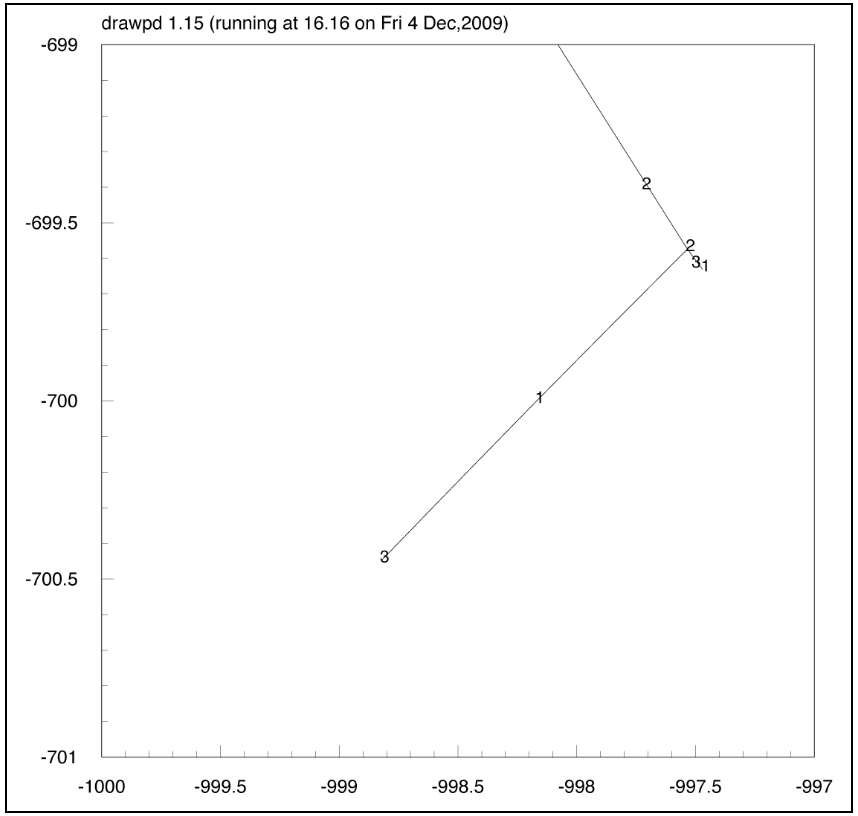
```
which phases : sa sill
no phases in excess (from script)
variance of required equilibrium (2?) : 2

specification of PT window:
at fixed P = 9.0 kbar and T = 1020.0?C (from script)
mu(MgO): low, high : -701 -699
? window : -701.0 <-> -699.0 :
? interval : 0.2
<==================================================>
phases : sa, sill, (mu(MgO))

--------------------------------------------------------------------
 P(kbar)     T(?C)    y(sa)
    9.0    1020.0   0.3121

  mu       SiO2    Al2O3      MgO
       -999.61 -1810.92  -701.00
--------------------------------------------------------------------
 P(kbar)     T(?C)    y(sa)
    9.0    1020.0   0.3027

  mu       SiO2    Al2O3      MgO
       -999.33 -1811.21  -700.80
--------------------------------------------------------------------
```

etc

This line runs from i2 to i3. Normally you would have to think about the topology of the diagram which has to follow Schreinemakers rules. If you don’t understand Schreinemakers rules, then look at the “introduction to phase diagrams” page, any metamorphic textbook or take up palaeontology. For this diagram its pretty easy as knowing the sa-sill line and sill-opx line both connect the points i2-i3 and i1-i2 respectively tell us where the sill field is and this part of the diagram must look like



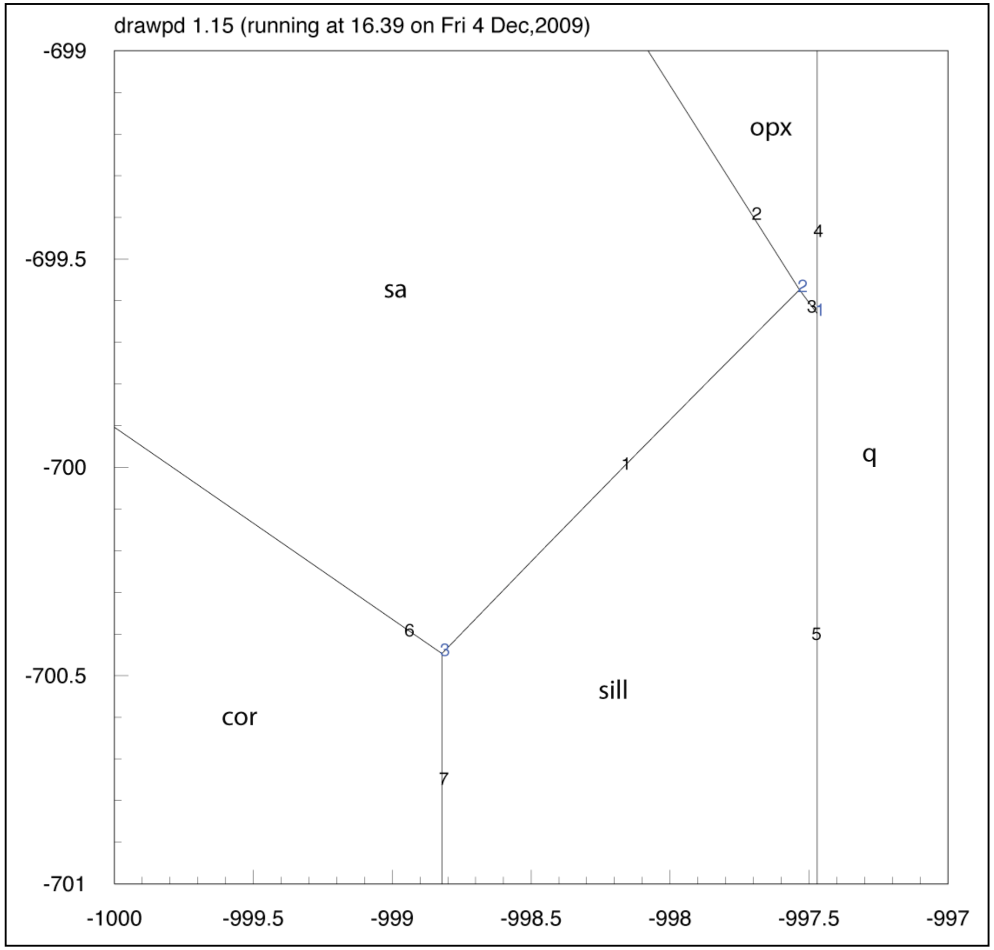
So we can calculate the sa-opx and sill-opx lines
(note; the sill-opx line is quite short so you will need small increments).
The diagram should look like that to the right:



Now the opx-q and opx-sill lines need to be calculated. The first one (opx-q) is straightforward and must be a vertical line as quartz fixes µSiO2 at a single value (that of µSiO2 at i1). But you won’t be able to calculate the sill-q line as it is degenerate and THERMOCALC can’t write a reaction. However as it is vertical and at the same µSiO2 of the opx-q line we can just calculate the metastable extension of the opx-q line and use this as the boundary for sill-q. The sa-cor line is straightforward to calculate, but like with sill-q, the cor-sill line can’t be calculated. Given that both cor and sill are nominally pure phases and contain no MgO (in terms of the model compositions) the boundary between the two must be vertical (ie at constant µSiO2) and the value of µSiO2 for this line is that of i3, then we can just manually make a line using the information from i3 and just adjusting the µMgO value. The list I made looks like:

```
% ------------------------------
u7   sa sill cor   divariant % modified to make cor-sill line

        %        SiO2       Al2O3         MgO
9.000 1020.00
             -998.8209  -1811.7113   -701.0000
9.000 1020.00
             -998.8209  -1811.7113   -700.7500
9.000 1020.00
             -998.8209  -1811.7113   -700.5000
9.000 1020.00
             -998.8209  -1811.7113   -700.2500
```

The finished and labelled diagram looks like:



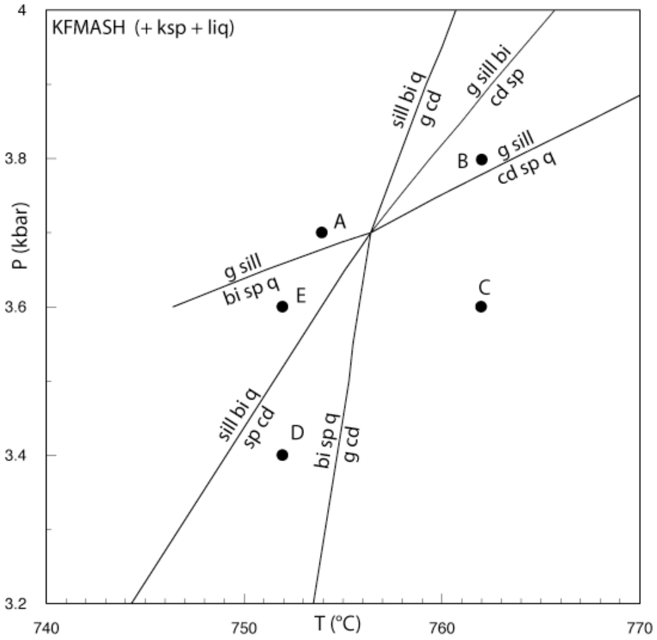
You could now calculate the μMgO–μSiO2 diagram for 1040°C where sa-q assemblages are stable (see White *et al.*, 2008 Fig. 3a for the resultant diagram). Note you will have to change your x & y ranges as the whole diagram also shifts in μMgO–μSiO2 space as well as changing topology. The following values should work

```
window -1002 -1000 -703 -700
```

```
bigticks 0.5 -1002 0.5 -703
```

Part 2. Calculations in a bigger system.

Calculating μ-μ sections in larger systems requires the system be effectively reduced to 3 components (the two components used in the axes and one unconstrained component). The system can be reduced in two ways, one by setting excess phases, the other by setting μ values. Both approaches can be used but the effects are typically different (an important exception is where a phase is also a component eg quartz/SiO2). In the following these differences are highlighted. In the following examples the calculations are undertaken in KFMASH, looking at equilibria involving g, sill, sp, cd, ksp, liq & q at low P. As a starting point the univariant equilibria under consideration are shown below:



To calculate a μ-μ diagram for point C (3.6kbar 762°C) above for example, we have to reduce the 6 component system to 3 components. We can do this relatively easily by setting excess phases, and in this example they will be quartz, K-feldspar and melt (liq) leaving Al2O3, FeO and MgO. Leaving Al2O3 as our dependent variable we have μFeO and μMgO as our axes. The input files to use here are:

tc-mu2	The script file
tc-KFMASHp	The a-x file
dr-mu2	The drawpd input file

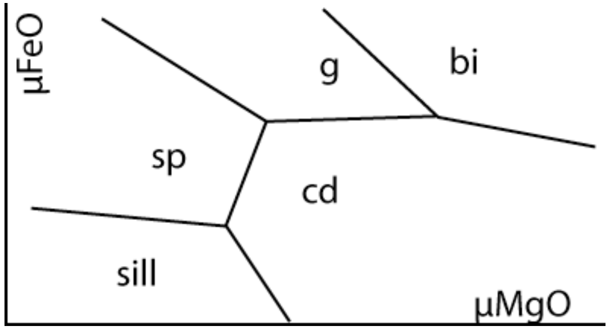
you should also make sure the script in the tc-prefs file is set to ds55 ie `dataset 55`

so running THERMOCALC with the above input files (where the in-excess phases and P-T conditions are already set) you can start to calculate the divariant points, which from the grid above are sp-cd-sill, sp-cd-g and g-cd-bi.

```
<================================================>
phases : cd, sp, sill, (liq, ksp, q)
--------------------------------------------------------------------
 P(kbar)     T(°C)    x(cd)    h(cd)    x(sp)     q(L)   fsp(L)    ol(L)     x(L)   h2o(L)
    3.60     762.0   0.7590   0.5043   0.9537   0.2636   0.2705 0.003527   0.9149   0.4346

  mu        H2O     SiO2    Al2O3      MgO      FeO      K2O
       -390.06  -977.34 -1776.14  -702.96  -366.47  -965.49

<================================================>
phases : cd, g, sp, (liq, ksp, q)
--------------------------------------------------------------------
 P(kbar)     T(°C)    x(cd)    h(cd)     x(g)    x(sp)     q(L)   fsp(L)    ol(L)     x(L)   h2o(L)
    3.60     762.0   0.7594   0.5047   0.9496   0.9538   0.2637   0.2707 0.003920   0.9150   0.4351

  mu        H2O     SiO2    Al2O3      MgO      FeO      K2O
       -390.05  -977.34 -1776.36  -702.75  -366.24  -965.26

<================================================>
phases : bi, cd, g, (liq, ksp, q)
--------------------------------------------------------------------
 P(kbar)     T(°C)    x(bi)    y(bi)    Q(bi)    x(cd)    h(cd)     x(g)     q(L)   fsp(L)    ol(L)     x(L)   h2o(L)
    3.60     762.0   0.8657   0.5889  0.04525   0.7085   0.5062   0.9353   0.2642   0.2715 0.004559   0.8973   0.4368

  mu        H2O     SiO2    Al2O3      MgO      FeO      K2O
       -389.99  -977.34 -1777.09  -700.39  -366.13  -964.54
```

The first thing to notice is that by setting (+q) we have fixed μSiO2 (-977.39), but the other components effectively removed from the system (K2O & H2O by projecting from ksp and liq respectively) are different at each calculated point. In other words setting these two excess phases constrains the chemical potentials of K2O and H2O (as they must for a divariant assemblage) but does not fix them at a single value. The consequences of this will hopefully become more apparent later in the tutorial where these components are removed from the effective system by fixing their chemical potentials.

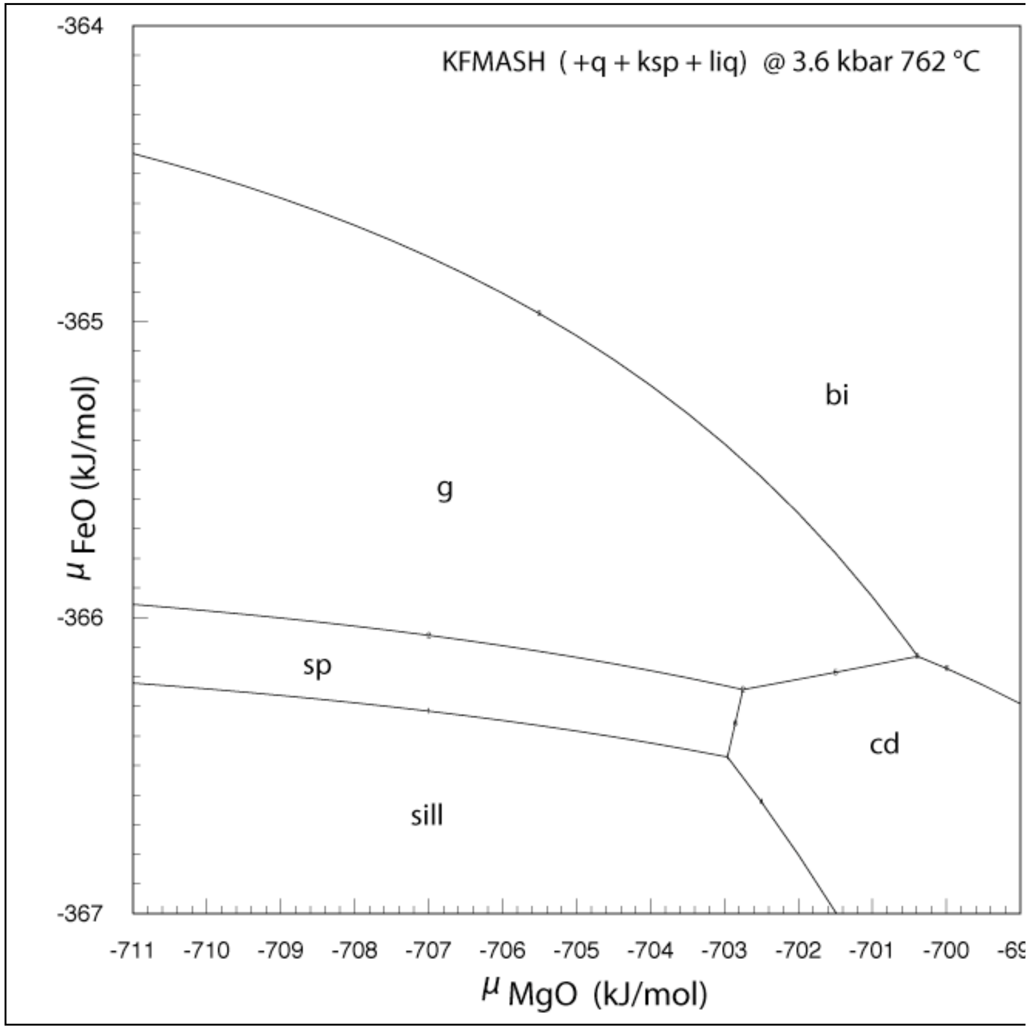
Just from the positions of these points we can constrain much of the topology of the diagram as the lines that connect these points in part define the cd field which must have its boundaries forming angles less than 180°. Ie this part of the diagram has to look something like that below:



Calculating the lines requires setting μFeO or μMgO to a range of values as done in the first example. Here, I set μMgO as it turns out that the lines are all fairly flat. So for the sill-sp line, I got

```
which phases : sill sp
variance of required equilibrium (2?) :

specification of PT window:
at fixed P = - kbar and T = 762.0?C (from script)
mu(MgO): low, high : -711 -700
? window : -711.0 <-> -700.0 :
? interval : 0.5
<==================================================>
phases : sp, sill, (liq, ksp, q, mu(MgO))

--------------------------------------------------------------------
 P(kbar)     T(?C)    x(sp)     q(L)   fsp(L)    ol(L)     x(L)   h2o(L)
     3.6     762.0   0.9818   0.2637   0.2707 0.003134   0.9587   0.4348

  mu        H2O     SiO2    Al2O3      MgO      FeO      K2O
        -390.05  -977.34 -1776.14  -711.00  -366.22  -965.49
--------------------------------------------------------------------
 P(kbar)     T(?C)    x(sp)     q(L)   fsp(L)    ol(L)     x(L)   h2o(L)
     3.6     762.0   0.9807   0.2637   0.2706 0.003152   0.9568   0.4348

  mu        H2O     SiO2    Al2O3      MgO      FeO      K2O
        -390.06  -977.34 -1776.14  -710.50  -366.23  -965.49
--------------------------------------------------------------------
 P(kbar)     T(?C)    x(sp)     q(L)   fsp(L)    ol(L)     x(L)   h2o(L)
     3.6     762.0   0.9796   0.2637   0.2706 0.003170   0.9548   0.4348

  mu        H2O     SiO2    Al2O3      MgO      FeO      K2O
        -390.06  -977.34 -1776.14  -710.00  -366.24  -965.49
etc
```

Calculating the other lines gives the finished diagram to the right. For the sp-cd line here, it's easiest to just use the "connect" code in drawpd rather than trying to calculate it. Alternatively, you can set values of μFeO to calculate it.



In contrast to setting excess phases we may want to fix one or more μ’s. In your own calculations which way you do it will depend on the problem you are trying to solve and what your petrography tells you. As an example, imagine that the part of your rock you are considering is not actually melt bearing, but there is lots of melt nearby and you infer that H2O from that melt can diffuse into that part of the rock, but other components in the melt cannot. Here, setting μH2O would be more sensible than setting melt to be in excess.

For the example here μH2O is set to -389.99 which is the value at the g-bi-cd point. To set this μ in your script file use the script:

```
setmu   H2O -389.99
```

You also need to remove “liq” from the list of in-excess phases. Running the divariant points gives

```
% ------------------------------
i1  cd sp sill   divariant

        %         H2O        SiO2       Al2O3         MgO         FeO         K2O
3.600 762.00
             -389.9900   -977.3851  -1775.9962   -702.9144   -366.5264   -965.5079

% ------------------------------
i2   cd g sp   divariant

        %         H2O        SiO2       Al2O3         MgO         FeO         K2O
3.600 762.00
              -389.9900   -977.3351  -1776.3636   -702.8216   -366.2396   -965.2606
% ------------------------------
i3
   bi cd g   divariant

        %         H2O        SiO2       Al2O3         MgO         FeO         K2O
3.600 762.00
              -389.9900   -977.3351  -1777.0814   -700.4075   -366.1317   -964.5427
```

which are very similar to the results with excess liq, though still different

To calculate the trivariant lines you also need to set μMgO at a range of values. To do this you need to set the following script

```
setmu   H2O -389.99 MgO
```

Trying to calculate the trivariant lines, some odd things will happen. Firstly, THERMOCALC will suggest v=1 (rather than 2) for the sp-sill and sp-g lines, this is because with μH2O set, there are no reactions between endmembers that can be written involving H2O (ie a degeneracy) and the system is effectively reduced by one component. Ignore THERMOCALC and enter the variance as 2 anyway (if you enter v=1 you will be prompted for a temperature range which is not what you want). This also means the output for these lines will lack a μH2O column and will look like

```
% -----------------------------
u1   sp sill   divariant

begin i1

        %     SiO2       Al2O3         MgO         FeO         K2O
3.600 762.00
             -977.3351  -1776.1362   -711.0000   -366.2215   -965.4879
3.600 762.00
             -977.3351  -1776.1362   -710.0000   -366.2411   -965.4879
3.600 762.00
             -977.3351  -1776.1362   -709.0000   -366.2633   -965.4879
3.600 762.00
             -977.3351  -1776.1362   -708.0000   -366.2882   -965.4879
etc
```

you will have to manually add the µH2O numbers (-389.99) here to give this output the right number of columns so the modified data in the drawpd input file looks like:

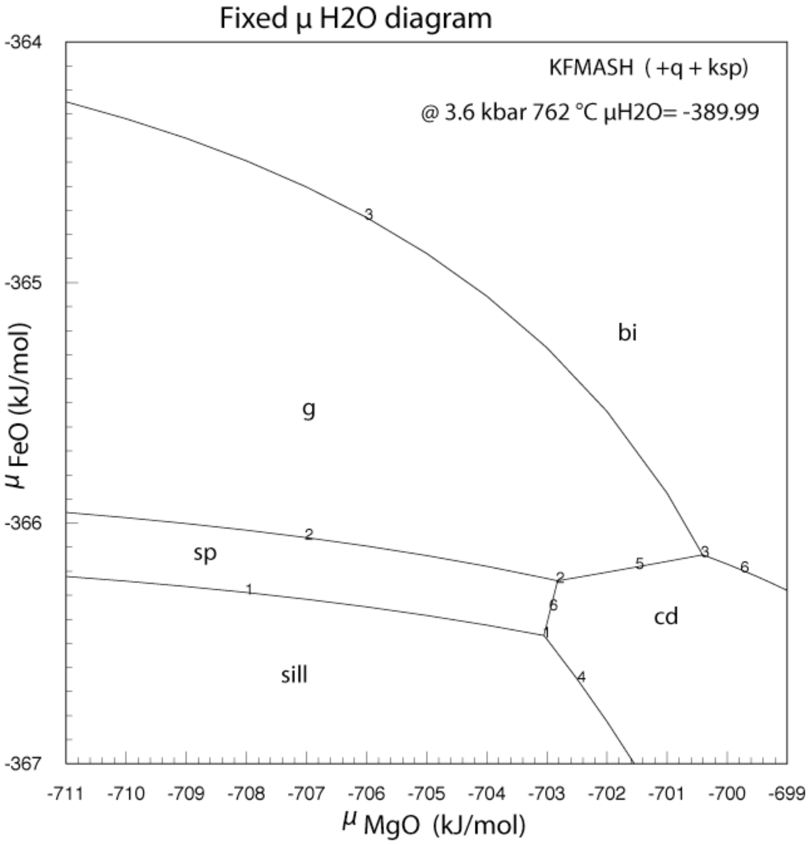
```
% -----------------------------
u1   sp sill   divariant

begin i1

        %        H2O        SiO2       Al2O3         MgO         FeO         K2O
3.600 762.00
             -389.9900   -977.3351  -1776.1362   -711.0000   -366.2215   -965.4879
3.600 762.00
             -389.9900   -977.3351  -1776.1362   -710.0000   -366.2411   -965.4879
3.600 762.00
             -389.9900   -977.3351  -1776.1362   -709.0000   -366.2633   -965.4879
3.600 762.00
             -389.9900   -977.3351  -1776.1362   -708.0000   -366.2882   -965.4879
etc
```

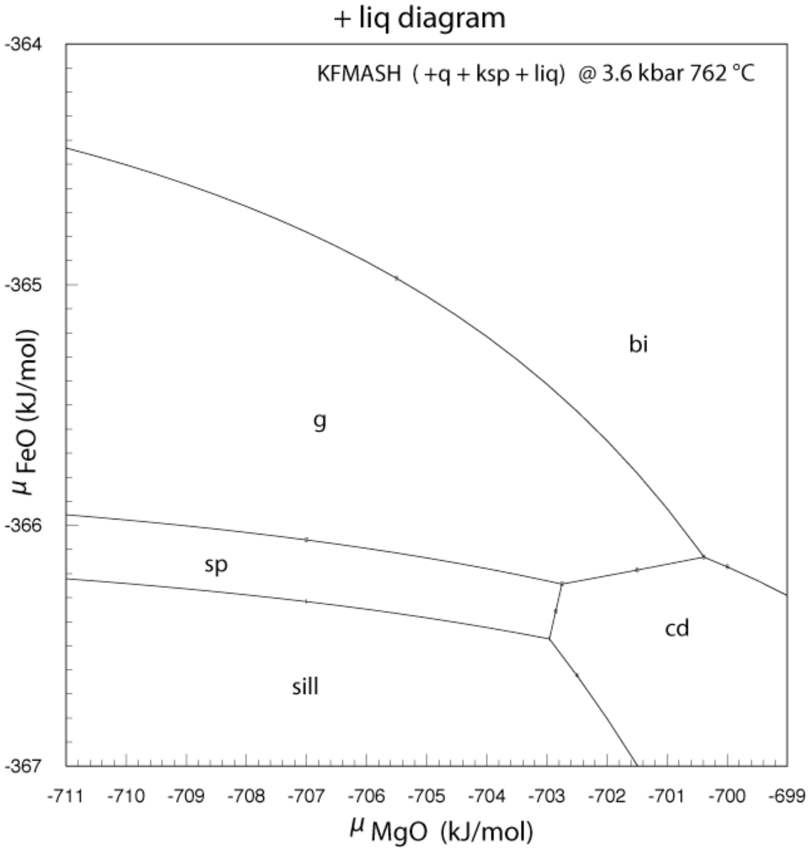
The sp-cd line returns an even stranger result, being:

```
at fixed P = - kbar and T = 762.0?C (from script)
mu(MgO): low, high : -703 -702.5
? window : -703.0 <-> -702.5 :
? interval : 0.05
<==================================================>
phases : cd, sp, (ksp, q, mu(H2O), mu(MgO))

equilibrium does not depend on mu(MgO)
--------------------------------------------------------------------
 P(kbar)     T(?C)    x(cd)    h(cd)    x(sp)
     3.6     762.0   0.7610   0.5064   0.9542

  mu        H2O     SiO2    Al2O3      MgO      FeO      K2O
        -389.99  -977.34 -1776.19  -703.00  -366.42  -965.44
```

Here, the best solution is to use the connect code between i1 & i2 for this line.

Overall the diagram looks much the same (see below), though the positions of the points have changed. The greater the difference between the fixed value of μH2O and that at any divariant point with +liq the more different the two diagrams.


Fixed μ H2O diagram


+ liq diagram

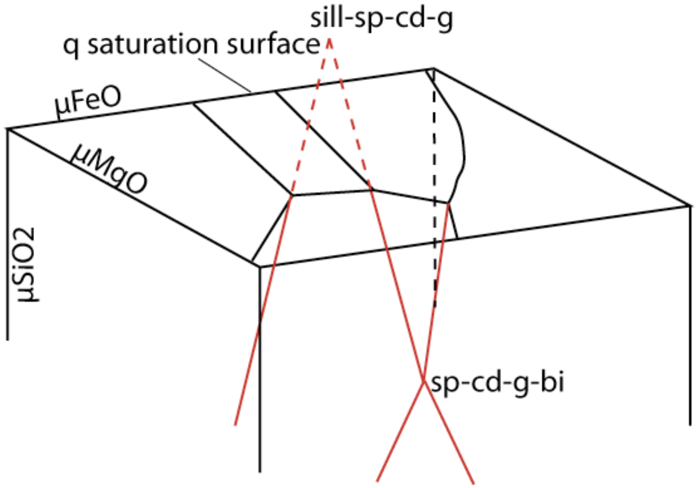
Controls of µSiO2 on the topology in 3D

Before starting this, return “liq” to the in-excess list and remove “q” from it in the script file. Also remove the fixed µH2O value from the setmu script

Lets consider that quartz is not in excess and that quartz-absent equilibria are to be considered. Quartz-absent equilibria can be considered by looking at the effects of varying µSiO2. Here, the chemical potential relationships have to be considered in 3 dimensions (µFeO-µMgO-µSiO2) even though we may only ever present 2D slices through this 3D space. The maximum stable µSiO2 value is represented by the quartz saturation surface and the relationships for this were calculated in the first diagram in part 2 of this tutorial. To lower µSiO2 (in 3D), several key changes can happen to the diagram. Firstly, the quartz-bearing divariant points become quartz-absent lines that extend to lower µSiO2, though with one less phase present (q) they are now trivariant. These lines may just continue off to lower µSiO2, may intersect to form a point or may involve the appearance of a new phase to form a point. Constraining where these changes occur is important as through these points the topology of the diagram changes. For the case of lines intersecting at a point the two possibilities are the points sill-sp-cd-g and sp-cd-g-bi. The lines sill-sp-cd and g-cd-bi cannot intersect at a stable point. The results for the two points are:

```
<==================================================>
phases : cd, g, sp, sill, (liq, ksp)

--------------------------------------------------------------------
 P(kbar)     T(?C)    x(cd)    h(cd)     x(g)    x(sp)     q(L)   fsp(L)    ol(L)     x(L)   h2o(L)
    3.60     762.0   0.7781   0.4974   0.9544   0.9583   0.2748   0.2698 0.003624   0.9213   0.4245

  mu        H2O     SiO2    Al2O3      MgO      FeO      K2O
        -390.30  -977.24 -1776.23  -703.75  -366.34  -965.95

<==================================================>
phases : bi, cd, g, sp, (liq, ksp)

--------------------------------------------------------------------
 P(kbar)     T(?C)    x(bi)    y(bi)    Q(bi)    x(cd)    h(cd)     x(g)    x(sp)     q(L)   fsp(L)    ol(L)     x(L)   h2o(L)
    3.60     762.0   0.8889   0.6181  0.03410   0.7446   0.5102   0.9456   0.9502   0.2552   0.2715 0.004171   0.9100   0.4432

  mu        H2O     SiO2    Al2O3      MgO      FeO      K2O
        -389.86  -977.41 -1776.47  -701.99  -366.17  -964.71
```

This output highlights the importance of looking at the output carefully. Look at the value of µSiO2 for the sill-sp-cd-g point (ie the top result). This value (-977.24) is higher than that for the quartz saturation surface (-977.33) this means this assemblage is metastable relative to quartz. In terms of what the diagram must look like in 3D this means the sp-sill-cd and sp-g-cd lines diverge to lower µSiO2. In contrast the sp-cd-g-bi point is at µSiO2 lower than that of the quartz saturation surface. A sketch of these relationships is shown below



It is also possible that the divariant lines end at a univariant point involving a new phase, which with decreasing μSiO2 is likely to be corundum (cor). The points involving cor are as follows:

```
<==================================================>
phases : cd, sp, sill, cor, (liq, ksp)

--------------------------------------------------------------------
 P(kbar)    T(?C)    x(cd)    h(cd)    x(sp)     q(L)   fsp(L)    ol(L)     x(L)   h2o(L)
    3.60    762.0   0.4755   0.5727   0.8558   0.1342   0.2796 0.002041   0.7991   0.5512

  mu        H2O     SiO2    Al2O3      MgO      FeO      K2O
        -387.69  -978.83 -1774.64  -694.67  -368.90  -958.03

<==================================================>
phases : cd, g, sp, cor, (liq, ksp)

--------------------------------------------------------------------
 P(kbar)    T(?C)    x(cd)    h(cd)     x(g)    x(sp)     q(L)   fsp(L)    ol(L)     x(L)   h2o(L)
    3.60    762.0   0.9849   0.3603   0.9975   0.9977   0.4378   0.2536 0.001302   0.9918   0.2708

  mu        H2O     SiO2    Al2O3      MgO      FeO      K2O
        -395.15  -976.15 -1774.64  -730.15  -367.58  -974.06

<==================================================>
phases : bi, cd, g, cor, (liq, ksp)

--------------------------------------------------------------------
 P(kbar)    T(?C)    x(bi)    y(bi)    Q(bi)    x(cd)    h(cd)     x(g)     q(L)   fsp(L)    ol(L)     x(L)   h2o(L)
    3.60    762.0   0.9488   0.6910  0.01193   0.8610   0.5174   0.9738   0.2331   0.2704 0.003113   0.9487   0.4567

  mu        H2O     SiO2    Al2O3      MgO      FeO      K2O
        -389.61  -977.60 -1774.64  -708.65  -366.34  -965.41
```

The first of these at this stage appears stable (though this changes as shown below), the second is at µSiO2 above the quartz saturation surface so is metastable, and the third is below the sp-cd-g-bi point so is metastable with respect to that point.

Now that we have established the stability of the sp-cd-g-bi point we need to work out what the diagram looks like below this. The point can be viewed as the reaction g + cd = bi + sp so the stable lines emanating from this point to lower µSiO2 are sp-bi-g and sp-bi-cd. These two lines may still terminate at a cor-bearing point so we have to check the sp-bi-cd-cor and sp-bi-g-cor points. These are:

```
<==================================================>
phases : bi, cd, sp, cor, (liq, ksp)

--------------------------------------------------------------------
 P(kbar)     T(?C)    x(bi)    y(bi)    Q(bi)    x(cd)    h(cd)    x(sp)     q(L)   fsp(L)    ol(L)     x(L)   h2o(L)
    3.60     762.0   0.7913   0.6748  0.05139   0.5864   0.5498   0.9027   0.1780   0.2754 0.001964   0.8504   0.5096

  mu        H2O     SiO2    Al2O3      MgO      FeO      K2O
       -388.49  -978.20 -1774.64  -698.05  -368.44  -961.79

<==================================================>
phases : bi, g, sp, cor, (liq, ksp)

--------------------------------------------------------------------
 P(kbar)     T(?C)    x(bi)    y(bi)    Q(bi)     x(g)    x(sp)     q(L)   fsp(L)    ol(L)     x(L)   h2o(L)
    3.60     762.0   0.4112   0.4601   0.2175   0.6671   0.6990   0.3846   0.2583 0.002663   0.6514   0.3174

  mu        H2O     SiO2    Al2O3      MgO      FeO      K2O
       -393.40  -976.46 -1774.64  -688.33  -370.64  -972.22
```

Of these only the first one can be possibly stable, the second one is above the quartz saturation surface.

Another possibility is that the sp-bi-cd line (in 3D) intersects the cd-sp-sill line to make a cd-sp-sill-bi point, which, when calculated, gives:

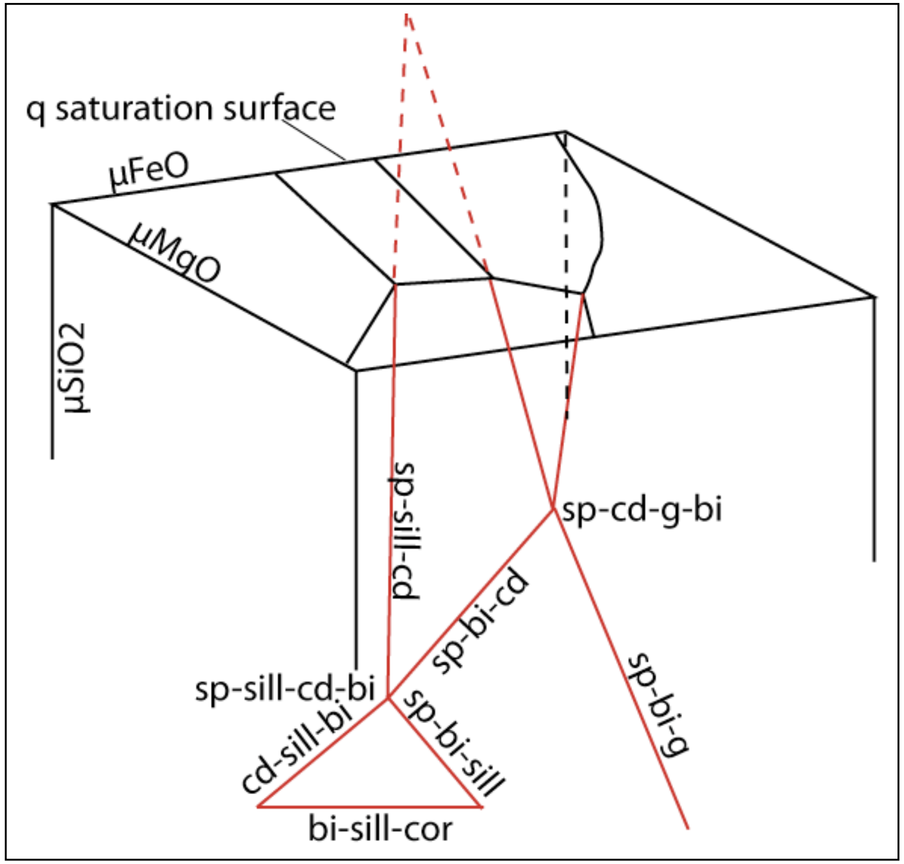
```
<==================================================>
phases : bi, cd, sp, sill, (liq, ksp)

--------------------------------------------------------------------
 P(kbar)     T(?C)    x(bi)    y(bi)    Q(bi)    x(cd)    h(cd)    x(sp)     q(L)   fsp(L)    ol(L)     x(L)   h2o(L)
    3.60     762.0   0.8546   0.6422  0.04083   0.6832   0.5279   0.9339   0.2228   0.2733 0.003135   0.8882   0.4715

  mu        H2O     SiO2    Al2O3      MgO      FeO      K2O
       -389.25  -977.71 -1775.76  -700.25  -367.03  -963.62
```

Thus, from the µSiO2 values, this point appears to be stable, which makes the sp-bi-cd-cor and cd-sp-sill-cor points above, metastable. One final possibility is that the sp-bi-sill and sp-bi-g lines converge to a sp-bi-sill-g point. However, when calculated this point (µSiO2 = -977.27) is above the quartz saturation surface, so is metastable. Now we have to check for corundum-bearing points, namely cd-sill-bi-cor and sp-bi-sill-cor. These both occur at the same µSiO2 due to both containing corundum and sillimanite.

```
<==================================================>
phases : bi, cd, sill, cor, (liq, ksp)

--------------------------------------------------------------------
 P(kbar)     T(?C)    x(bi)    y(bi)    Q(bi)    x(cd)    h(cd)     q(L)   fsp(L)    ol(L)     x(L)   h2o(L)
    3.60     762.0   0.5325   0.6314   0.1215   0.3373   0.5732   0.1344   0.28000.0008998   0.7147   0.5517

  mu        H2O     SiO2    Al2O3      MgO      FeO      K2O
        -387.67  -978.83 -1774.64  -692.66  -371.86  -958.03


<==================================================>
phases : bi, sp, sill, cor, (liq, ksp)

--------------------------------------------------------------------
 P(kbar)     T(?C)    x(bi)    y(bi)    Q(bi)    x(sp)     q(L)   fsp(L)    ol(L)     x(L)   h2o(L)
    3.60     762.0   0.9062   0.7247  0.01885   0.9550   0.1343   0.2797 0.001592   0.9169   0.5514

  mu        H2O     SiO2    Al2O3      MgO      FeO      K2O
        -387.68  -978.83 -1774.64  -704.69  -367.95  -958.03
```

However, I'm not going to do any further calculations of corundum-bearing equlibria in this tutorial

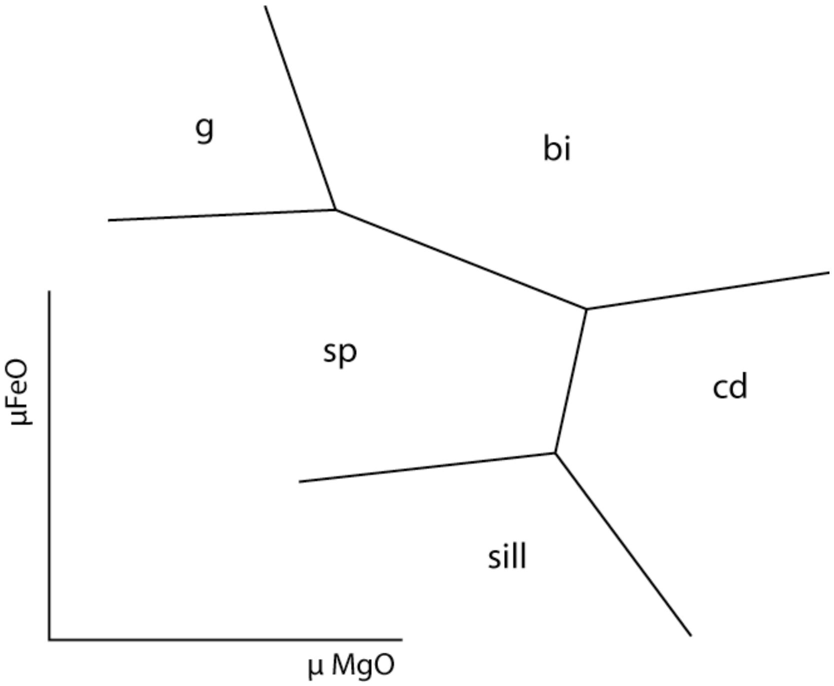
Now that we have an idea of the general topology we can consider a series of μFeO-μMgO diagrams at fixed but different values of μSiO2. Firstly we can consider the topology of the μFeO-μMgO diagrams to fall into four basic forms corresponding to different μSiO2 ranges. The first form is the same topology as the quartz-saturated diagram and extends down to the g-cd-sp-bi point at μSiO2 ≈ -977.47. The second form involves a stable sp-bi line (or plane in 3D) and extends from the g-cd-sp-bi point down to the cd-sp-sill-bi point. Below this (the third form), there are the lines cd-sill-bi, sp-bi-sill and sp-bi-g until corundum becomes stable. To the right is a very rough sketch of the relations in 3D.



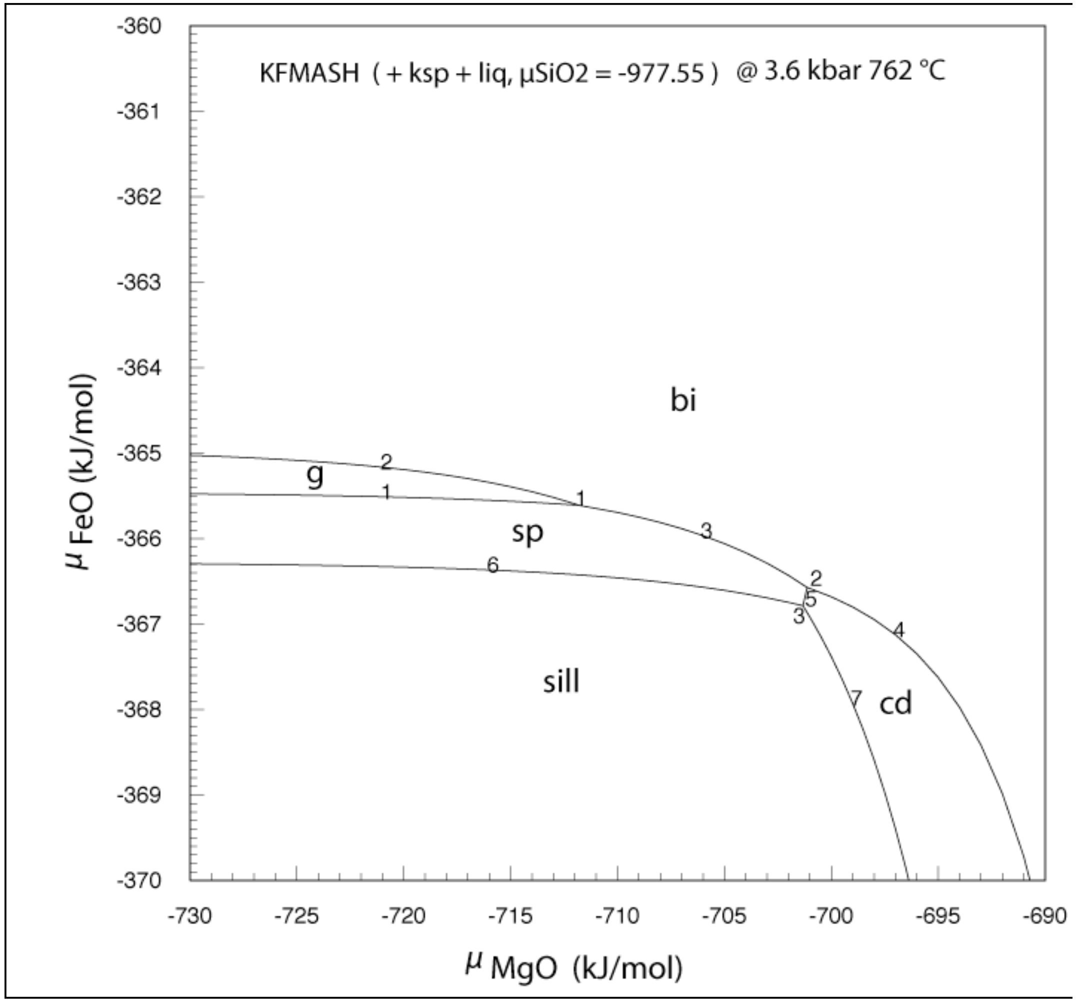
I won't bother calculating the diagram above the g-cd-sp-bi point as the topology there is known, so I will start with a diagram at a fixed μSiO2 = -977.55 which is between the g-cd-sp-bi and sp-sill-cd-bi points (you will need the "`setmu SiO2 -977.55`" script in your script file. Here the 3 stable points (at fixed μSiO2, ie the intersection of lines in 3D with a plane at fixed μSiO2) are sp-bi-g, sp-bi-cd and sp-cd-sill, giving the values below

```
% ------------------------------
i1   bi g sp   divariant

        %         H2O        SiO2       Al2O3         MgO         FeO         K2O
3.600 762.00
             -389.5098   -977.5500  -1776.7223   -711.8027   -365.6117   -963.6124

% ------------------------------
i2   bi cd sp   divariant

        %         H2O        SiO2       Al2O3         MgO         FeO         K2O
3.600 762.00
             -389.5557   -977.5500  -1776.1334   -701.1274   -366.5739   -964.2014

% ------------------------------
i3   cd sp sill   divariant

        %         H2O        SiO2       Al2O3         MgO         FeO         K2O
3.600 762.00
             -389.5702   -977.5500  -1775.9214   -701.3239   -366.7868   -964.4134
```

Again, seeing where these plot relative to each other gives away much of the topology in a general sense. The overall topology must look something like:



Calculating the lines, gives the final diagram, to the right



Below the sp-sill-cd-bi point, do the calculations for yourself at μSiO2 = -978.00. This plane is below the sp-sill-cd-bi point but above the two corundum-bearing points