

# P-T pseudosection tutorial

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This tutorial is a base level instruction for constructing a P-T pseudosection. It starts with the very basics. This tutorial is based around calculating and drawing the NCKFMASH pseudosection Fig. 8b in White, R.W., Powell, R. & Holland T.J.B., 2007. Progress relating to calculation of partial melting equilibria for metapelites. *Journal of Metamorphic Geology*, **25**, 511–527.

As with that figure, I have not bothered to calculate the muscovite-bearing assemblages that would occur in the top left of the diagram. A copy of the finished diagram is included in this tutorial download.

This tutorial was made using THERMOCALC v3.30i on a mac (a version modified for THERMOCALC 3.33 and drawpd 1.15 is also available in the download)

In the following description assemblages are given as lists of phases separated by dashes (e.g. cd-bi-sill-pl ) and phases set to zero to calculate lines and points are given in brackets (e.g. (cd) or (cd sill) )

Before starting this tutorial you should look at the “getting started” section of the webpage and the documentation.

In your THERMOCALC folder you will need the following files

tc-ptpstute                ( this is the script file)  
tc-NCKFMASHp            ( this is the a-x file)

dr dfin      For mac drawpd 1.11    (in whatever folder you have drawpd)  
dr-pfin      For mac drawpd 1.12    (in whatever folder you have drawpd)  
drdfin      For pc drawpd 1.11    (in whatever folder you have drawpd)

The above files are the finished (but not filled in) drawpd files

dr dptpstute    For mac drawpd 1.11    (in whatever folder you have drawpd)  
dr-ptpstute    For mac drawpd 1.12    (in whatever folder you have drawpd)  
drdtut          For pc drawpd 1.11    (in whatever folder you have drawpd)

The above files are blank drawpd files with the P-T window etc preset for this exercise

In your tc-prefs file use the scripts;

calcmode 1

scriptfile ptpstute

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

Start up THERMOCALC, you will be given a block of information listing all the minerals in the ax file followed by a prompt:

```
choose from: ged anth bi cd st ctd chl g sp mu pa opx. . . .  
which phases :
```

Normally, you will have calculated a T-X section from a known composition to this one, which would provide you with some equilibria to start with. In this example we can pretend we have done this. Otherwise we can use logic, in this case assuming this metapelite sees the reaction  $bi + sill = g + cd$  in some form (as most pelites must!).

Here we type in the phases we wish to use (separated by a space) and hit return.

```
which phases : g sill bi cd ksp pl q liq
```

any in-excess phases that you have given in the script file will be listed, Next you are prompted for the variance (yes I know the program should be able to work that out! But doing it yourself is character-building....honest!). We are in NCKFMASH so V=2. Enter the variance and hit return.

The next question regards which phase or phases to set to zero to calculate a field boundary. Again you normally would know this from the T-X diagram. In this case the phase to set to zero mode is cd. So enter cd and hit return. For this equilibria (in normal pelites) the low-T boundaries of the field will always involve a (cd) and a (g) line (if this does not make sense, sketch an appropriate AFM diagram (+ q +ksp + liq) for either side of the reaction  $bi + sill = g + cd$ ).

```
which to set : cd
```

now we have to decide to calculate T at a series of P's or visa versa. Typically you hit yes (or just hit return) to this prompt unless the boundary is likely to be near isobaric.

```
calculate T at P (rather than P at T) ? yes
```

you are now prompted for a P window, T window and P increments

```
specification of PT window:  
P range over which T of reactions to be calculated  
P window: P low,high : 3 7 <return>  
T window within which reactions expected to lie  
T window: T low,high : 600 900 <return>  
P window :3 <-> 7 kbar :P interval : 0.25 <return>
```

Once you have entered the P increment and hit return the calculation will take place. I picked those ranges of P &T to ensure I found the equilibria somewhere.

## THERMOCALC will have returned the output

```
composition (from script)
  H2O SiO2 Al2O3  CaO  MgO  FeO  K2O  Na2O
  5.92 69.11  8.82  0.27 3.59  8.80  2.93  0.56
<=====>
phases : bi, cd, g, liq, ksp, pl, sill, q

77777777-----
P(kbar)    T(?C)    x(bi)    y(bi)    Q(bi)    x(cd)    h(cd)    x(g)    z(g)    q(L)    fsp(L)    na(L)    an(L)    ol(L)    x(L)    h2o(L)    na(ksp)    ca(ksp)    ca(pl)    k(pl)
  5.00     738.5    0.6831   0.5585   0.07066  0.4472   0.5987   0.8427  0.02130  0.1713   0.3001   0.4652  0.007999 0.002780  0.8100  0.5017   0.2328   0.01137  0.3543  0.03956

mode       bi      cd      g      liq      ksp      pl      sill      q
      0.3132      0  0.04950  0.08484  0.05735  0.02046  0.03918  0.4355
-----
P(kbar)    T(?C)    x(bi)    y(bi)    Q(bi)    x(cd)    h(cd)    x(g)    z(g)    q(L)    fsp(L)    na(L)    an(L)    ol(L)    x(L)    h2o(L)    na(ksp)    ca(ksp)    ca(pl)    k(pl)
  5.25     747.1    0.6474   0.5485   0.07988  0.4190   0.6083   0.8247  0.02641  0.1764   0.2950   0.4118  0.01055 0.002966  0.7963  0.4984   0.1879   0.01161  0.4606  0.02993

mode       bi      cd      g      liq      ksp      pl      sill      q
      0.2428      0  0.1040  0.1333  0.08345  0.006229  0.03526  0.3950
77777777
more phase diagram calculations ?
```

In this calculation the line was found at 2 pressures (5 & 5.25 kbar). We will want more points to define our line in drawpd so we can refine this result by rerunning the same equilibria.

So hit return, and you are again prompted for the phases.

To save typing you can enter the “=” sign to run the same equilibria (THERMOCALC 3.30 and above) and hit return at the “omit” prompt, and answer the prompts as before, except now calculate over the P range 4.6 to 5.6 and set the P interval to 0.1

```
choose from: ged anth bi cd st ctd chl g sp mu pa opx liq ksp pl osm ky sill and q H2O
which phases : =
use same phases - of these: bi cd g liq ksp pl sill q
omit :
no phases in excess (from script)

variance of required equilibria :
```

to get this output

```
777-----
P(kbar)    T(?C)    x(bi)    y(bi)    Q(bi)    x(cd)    h(cd)    x(g)    z(g)    q(L)    fsp(L)    na(L)    an(L)    ol(L)    x(L)    h2o(L)    na(ksp)    ca(ksp)    ca(pl)    k(pl)
  4.90     735.0    0.6971   0.5623   0.06704  0.4588   0.5949   0.8495  0.01898  0.1690   0.3024   0.4874  0.006948 0.002703  0.8155  0.5031   0.2561   0.01123  0.3044  0.04599

mode       bi      cd      g      liq      ksp      pl      sill      q
      0.3453      0  0.02484  0.06303  0.04314  0.02892  0.04099  0.4538
```

P(kbar)	T(?C)	x(bi)	y(bi)	Q(bi)	x(cd)	h(cd)	x(g)	z(g)	q(L)	fsp(L)	na(L)	an(L)	ol(L)	x(L)	h2o(L)	na(ksp)	ca(ksp)	ca(pl)	k(pl)
5.00	738.5	0.6831	0.5585	0.07066	0.4472	0.5987	0.8427	0.02130	0.1713	0.3001	0.4652	0.007999	0.002780	0.8100	0.5017	0.2328	0.01137	0.3543	0.03956
mode	bi	cd	g	liq	ksp	pl	sill	q											
	0.3132	0	0.04950	0.08484	0.05735	0.02046	0.03918	0.4355											
P(kbar)	T(?C)	x(bi)	y(bi)	Q(bi)	x(cd)	h(cd)	x(g)	z(g)	q(L)	fsp(L)	na(L)	an(L)	ol(L)	x(L)	h2o(L)	na(ksp)	ca(ksp)	ca(pl)	k(pl)
5.10	742.0	0.6690	0.5546	0.07431	0.4358	0.6026	0.8356	0.02350	0.1735	0.2979	0.4431	0.009048	0.002856	0.8046	0.5004	0.2126	0.01148	0.4007	0.03480
mode	bi	cd	g	liq	ksp	pl	sill	q											
	0.2835	0	0.07238	0.1051	0.06905	0.01389	0.03753	0.4185											
P(kbar)	T(?C)	x(bi)	y(bi)	Q(bi)	x(cd)	h(cd)	x(g)	z(g)	q(L)	fsp(L)	na(L)	an(L)	ol(L)	x(L)	h2o(L)	na(ksp)	ca(ksp)	ca(pl)	k(pl)
5.20	745.4	0.6546	0.5506	0.07801	0.4246	0.6064	0.8284	0.02549	0.1755	0.2959	0.4218	0.01006	0.002930	0.7990	0.4991	0.1954	0.01157	0.4420	0.03131
mode	bi	cd	g	liq	ksp	pl	sill	q											
	0.2559	0	0.09377	0.1242	0.07898	0.008562	0.03599	0.4026											
P(kbar)	T(?C)	x(bi)	y(bi)	Q(bi)	x(cd)	h(cd)	x(g)	z(g)	q(L)	fsp(L)	na(L)	an(L)	ol(L)	x(L)	h2o(L)	na(ksp)	ca(ksp)	ca(pl)	k(pl)
5.30	748.7	0.6401	0.5464	0.08176	0.4135	0.6102	0.8210	0.02727	0.1772	0.2942	0.4021	0.01103	0.003001	0.7935	0.4978	0.1810	0.01165	0.4779	0.02875
mode	bi	cd	g	liq	ksp	pl	sill	q											
	0.2301	0	0.1139	0.1422	0.08764	0.004066	0.03455	0.3876											
P(kbar)	T(?C)	x(bi)	y(bi)	Q(bi)	x(cd)	h(cd)	x(g)	z(g)	q(L)	fsp(L)	na(L)	an(L)	ol(L)	x(L)	h2o(L)	na(ksp)	ca(ksp)	ca(pl)	k(pl)
5.40	751.9	0.6254	0.5421	0.08554	0.4025	0.6139	0.8133	0.02885	0.1787	0.2928	0.3841	0.01194	0.003071	0.7878	0.4967	0.1690	0.01174	0.5088	0.02684
mode	bi	cd	g	liq	ksp	pl	sill	q											
	0.2058	0	0.1328	0.1592	0.095340	0.001356	0.03317	0.3735											

77

in this list of information, the mode info is critical for working out why a line starts and ends. We can see that to lower P the mode of garnet is approaching zero and to higher P the mode of plagioclase is approaching zero. This means that the line terminates at a (cd g) and a (cd pl) point at either end.

To calculate these points we run the same equilibria again and set two phases to zero for each point. For the (cd g) point

choose from: ged anth bi cd st ctd chl g sp mu pa opx liq ksp pl osm ky sill and q H2O

which phases : =

use same phases - of these: bi cd g liq ksp pl sill q

omit :

no phases in excess (from script)

variance of required equilibria :

0 = invariant

1 = univariant

2 = divariant

...

n = n-variant

variance : 2

you may set zero modal proportions, from:bi cd g liq ksp pl sill q

which to set : cd g

```

specification of PT window:
PT window within which invariant points expected to lie
T low,high, P low,high :
composition (from script)
  H2O  SiO2  Al2O3   CaO   MgO   FeO   K2O   Na2O
  5.92 69.11  8.82  0.27  3.59  8.80  2.93  0.56
<=====>
phases : bi, cd, g, liq, ksp, pl, sill, q

```

```

-----
P(kbar)    T(?C)    x(bi)    y(bi)    Q(bi)    x(cd)    h(cd)    x(g)    z(g)    q(L)    fsp(L)    na(L)    an(L)    ol(L)    x(L)    h2o(L)    na(ksp)    ca(ksp)    ca(pl)    k(pl)
   4.81     731.8    0.7101   0.5659   0.06370  0.4700   0.5912   0.8558  0.01678  0.1670   0.3044   0.5069  0.006007  0.002631  0.8205   0.5042   0.2799   0.01105   0.2573   0.05377

mode       bi      cd      g      liq      ksp      pl      sill      q
         0.3778      0      0  0.04116  0.02680  0.03927  0.04283  0.4721

```

The output for the (cd pl) point will be

```

phases : bi, cd, g, liq, ksp, pl, sill, q

```

```

-----
P(kbar)    T(?C)    x(bi)    y(bi)    Q(bi)    x(cd)    h(cd)    x(g)    z(g)    q(L)    fsp(L)    na(L)    an(L)    ol(L)    x(L)    h2o(L)    na(ksp)    ca(ksp)    ca(pl)    k(pl)
   5.40     752.0    0.6248   0.5420   0.08568  0.4021   0.6140   0.8130  0.02891  0.1787   0.2928   0.3835  0.01198  0.003073  0.7876   0.4966   0.1685   0.01174   0.5099   0.02678

mode       bi      cd      g      liq      ksp      pl      sill      q
         0.2049      0  0.1335  0.1599  0.09561      0  0.03312  0.3730

```

now we have two points and a line which we can put into drawpd. To do this you need to open up the tc-tpstute-dr file and copy and paste the relevant info into your drawpd file. My personal preference is to keep all the points together separate from all the lines, so that's how I will do it here. See the drawpd documentation on how to use it. Once you have numbered each point and line and given the start and finish points for line u1 in the dr dpsstute file they will look like this:

```

% -----
i1  bi liq ksp pl sill q - cd g

4.81 731.8 % cd = 0g = 0

% -----
i2  bi g liq ksp sill q - cd pl

5.40 752.0 % cd = 0pl = 0

% -----
u1  bi g liq ksp pl sill q - cd

i1 i2

4.90 735.0 % cd = 0
5.00 738.5 % cd = 0
5.10 742.0 % cd = 0

```

```
5.20 745.4 % cd = 0
5.30 748.7 % cd = 0
5.40 751.9 % cd = 0
```

before running drawpd we can calculate some more lines from the same equilibria. From the (cd g) point there will be a (g) line. I used the following ranges

```

specification of PT window:
P range over which T of reactions to be calculated
P window: P low,high : 4 5
T window within which reactions expected to lie
T window: T low,high :
P window :4 <=> 5 kbar :P interval : 0.1

```

and got the result

77777-----

[illegible]

77

again, looking at the modes we can see that this line stops at a (g sill) point to lower P

[illegible]

from which emanates a (sill) line

77777-----																			
P(kbar)	T(?C)	x(bi)	y(bi)	Q(bi)	x(cd)	h(cd)	x(g)	z(g)	q(L)	fsp(L)	na(L)	an(L)	ol(L)	x(L)	h2o(L)	na(ksp)	ca(ksp)	ca(pl)	k(pl)
4.50	731.3	0.7568	0.5815	0.05070	0.5177	0.5745	0.8789	0.02185	0.1797	0.2978	0.4482	0.007822	0.002550	0.8405	0.4953	0.2192	0.01093	0.3828	0.03544
mode	bi	cd	g	liq	ksp	pl	sill	q											
	0.2873	0.1252	0.009111	0.06557	0.07985	0.02290	0	0.4101											
P(kbar)	T(?C)	x(bi)	y(bi)	Q(bi)	x(cd)	h(cd)	x(g)	z(g)	q(L)	fsp(L)	na(L)	an(L)	ol(L)	x(L)	h2o(L)	na(ksp)	ca(ksp)	ca(pl)	k(pl)
4.60	734.4	0.7437	0.5780	0.05398	0.5046	0.5792	0.8726	0.02387	0.1815	0.2955	0.4277	0.008729	0.002619	0.8351	0.4946	0.2010	0.01100	0.4258	0.03156
mode	bi	cd	g	liq	ksp	pl	sill	q											
	0.2587	0.1200	0.03362	0.08665	0.09017	0.01697	0	0.3939											
P(kbar)	T(?C)	x(bi)	y(bi)	Q(bi)	x(cd)	h(cd)	x(g)	z(g)	q(L)	fsp(L)	na(L)	an(L)	ol(L)	x(L)	h2o(L)	na(ksp)	ca(ksp)	ca(pl)	k(pl)
4.70	737.4	0.7303	0.5743	0.05738	0.4918	0.5838	0.8662	0.02571	0.1831	0.2934	0.4084	0.009598	0.002686	0.8296	0.4940	0.1855	0.01107	0.4638	0.02869
mode	bi	cd	g	liq	ksp	pl	sill	q											
	0.2321	0.1152	0.05646	0.1063	0.09907	0.01205	0	0.3788											
P(kbar)	T(?C)	x(bi)	y(bi)	Q(bi)	x(cd)	h(cd)	x(g)	z(g)	q(L)	fsp(L)	na(L)	an(L)	ol(L)	x(L)	h2o(L)	na(ksp)	ca(ksp)	ca(pl)	k(pl)
4.80	740.3	0.7166	0.5704	0.06090	0.4790	0.5883	0.8596	0.02737	0.1845	0.2916	0.3906	0.01042	0.002751	0.8240	0.4935	0.1726	0.01113	0.4967	0.02656
mode	bi	cd	g	liq	ksp	pl	sill	q											
	0.2073	0.1107	0.07784	0.1247	0.1069	0.007829	0	0.3647											
P(kbar)	T(?C)	x(bi)	y(bi)	Q(bi)	x(cd)	h(cd)	x(g)	z(g)	q(L)	fsp(L)	na(L)	an(L)	ol(L)	x(L)	h2o(L)	na(ksp)	ca(ksp)	ca(pl)	k(pl)
4.90	743.0	0.7027	0.5665	0.06453	0.4665	0.5928	0.8527	0.02885	0.1855	0.2901	0.3744	0.01119	0.002814	0.8184	0.4930	0.1617	0.01119	0.5249	0.02495
mode	bi	cd	g	liq	ksp	pl	sill	q											
	0.1842	0.1066	0.09788	0.1418	0.1139	0.004108	0	0.3515											
P(kbar)	T(?C)	x(bi)	y(bi)	Q(bi)	x(cd)	h(cd)	x(g)	z(g)	q(L)	fsp(L)	na(L)	an(L)	ol(L)	x(L)	h2o(L)	na(ksp)	ca(ksp)	ca(pl)	k(pl)
5.00	745.7	0.6884	0.5623	0.06826	0.4541	0.5972	0.8457	0.03016	0.1863	0.2888	0.3599	0.01192	0.002876	0.8128	0.4926	0.1526	0.01126	0.5490	0.02373
mode	bi	cd	g	liq	ksp	pl	sill	q											
	0.1625	0.1026	0.1167	0.1580	0.12020	0.007557	0	0.3392											

which ends at a (sill pl) point

-----																			
P(kbar)	T(?C)	x(bi)	y(bi)	Q(bi)	x(cd)	h(cd)	x(g)	z(g)	q(L)	fsp(L)	na(L)	an(L)	ol(L)	x(L)	h2o(L)	na(ksp)	ca(ksp)	ca(pl)	k(pl)
5.02	746.4	0.6849	0.5613	0.06917	0.4512	0.5982	0.8440	0.03045	0.1865	0.2886	0.3567	0.01209	0.002890	0.8114	0.4925	0.1507	0.01128	0.5542	0.02349
mode	bi	cd	g	liq	ksp	pl	sill	q											
	0.1576	0.1017	0.1210	0.1617	0.1216	0	0	0.3364											

we now have both the (cd pl) and (sill pl) points that will be connected by the (pl) line, which from looking at the P-T conditions of those two points is a fairly short line.

```

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P(kbar)    T(?C)    x(bi)    y(bi)    Q(bi)    x(cd)    h(cd)    x(g)    z(g)    q(L)    fsp(L)    na(L)    an(L)    ol(L)    x(L)    h2o(L)    na(ksp)    ca(ksp)    ca(pl)    k(pl)
  5.10      747.4    0.6731    0.5576    0.07242   0.4409   0.6015   0.8380   0.03018   0.1849   0.2894   0.3620   0.01207  0.002926   0.8066   0.4935   0.1541   0.01136   0.5456   0.02409

mode        bi        cd        g        liq        ksp        pl        sill        q
         0.1672   0.08168   0.1233   0.1609   0.1165         0  0.006516   0.3439
-----
P(kbar)    T(?C)    x(bi)    y(bi)    Q(bi)    x(cd)    h(cd)    x(g)    z(g)    q(L)    fsp(L)    na(L)    an(L)    ol(L)    x(L)    h2o(L)    na(ksp)    ca(ksp)    ca(pl)    k(pl)
  5.20      748.9    0.6573    0.5525    0.07676   0.4278   0.6058   0.8300   0.02979   0.1828   0.2904   0.3690   0.01204  0.002973   0.8004   0.4946   0.1587   0.01148   0.5340   0.02491

mode        bi        cd        g        liq        ksp        pl        sill        q
         0.1797   0.05513   0.1265   0.1602   0.1097         0  0.01515   0.3536
-----
P(kbar)    T(?C)    x(bi)    y(bi)    Q(bi)    x(cd)    h(cd)    x(g)    z(g)    q(L)    fsp(L)    na(L)    an(L)    ol(L)    x(L)    h2o(L)    na(ksp)    ca(ksp)    ca(pl)    k(pl)
  5.30      750.4    0.6414    0.5474    0.08113   0.4150   0.6099   0.8217   0.02937   0.1808   0.2915   0.3761   0.01201  0.003022   0.7941   0.4957   0.1634   0.01161   0.5223   0.02580

mode        bi        cd        g        liq        ksp        pl        sill        q
         0.1921   0.02826   0.1299   0.1599   0.1029         0  0.02391   0.3632
-----
P(kbar)    T(?C)    x(bi)    y(bi)    Q(bi)    x(cd)    h(cd)    x(g)    z(g)    q(L)    fsp(L)    na(L)    an(L)    ol(L)    x(L)    h2o(L)    na(ksp)    ca(ksp)    ca(pl)    k(pl)
  5.40      751.9    0.6254    0.5422    0.08552   0.4025   0.6139   0.8133   0.02892   0.1788   0.2927   0.3832   0.01198  0.003071   0.7878   0.4966   0.1684   0.01174   0.5103   0.02675

mode        bi        cd        g        liq        ksp        pl        sill        q
         0.2044  0.001007   0.1334   0.1598   0.09587         0  0.03279   0.3726
7

```

with this data we can now enclose the first field, from the data in our dr d file that should look like:

```

% -----
i1  bi liq ksp pl sill q  - cd g

4.81 731.8 % cd = 0g = 0

% -----
i2  bi g liq ksp sill q  - cd pl

5.40 752.0 % cd = 0pl = 0

% -----
i3  bi cd liq ksp pl q  - g sill

4.46 730.2 % g = 0sill = 0

% -----
i4  bi cd g liq ksp q  - pl sill

5.02 746.4 % pl = 0sill = 0

%Lines

% -----

```



```
u1  bi g liq ksp pl sill q  - cd
```

```
i1 i2
```

```
4.90 735.0 % cd = 0
```

```
5.00 738.5 % cd = 0
```

```
5.10 742.0 % cd = 0
```

```
5.20 745.4 % cd = 0
```

```
5.30 748.7 % cd = 0
```

```
5.40 751.9 % cd = 0
```

```
% -----  
u2  bi cd liq ksp pl sill q  - g
```

```
i3 i1
```

```
4.50 730.3 % g = 0
```

```
4.60 730.7 % g = 0
```

```
4.70 731.1 % g = 0
```

```
4.80 731.7 % g = 0
```

```
% -----  
u3  bi cd g liq ksp pl q  - sill
```

```
i3 i4
```

```
4.50 731.3 % sill = 0
```

```
4.60 734.4 % sill = 0
```

```
4.70 737.4 % sill = 0
```

```
4.80 740.3 % sill = 0
```

```
4.90 743.0 % sill = 0
```

```
5.00 745.7 % sill = 0
```

```
% -----  
u4  bi cd g liq ksp sill q  - pl
```

```
i4 i2
```

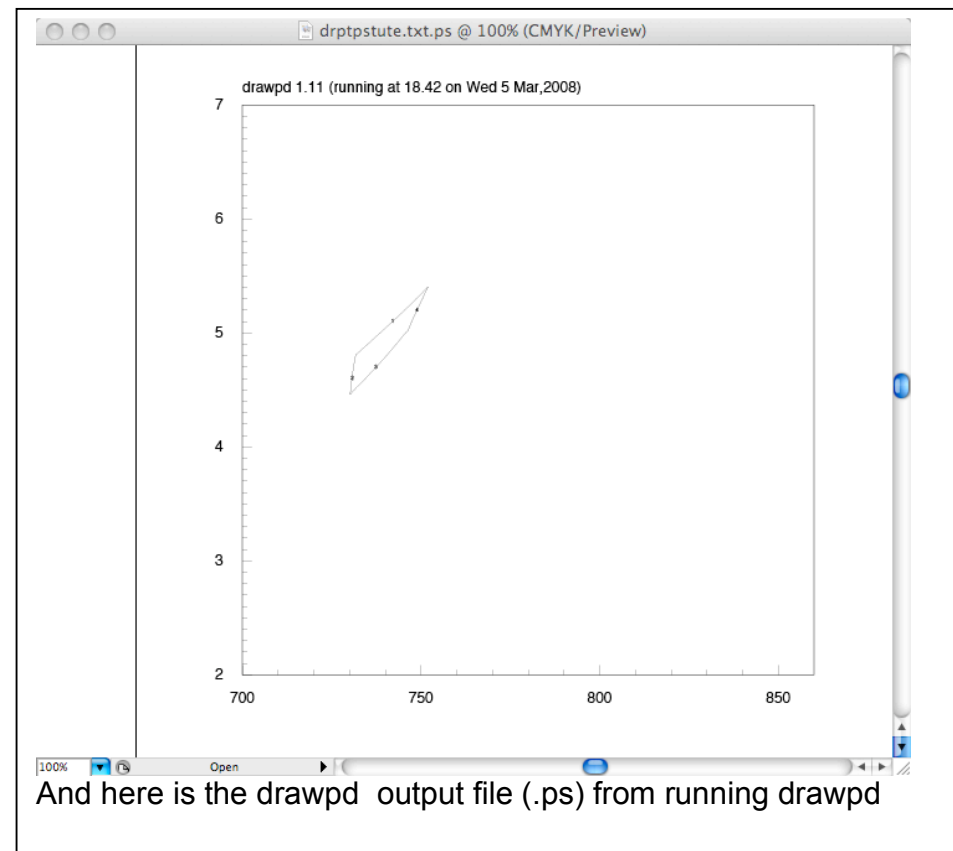
```
5.10 747.4 % pl = 0
```

```
5.20 748.9 % pl = 0
```

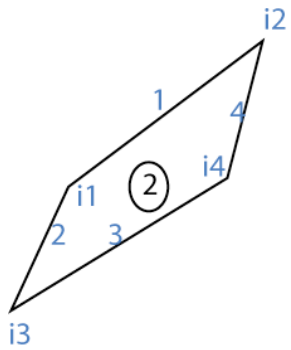
```
5.30 750.4 % pl = 0
```

```
5.40 751.9 % pl = 0
```

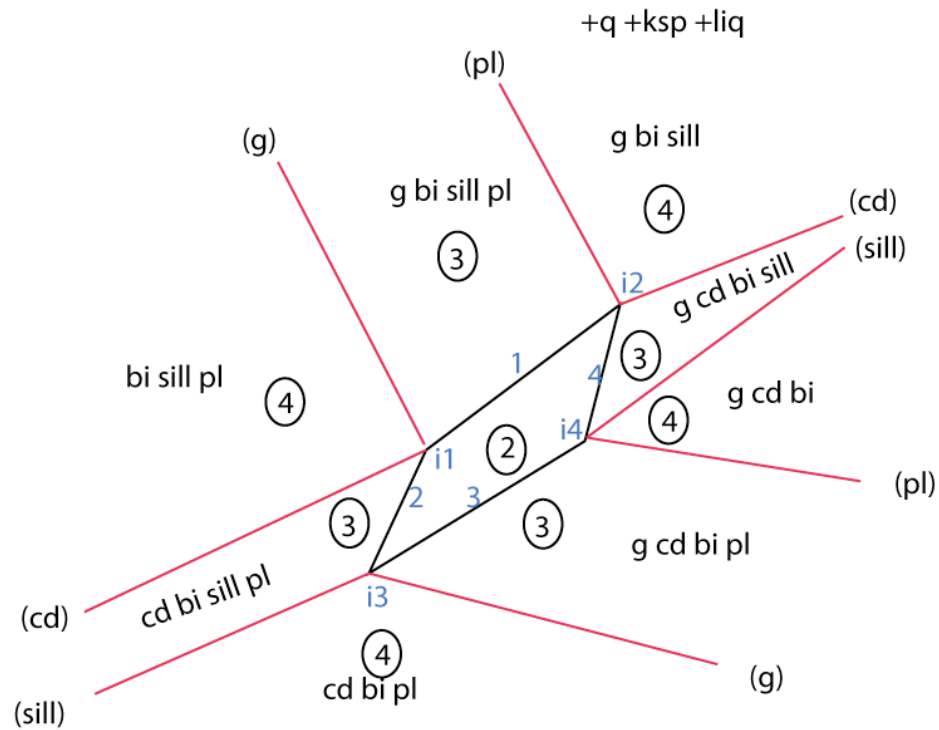
to keep track of what we are doing it is best to do a sketch as you go.  
Here is my sketch of the diagram so far.



+q +ksp +liq



Each of the points we have calculated must have 4 lines that come off them and we can predict what those extra lines will be (though not their exact slopes). Below is a sketch of what the other lines and fields must roughly look like.



here the red lines are those we are yet to calculate, the numbers in circles are the variances of the fields and the minerals in brackets signify the phase that goes to zero for each line. The blue labeling is the line and point numbering

Starting with the trivariant field cd-bi-sill-pl-ksp-q-liq, we need to calculate the (cd) and the (sill) line. We can type in the trivariant assemblage and run with that, but if we still have the divariant assemblage as the assemblage we get when we hit “=” then we can use it and the “omit” option.

```
reading a-x datafile, "tc-NCKFMAShp.txt"...
ged anth bi cd st ctd chl g sp mu pa opx liq ksp pl osm
ky sill and q H2O
choose from: ged anth bi cd st ctd chl g sp mu pa opx liq ksp pl osm ky sill and q H2O
which phases : =
use same phases - of these: bi cd g liq ksp pl sill q
omit : g
no phases in excess (from script)

variance of required equilibria :
    0 = invariant
    1 = univariant
    2 = divariant
    ...
    n = n-variant
variance : 3
you may set zero modal proportions, from:bi cd liq ksp pl sill q
which to set : cd
calculate T at P (rather than P at T) ?

specification of PT window:
P range over which T of reactions to be calculated
P window: P low,high : 2 5
T window within which reactions expected to lie
T window: T low,high :
P window :2 <-> 5 kbar :P interval : 0.25
```

here, garnet was entered into the “omit” prompt (highlighted) to make the trivariant assmblage we wanted. The results look like:

```
<=====>
phases : bi, cd, liq, ksp, pl, sill, q
```

P(kbar)	T(?C)	x(bi)	y(bi)	Q(bi)	x(cd)	h(cd)	q(L)	fsp(L)	na(L)	an(L)	ol(L)	x(L)	h2o(L)	na(ksp)	ca(ksp)	ca(pl)	k(pl)
2.00	600.9	0.7102	0.6699	0.05106	0.4059	0.5567	0.1863	0.2310	0.4907	0.001875	4.353e-5	0.7587	0.5718	0.2153	0.003917	0.2209	0.03489
mode	bi	cd	liq	ksp	pl	sill	q										
	0.3897	0	0.02400	0.01929	0.04819	0.02965	0.4891										

P(kbar)	T(?C)	x(bi)	y(bi)	Q(bi)	x(cd)	h(cd)	q(L)	fsp(L)	na(L)	an(L)	ol(L)	x(L)	h2o(L)	na(ksp)	ca(ksp)	ca(pl)	k(pl)
2.25	612.6	0.7102	0.6602	0.05232	0.4124	0.5625	0.1830	0.2381	0.4940	0.002079	6.468e-5	0.7659	0.5673	0.2219	0.004349	0.2235	0.03657
mode	bi	cd	liq	ksp	pl	sill	q										
	0.3886	0	0.02523	0.02009	0.04751	0.03095	0.4876										

P(kbar)	T(?C)	x(bi)	y(bi)	Q(bi)	x(cd)	h(cd)	q(L)	fsp(L)	na(L)	an(L)	ol(L)	x(L)	h2o(L)	na(ksp)	ca(ksp)	ca(pl)	k(pl)
---------	-------	-------	-------	-------	-------	-------	------	--------	-------	-------	-------	------	--------	---------	---------	--------	-------

2.50	624.4	0.7102	0.6506	0.05355	0.4188	0.5677	0.1801	0.2451	0.4968	0.002306	9.547e-5	0.7728	0.5624	0.2284	0.004818	0.2263	0.03825
mode	bi	cd	liq	ksp	pl	sill	q										
	0.3875	0	0.02650	0.02086	0.04681	0.03222	0.4861										
-----																	
P(kbar)	T(?C)	x(bi)	y(bi)	Q(bi)	x(cd)	h(cd)	q(L)	fsp(L)	na(L)	an(L)	ol(L)	x(L)	h2o(L)	na(ksp)	ca(ksp)	ca(pl)	k(pl)
2.75	636.1	0.7102	0.6410	0.05475	0.4250	0.5723	0.1776	0.2521	0.4992	0.0025590	0.0001400	0.7792	0.5573	0.2347	0.005324	0.2291	0.03994
mode	bi	cd	liq	ksp	pl	sill	q										
	0.3865	0	0.02781	0.02161	0.04609	0.03347	0.4846										
-----																	
1-P(kbar)	T(?C)	x(bi)	y(bi)	Q(bi)	x(cd)	h(cd)	q(L)	fsp(L)	na(L)	an(L)	ol(L)	x(L)	h2o(L)	na(ksp)	ca(ksp)	ca(pl)	k(pl)
3.25	659.7	0.7102	0.6223	0.05706	0.4370	0.5799	0.1732	0.2658	0.5032	0.0031540	0.0002966	0.7911	0.5460	0.2471	0.006462	0.2353	0.04336
mode	bi	cd	liq	ksp	pl	sill	q										
	0.3844	0	0.03059	0.02303	0.04457	0.03588	0.4816										
-----																	
P(kbar)	T(?C)	x(bi)	y(bi)	Q(bi)	x(cd)	h(cd)	q(L)	fsp(L)	na(L)	an(L)	ol(L)	x(L)	h2o(L)	na(ksp)	ca(ksp)	ca(pl)	k(pl)
3.50	671.4	0.7102	0.6130	0.05818	0.4427	0.5829	0.1715	0.2724	0.5046	0.0035010	0.0004275	0.7966	0.5400	0.2530	0.007091	0.2385	0.04507
mode	bi	cd	liq	ksp	pl	sill	q										
	0.3833	0	0.03206	0.02370	0.04378	0.03704	0.4801										
-----																	
P(kbar)	T(?C)	x(bi)	y(bi)	Q(bi)	x(cd)	h(cd)	q(L)	fsp(L)	na(L)	an(L)	ol(L)	x(L)	h2o(L)	na(ksp)	ca(ksp)	ca(pl)	k(pl)
3.75	683.0	0.7102	0.6039	0.05927	0.4483	0.5855	0.1701	0.2789	0.5057	0.0038860	0.0006125	0.8017	0.5337	0.2587	0.007761	0.2419	0.04677
mode	bi	cd	liq	ksp	pl	sill	q										
	0.3823	0	0.03361	0.02434	0.04296	0.03819	0.4786										
-----																	
P(kbar)	T(?C)	x(bi)	y(bi)	Q(bi)	x(cd)	h(cd)	q(L)	fsp(L)	na(L)	an(L)	ol(L)	x(L)	h2o(L)	na(ksp)	ca(ksp)	ca(pl)	k(pl)
4.00	694.6	0.7102	0.5948	0.06035	0.4537	0.5876	0.1690	0.2852	0.5065	0.0043110	0.0008722	0.8066	0.5272	0.2641	0.008473	0.2453	0.04846
mode	bi	cd	liq	ksp	pl	sill	q										
	0.3813	0	0.03523	0.02496	0.04213	0.03932	0.4771										
-----																	
P(kbar)	T(?C)	x(bi)	y(bi)	Q(bi)	x(cd)	h(cd)	q(L)	fsp(L)	na(L)	an(L)	ol(L)	x(L)	h2o(L)	na(ksp)	ca(ksp)	ca(pl)	k(pl)
4.25	706.2	0.7102	0.5857	0.06140	0.4589	0.5893	0.1682	0.2914	0.5070	0.004780	0.001235	0.8112	0.5204	0.2693	0.009226	0.2489	0.05013
mode	bi	cd	liq	ksp	pl	sill	q										
	0.3802	0	0.03694	0.02555	0.04127	0.04043	0.4756										
-----																	
P(kbar)	T(?C)	x(bi)	y(bi)	Q(bi)	x(cd)	h(cd)	q(L)	fsp(L)	na(L)	an(L)	ol(L)	x(L)	h2o(L)	na(ksp)	ca(ksp)	ca(pl)	k(pl)
4.50	717.7	0.7102	0.5768	0.06244	0.4640	0.5905	0.1675	0.2974	0.5071	0.005298	0.001740	0.8155	0.5133	0.2742	0.01002	0.2526	0.05178
mode	bi	cd	liq	ksp	pl	sill	q										
	0.3792	0	0.03876	0.02612	0.04039	0.04152	0.4740										
-----																	
P(kbar)	T(?C)	x(bi)	y(bi)	Q(bi)	x(cd)	h(cd)	q(L)	fsp(L)	na(L)	an(L)	ol(L)	x(L)	h2o(L)	na(ksp)	ca(ksp)	ca(pl)	k(pl)
4.75	729.1	0.7101	0.5679	0.06346	0.4689	0.5912	0.1671	0.3031	0.5070	0.005868	0.002438	0.8196	0.5060	0.2789	0.01086	0.2564	0.05340
mode	bi	cd	liq	ksp	pl	sill	q										
	0.3781	0	0.04070	0.02667	0.03948	0.04259	0.4725										
-----																	
P(kbar)	T(?C)	x(bi)	y(bi)	Q(bi)	x(cd)	h(cd)	q(L)	fsp(L)	na(L)	an(L)	ol(L)	x(L)	h2o(L)	na(ksp)	ca(ksp)	ca(pl)	k(pl)
5.00	740.5	0.7100	0.5591	0.06448	0.4737	0.5913	0.1668	0.3087	0.5066	0.006496	0.003400	0.8235	0.4983	0.2832	0.01173	0.2604	0.05499

mode	bi	cd	liq	ksp	pl	sill	q
	0.3770	0	0.04280	0.02721	0.03853	0.04365	0.4709

Notice how the result at 3kbar could not be calculated. This is not a serious problem and it does not affect the line.

We can now repeat the procedure for the (sill) line

```
reading a-x datafile, "tc-NCKFMAShp.txt"...
ged anth bi cd st ctd chl g sp mu pa opx liq ksp pl osm
ky sill and q H2O
choose from: ged anth bi cd st ctd chl g sp mu pa opx liq ksp pl osm ky sill and q H2O
which phases : =
use same phases - of these: bi cd g liq ksp pl sill q
omit : g
no phases in excess (from script)

variance of required equilibria :
    0 = invariant
    1 = univariant
    2 = divariant
    ...
    n = n-variant
variance : 3
you may set zero modal proportions, from:bi cd liq ksp pl sill q
which to set : sill
calculate T at P (rather than P at T) ?

specification of PT window:
P range over which T of reactions to be calculated
P window: P low,high : 2 5
T window within which reactions expected to lie
T window: T low,high :
P window :2 <-> 5 kbar :P interval : 0.25
composition (from script)
```

Make the (cd) line u5 and the (sill) line u6 in your drawpd file. u5 goes from begin to i1 and u6 from begin to i3

```
% -----
u5  bi liq ksp pl sill q - cd

begin i1

2.00 600.9 % cd = 0
2.25 612.6 % cd = 0
2.50 624.4 % cd = 0
2.75 636.1 % cd = 0
3.25 659.7 % cd = 0
3.50 671.4 % cd = 0
3.75 683.0 % cd = 0
4.00 694.6 % cd = 0
```

```

4.25 706.2 % cd = 0
4.50 717.7 % cd = 0
4.75 729.1 % cd = 0
5.00 740.5 % cd = 0

% -----
u6  bi cd liq ksp pl q  - sill

begin i3

2.00 612.8 % sill = 0
2.25 624.9 % sill = 0
2.50 637.1 % sill = 0
2.75 649.1 % sill = 0
3.00 661.1 % sill = 0
3.25 673.1 % sill = 0
3.50 684.9 % sill = 0
3.75 696.7 % sill = 0
4.00 708.5 % sill = 0
4.25 720.2 % sill = 0
4.50 731.8 % sill = 0
4.75 743.3 % sill = 0
5.00 754.8 % sill = 0

```

You can do the same for the g-sill-bi-pl-ksp-q-liq (ie omit cd) and g-cd-bi-pl-ksp-q-liq (ie omit sill) fields and put them in the dr d file as these are fairly straightforward. The resulting line numbers and start/finish points being

```

% -----
u7  bi liq ksp pl sill q  - g

i1  end

% -----
u8  bi g liq ksp sill q  - pl

i2  end

% -----
u9  bi cd liq ksp pl q  - g

begin i3

% -----
u10 bi cd g liq ksp q  - pl

begin i4

```

The g-cd-sill-bi field is a little more complex with the (cd) line terminating at a (cd bi) point and the (sill) line terminating at a (sill bi) point. These two points must be joined by a (bi) line. Below are the points output line numbers and start/finish points for these lines

```

% -----
i5   cd g liq ksp q  - bi sill

6.21 782.8 % bi = 0sill = 0

% -----
i6   g liq ksp sill q  - bi cd

6.58 792.8 % bi = 0cd = 0

% -----
u11  bi g liq ksp sill q  - cd

i2   i6

% -----
u12  bi cd g liq ksp q  - sill

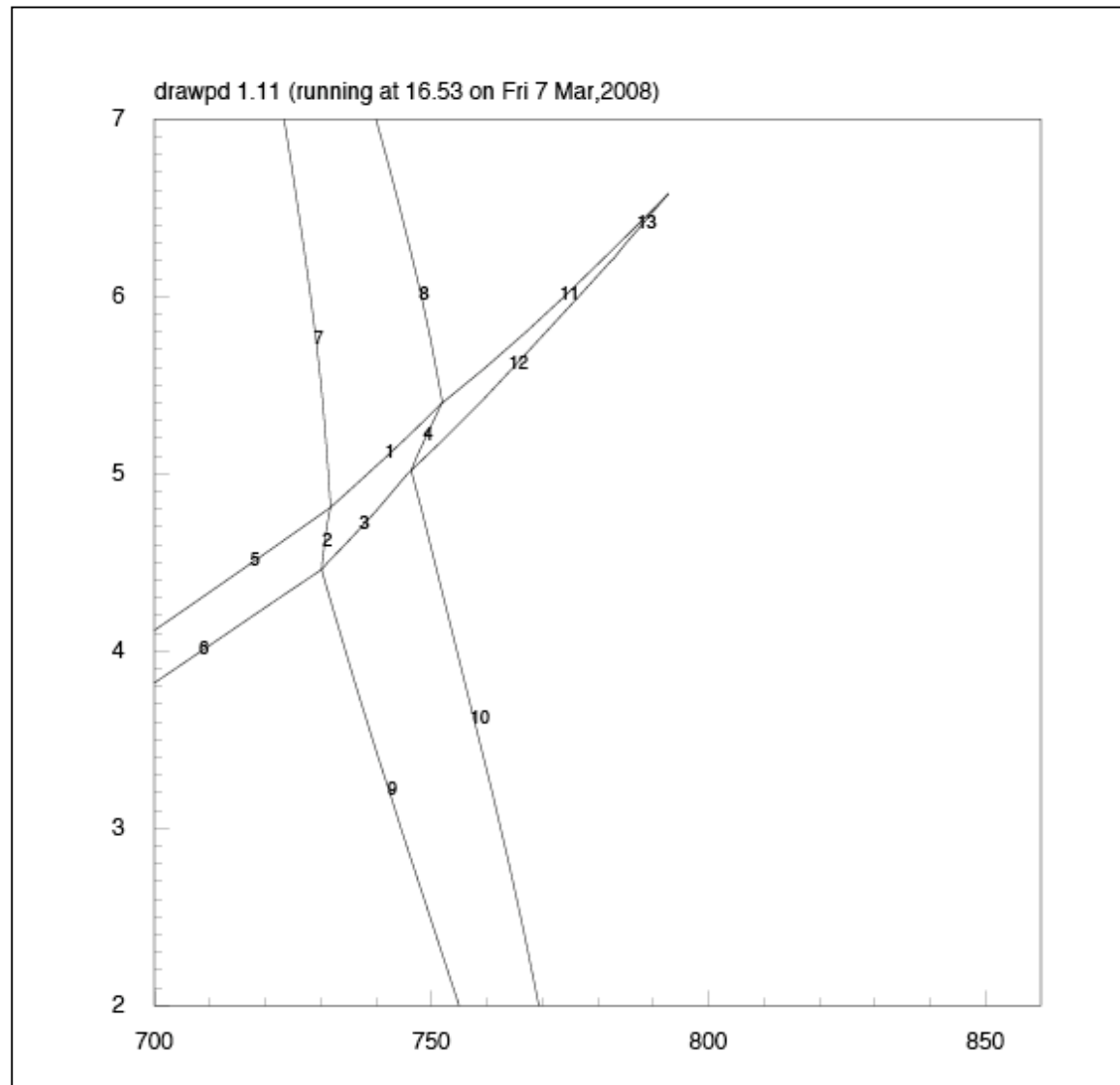
i4   i5

% -----
u13  cd g liq ksp sill q  - bi

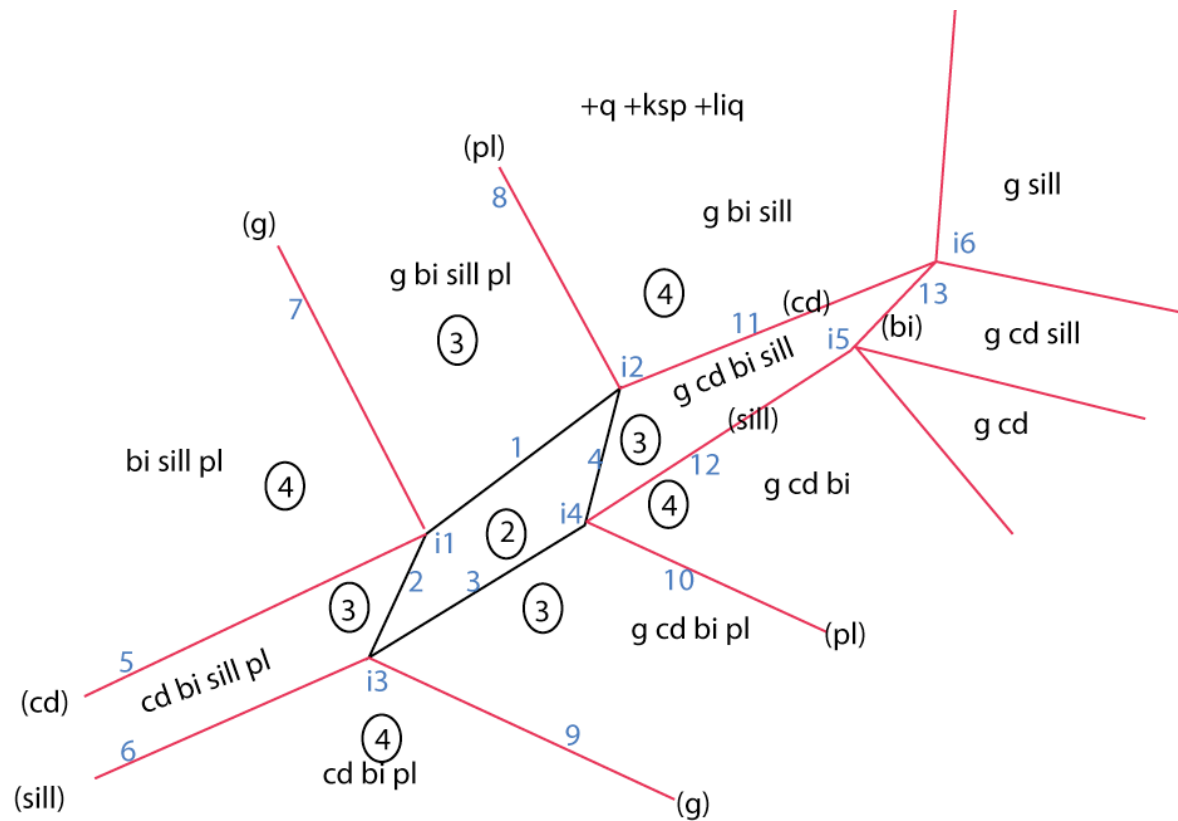
i5   i6

```

Running drawpd, the diagram should look like:



We now need to calculate the higher variance lines that emanate from the (cd bi) and (sill bi) points we just calculated, and the diagram should look something like this.



calculating the (bi) line from the g-bi-sill field is straight forward

```
% -----
u14  g liq ksp sill q - bi
i6  end
```

but the (cd) line from g-cd-sill-ksq-liq gives odd looking results that are well outside our window of interest

```
reading a-x datafile, "tc-NCKFMASHp.txt"...
ged anth bi cd st ctd chl g sp mu pa opx liq ksp pl osm
ky sill and q H2O
choose from: ged anth bi cd st ctd chl g sp mu pa opx liq ksp pl osm ky sill and q H2O
which phases : g cd sill ksp liq q
no phases in excess (from script)
```



variance of required equilibria :

0 = invariant  
1 = univariant  
2 = divariant  
...  
n = n-variant

variance : 4

you may set zero modal proportions, from:cd g liq ksp sill q

which to set : cd

calculate T at P (rather than P at T) ?

specification of PT window:

P range over which T of reactions to be calculated

P window: P low,high : 6 7

T window within which reactions expected to lie

T window: T low,high :

P window :6 <-> 7 kbar :P interval : 0.2

composition (from script)

H2O	SiO2	Al2O3	CaO	MgO	FeO	K2O	Na2O
5.92	69.11	8.82	0.27	3.59	8.80	2.93	0.56

<=====>

phases : cd, g, liq, ksp, sill, q

P(kbar)	T(?C)	x(cd)	h(cd)	x(g)	z(g)	q(L)	fsp(L)	na(L)	an(L)	ol(L)	x(L)	h2o(L)	na(ksp)	ca(ksp)
6.00	443.7	0.1026	0.8871	0.7104	0.02082	0.06078	0.1230	0.57590	0.00056920	0.0001453	0.3926	0.8151	0.099470	0.0004111
mode	cd	g	liq	ksp	sill	q								
	0	0.2951	0.1129	0.2436	0.02204	0.3264								

P(kbar)	T(?C)	x(cd)	h(cd)	x(g)	z(g)	q(L)	fsp(L)	na(L)	an(L)	ol(L)	x(L)	h2o(L)	na(ksp)	ca(ksp)
6.20	489.8	0.1273	0.8765	0.7104	0.02052	0.07033	0.1370	0.52720	0.00088790	0.0001920	0.4618	0.7908	0.097220	0.0006573
mode	cd	g	liq	ksp	sill	q								
	0	0.2950	0.1218	0.2383	0.02191	0.3230								

P(kbar)	T(?C)	x(cd)	h(cd)	x(g)	z(g)	q(L)	fsp(L)	na(L)	an(L)	ol(L)	x(L)	h2o(L)	na(ksp)	ca(ksp)
6.40	544.7	0.1583	0.8591	0.7104	0.01997	0.08444	0.1568	0.4678	0.0014750	0.0003055	0.5336	0.7555	0.09470	0.001074
mode	cd	g	liq	ksp	sill	q								
	0	0.2947	0.1358	0.2303	0.02164	0.3176								

P(kbar)	T(?C)	x(cd)	h(cd)	x(g)	z(g)	q(L)	fsp(L)	na(L)	an(L)	ol(L)	x(L)	h2o(L)	na(ksp)	ca(ksp)
6.60	622.2	0.2038	0.8228	0.7104	0.01867	0.1102	0.1911	0.3840	0.0028540	0.0006722	0.6147	0.6916	0.09188	0.001926
mode	cd	g	liq	ksp	sill	q								
	0	0.2940	0.1646	0.2142	0.02089	0.3063								

11

notice how this line is very flat in P-T space >200° / kbar. For flat lines like this it is best to calculate P at T by entering “no” at the prompt “calculate T at P (rather than P at T) ?”

rerunning this equilibria at given T’s gives:

reading a-x datafile, "tc-NCKFMASHp.txt"...

ged anth bi cd st ctd chl g sp mu pa opx liq ksp pl osm  
 ky sill and q H2O

choose from: ged anth bi cd st ctd chl g sp mu pa opx liq ksp pl osm ky sill and q H2O

which phases : =

use same phases - of these: cd g liq ksp sill q

omit :

no phases in excess (from script)

variance of required equilibria :

0 = invariant  
 1 = univariant  
 2 = divariant  
 ...  
 n = n-variant

variance : 4

you may set zero modal proportions, from:cd g liq ksp sill q

which to set : cd

calculate T at P (rather than P at T) ? no

specification of PT window:

T range over which P of reactions to be calculated

T window: T low,high : 780 870

P window within which reactions expected to lie

P window: P low,high :

T window : 780 <-> 870?C :T interval : 10

composition (from script)

H2O	SiO2	Al2O3	CaO	MgO	FeO	K2O	Na2O
5.92	69.11	8.82	0.27	3.59	8.80	2.93	0.56

<=====>

phases : cd, g, liq, ksp, sill, q

P(kbar)	T(?C)	x(cd)	h(cd)	x(g)	z(g)	q(L)	fsp(L)	na(L)	an(L)	ol(L)	x(L)	h2o(L)	na(ksp)	ca(ksp)
6.60	780.0	0.2958	0.6673	0.7101	0.01301	0.1826	0.2882	0.2351	0.007953	0.003873	0.7226	0.5004	0.08881	0.004188
mode	cd	g	liq	ksp	sill	q								
	0	0.2885	0.2949	0.1434	0.01555	0.2576								
P(kbar)	T(?C)	x(cd)	h(cd)	x(g)	z(g)	q(L)	fsp(L)	na(L)	an(L)	ol(L)	x(L)	h2o(L)	na(ksp)	ca(ksp)
6.58	790.0	0.3013	0.6512	0.7100	0.01250	0.1879	0.2956	0.2273	0.008304	0.004324	0.7275	0.4854	0.08866	0.004296
mode	cd	g	liq	ksp	sill	q								
	0	0.2877	0.3095	0.1356	0.01483	0.2524								
P(kbar)	T(?C)	x(cd)	h(cd)	x(g)	z(g)	q(L)	fsp(L)	na(L)	an(L)	ol(L)	x(L)	h2o(L)	na(ksp)	ca(ksp)
6.56	800.0	0.3068	0.6340	0.7098	0.01197	0.1933	0.3031	0.2197	0.008640	0.004825	0.7322	0.4699	0.08850	0.004390
mode	cd	g	liq	ksp	sill	q								
	0	0.2868	0.3255	0.1270	0.01403	0.2466								
P(kbar)	T(?C)	x(cd)	h(cd)	x(g)	z(g)	q(L)	fsp(L)	na(L)	an(L)	ol(L)	x(L)	h2o(L)	na(ksp)	ca(ksp)
6.53	810.0	0.3122	0.6157	0.7096	0.01143	0.1989	0.3107	0.2123	0.008956	0.005381	0.7367	0.4540	0.08834	0.004469
mode	cd	g	liq	ksp	sill	q								

	0	0.2858	0.3430	0.1177	0.01313	0.2404								
P(kbar)	T(?C)	x(cd)	h(cd)	x(g)	z(g)	q(L)	fsp(L)	na(L)	an(L)	ol(L)	x(L)	h2o(L)	na(ksp)	ca(ksp)
6.51	820.0	0.3175	0.5962	0.7094	0.01088	0.2045	0.3184	0.2051	0.009248	0.005996	0.7410	0.4378	0.08815	0.004531
mode	cd	g	liq	ksp	sill	q								
	0	0.2846	0.3623	0.1075	0.01213	0.2335								
P(kbar)	T(?C)	x(cd)	h(cd)	x(g)	z(g)	q(L)	fsp(L)	na(L)	an(L)	ol(L)	x(L)	h2o(L)	na(ksp)	ca(ksp)
6.48	830.0	0.3228	0.5754	0.7092	0.01032	0.2103	0.3262	0.1981	0.009511	0.006675	0.7451	0.4212	0.08795	0.004573
mode	cd	g	liq	ksp	sill	q								
	0	0.2832	0.3835	0.09627	0.01100	0.2260								
P(kbar)	T(?C)	x(cd)	h(cd)	x(g)	z(g)	q(L)	fsp(L)	na(L)	an(L)	ol(L)	x(L)	h2o(L)	na(ksp)	ca(ksp)
6.45	840.0	0.3279	0.5534	0.7088	0.009755	0.2161	0.3340	0.1914	0.009738	0.007425	0.7490	0.4043	0.08771	0.004594
mode	cd	g	liq	ksp	sill	q								
	0	0.2817	0.4069	0.08395	0.009727	0.2178								
P(kbar)	T(?C)	x(cd)	h(cd)	x(g)	z(g)	q(L)	fsp(L)	na(L)	an(L)	ol(L)	x(L)	h2o(L)	na(ksp)	ca(ksp)
6.42	850.0	0.3329	0.5300	0.7084	0.009182	0.2219	0.3419	0.1848	0.009924	0.008252	0.7528	0.3871	0.08744	0.004593
mode	cd	g	liq	ksp	sill	q								
	0	0.2799	0.4329	0.07034	0.008294	0.2086								
P(kbar)	T(?C)	x(cd)	h(cd)	x(g)	z(g)	q(L)	fsp(L)	na(L)	an(L)	ol(L)	x(L)	h2o(L)	na(ksp)	ca(ksp)
6.38	860.0	0.3378	0.5052	0.7080	0.008606	0.2278	0.3499	0.1784	0.01006	0.009162	0.7563	0.3696	0.08713	0.004567
mode	cd	g	liq	ksp	sill	q								
	0	0.2778	0.4617	0.05527	0.006672	0.1985								
P(kbar)	T(?C)	x(cd)	h(cd)	x(g)	z(g)	q(L)	fsp(L)	na(L)	an(L)	ol(L)	x(L)	h2o(L)	na(ksp)	ca(ksp)
6.35	870.0	0.3424	0.4791	0.7074	0.008030	0.2337	0.3578	0.1721	0.01015	0.01016	0.7597	0.3518	0.08675	0.004517
mode	cd	g	liq	ksp	sill	q								
	0	0.2753	0.4940	0.03850	0.004829	0.1873								

The (sill) boundary for the same field is also very flat so calculate this at a range of T's

As a general rule, this is one of the first things you should try if you can't calculate a line at a set of P's

The (bi) line from the assemblage g-cd-bi can also be calculated, but as it is steep it can be calculated at a series of P's.

The line numbers and start/finish points for these lines are given below

```
% -----
u14  g liq ksp sill q  - bi
i6  end
```

```
% -----
u15  g liq ksp sill q  - cd

i6  end
```

```
% -----
u16  cd g liq ksp q  - sill

i5  end
```

```
% -----
u17  cd g liq ksp q  - bi

begin i5
```

Now, the next step takes some intuition, this is where many people run into trouble. Looking at the finished pseudosection, there are a series of opx-bearing fields at lower-P /higher-T. You have to have some idea they are there to calculate them. In something like this sub aluminous metapelite, the opx fields could be inferred from a basic understanding of the AFM compatibility triangles for high-grade rocks and a basic knowledge of the published KFMASH grids. Some points based on this are listed below.

- 1) at these low pressures, opx will only be stable in ksp + liq +q bearing rocks in the absence of sillimanite (opx-sill restricted to higher P-T)
- 2) only assemblages that plot below the g-cd tie line in AFM for a given P-T may develop opx-bearing assemblages except at high P-T
- 3) the main KFMASH backbone reaction that brings in opx to higher T is the reaction  $bi + g = opx + cd$ , so any field with  $bi + g + cd$  is a sensible place to look

following this logic it would seem the g-cd-bi-pl trivariant field is a place to look for an opx-in line. I got the result

```
reading a-x datafile, "tc-NCKFMASHp.txt"...
ged anth bi cd st ctd chl g sp mu pa opx liq ksp pl osm
ky sill and q H2O
choose from: ged anth bi cd st ctd chl g sp mu pa opx liq ksp pl osm ky sill and q H2O
which phases : g bi cd pl opx ksp liq q
no phases in excess (from script)

variance of required equilibria :
  0 = invariant
  1 = univariant
  2 = divariant
  ...
  n = n-variant
variance : 2
you may set zero modal proportions, from:bi cd g opx liq ksp pl q
which to set : opx
calculate T at P (rather than P at T) ?

specification of PT window:
```

P range over which T of reactions to be calculated

P window: P low,high : 2.4 3

T window within which reactions expected to lie

T window: T low,high :

P window :2.4 <-> 3 kbar :P interval : 0.1

composition (from script)

H2O	SiO2	Al2O3	CaO	MgO	FeO	K2O	Na2O
5.92	69.11	8.82	0.27	3.59	8.80	2.93	0.56

<=====>

phases : bi, cd, g, opx, liq, ksp, pl, q

77-----

P(kbar)	T(?C)	x(bi)	y(bi)	Q(bi)	x(cd)	h(cd)	x(g)	z(g)	x(opx)	y(opx)	Q(opx)	q(L)	fsp(L)	na(L)	an(L)	ol(L)	x(L)	h2o(L)	na(ksp)
ca(ksp)	751.9	0.7598	0.4151	0.07753	0.5497	0.3950	0.8843	0.02816	0.7690	0.1407	0.2790	0.2415	0.3290	0.3536	0.01025	0.008872	0.8502	0.3995	0.1774
0.01244		ca(pl)	k(pl)																
		0.5270	0.02660																

mode	bi	cd	g	opx	liq	ksp	pl	q
	0.2349	0.1619	0.01791	0	0.1507	0.07967	0.01280	0.3421

P(kbar)	T(?C)	x(bi)	y(bi)	Q(bi)	x(cd)	h(cd)	x(g)	z(g)	x(opx)	y(opx)	Q(opx)	q(L)	fsp(L)	na(L)	an(L)	ol(L)	x(L)	h2o(L)	na(ksp)
ca(ksp)	754.6	0.7473	0.4131	0.08162	0.5367	0.4004	0.8783	0.02957	0.7587	0.1410	0.2892	0.2426	0.3268	0.3385	0.01097	0.008996	0.8450	0.3997	0.1652
0.01243		ca(pl)	k(pl)																
		0.5557	0.02496																

mode	bi	cd	g	opx	liq	ksp	pl	q
	0.2132	0.1544	0.03880	0	0.1724	0.08355	0.009180	0.3284

P(kbar)	T(?C)	x(bi)	y(bi)	Q(bi)	x(cd)	h(cd)	x(g)	z(g)	x(opx)	y(opx)	Q(opx)	q(L)	fsp(L)	na(L)	an(L)	ol(L)	x(L)	h2o(L)	na(ksp)
ca(ksp)	757.2	0.7348	0.4112	0.08569	0.5240	0.4058	0.8723	0.03079	0.7484	0.1412	0.2991	0.2433	0.3248	0.3253	0.01163	0.009099	0.8399	0.4000	0.1553
0.01243		ca(pl)	k(pl)																
		0.5795	0.02375																

mode	bi	cd	g	opx	liq	ksp	pl	q
	0.1932	0.1476	0.05802	0	0.1922	0.08701	0.005993	0.3160

P(kbar)	T(?C)	x(bi)	y(bi)	Q(bi)	x(cd)	h(cd)	x(g)	z(g)	x(opx)	y(opx)	Q(opx)	q(L)	fsp(L)	na(L)	an(L)	ol(L)	x(L)	h2o(L)	na(ksp)
ca(ksp)	759.6	0.7223	0.4094	0.08972	0.5117	0.4113	0.8662	0.03185	0.7383	0.1414	0.3085	0.2437	0.3231	0.3137	0.01223	0.009184	0.8348	0.4005	0.1470
0.01245		ca(pl)	k(pl)																
		0.5995	0.02283																

mode	bi	cd	g	opx	liq	ksp	pl	q
	0.1748	0.1413	0.07577	0	0.2102	0.09015	0.003131	0.3046

alternatively you could search for the bounding points to this line where it hits lines 9 and 10, which is useful if the (opx) line is likely to be rather short and hence hard to find

% -----  
i7 bi cd g liq ksp q - opx pl

3.02 762.3 % opx = 0pl = 0

% -----  
i8 bi cd liq ksp pl q - g opx

$$2.52 \quad 749.5 \quad \% g = \theta_{\text{opx}} = 0$$

the (opx) line being

```
% -----
u18  bi cd g liq ksp pl q  - opx
```

i7 i8

there will also be at least a (pl) and a (g) line bounding this field.

Calculating the (pl) line shows that it terminates at a (pl bi) point, and hence a (bi) line must also bound this field.

```
% -----
i9   cd g opx liq ksp q  - bi pl
```

2.57 762.9 % bi = 0pl = 0

Some of these lines are very short and can be hard to calculate, but calculating the (g) shows us that it ends at a (g bi) point.

When I tried to calculate the (g) line I got no results (calculating at P), but did find a result calculating at T.

specification of PT window:

T range over which P of reactions to be calculated

T window: T low,high : 750 800

P window within which reactions expected to lie

P window: P low,high :

T window : 750 <-> 800°C :T interval : 5

composition (from script)

H2O	SiO2	Al2O3	CaO	MgO	FeO	K2O	Na2O
-----	------	-------	-----	-----	-----	-----	------

5.92 69.11 8.82 0.27 3.59 8.80 2.93 0.56

◀=====▶

phases : bi, cd, g, opx, liq, ksp, pl, q

7-----

P(kbar)	T(?C)	x(bi)	y(bi)	Q(bi)	x(cd)	h(cd)	x(g)	z(g)	x(opx)	y(opx)	Q(opx)	q(L)	fsp(L)	na(L)	an(L)	ol(L)	x(L)	h2o(L)	na(ksf)
---------	-------	-------	-------	-------	-------	-------	------	------	--------	--------	--------	------	--------	-------	-------	-------	------	--------	---------

2.50	755.0	0.7704	0.4158	0.07385	0.5631	0.3873	0.8895	0.03227	0.7781	0.1411	0.2684	0.2541	0.3222	0.2994	0.01202	0.009152	0.8551	0.3914	0.1383
0.01207																			
		ca(pl)	k(pl)																
		0.6212	0.02133																
mode	bi	cd	g	opx	liq	ksp	pl	q											
	0.1713	0.1783	0	0.05147	0.2119	0.08987	0.009853	0.2873											
-----																			
P(kbar)	T(?C)	x(bi)	y(bi)	Q(bi)	x(cd)	h(cd)	x(g)	z(g)	x(opx)	y(opx)	Q(opx)	q(L)	fsp(L)	na(L)	an(L)	ol(L)	x(L)	h2o(L)	na(ksp)
ca(ksp)																			
2.48	760.0	0.7713	0.4149	0.07337	0.5659	0.3846	0.8900	0.03714	0.7791	0.1417	0.2661	0.2674	0.3132	0.2316	0.01433	0.009511	0.8558	0.3841	0.09783
0.01176																			
		ca(pl)	k(pl)																
		0.7242	0.01727																
mode	bi	cd	g	opx	liq	ksp	pl	q											
	0.05482	0.1920	0	0.1244	0.3281	0.1065	0.004096	0.1901											

Doing this calculation at smaller T increments shows that the line terminates at a (g bi) point

```
% -----
i10  cd opx liq ksp pl q  - bi g

2.48 761.6  % bi = 0g = 0
```

Thus the (bi) line must connect the (g bi) and (pl bi) points. Calculating these points shows that they are very close together

```
% -----
i9   cd g opx liq ksp q  - bi pl

2.57 762.9  % bi = 0pl = 0

% -----
i10  cd opx liq ksp pl q  - bi g

2.48 761.6  % bi = 0g = 0
```

Rather than bothering to calculate the short (bi) line you can use the “connect” code in drawpd to draw a line between the two terminating points

```
% -----
u21  cd g opx liq ksp pl q  - bi

i9 i10 connect
```

So, calculating all the lines and points closes off the divariant field.

You will notice that the divariant field has a different shape than that published in White et al 2007. This is because we are now using a slightly different garnet a-x model than used there

We now need to calculate the other lines that emanate from the points we have just calculated. You should notice that the two lines that bound the g-opx-pl field, (g) and (pl), connect to higher T at a (g pl) point. Likewise the lines bounding the bi-g-opx-cd-ksp-q-liq field connect at a (opx bi) point

Calculating these points and lines gives:

```
% -----
i11  cd opx liq ksp q  - g pl

2.56 776.6  % g = 0pl = 0

% -----
i12  cd g liq ksp q  - bi opx

4.74 797.2  % bi = 0opx = 0

% -----
u22  bi cd liq ksp pl q  - opx

begin i8

% -----
u23  cd opx liq ksp pl q  - bi

begin i10

% -----
u24  cd opx liq ksp pl q  - g

i10 i11

% -----
u25  cd g opx liq ksp q  - pl

i9 i11

% -----
u26  bi cd g liq ksp q  - opx

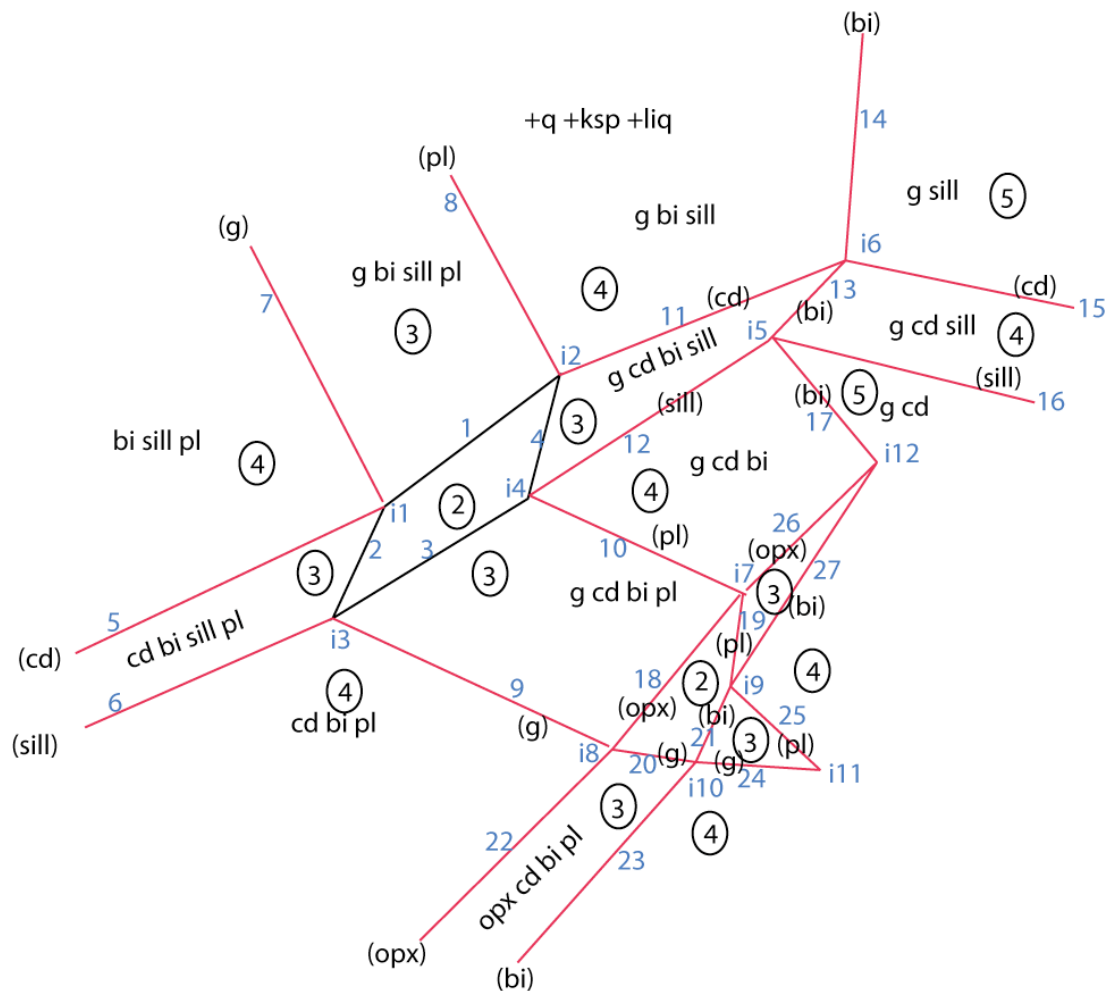
i7 i12

% -----
u27  cd g opx liq ksp q  - bi

i9 i12
```

Note that line u17 also now terminates at i12. The sketch of the diagram should now look something like:





we now need to calculate the remaining lines that emanate from i11 and i12. From i12 we have the assemblage g-opx-cd-ksp-q-liq and the (opx) boundary to this (calculate this at a set of T's). From i11 we have the (g) line from the same field and the (pl) from the opx-cd-pl-ksp-q-liq field

the (g) line bounding the g-opx-cd field terminates up T at a (g ksp) point, meaning there is also a (ksp) boundary to this field, giving the following points and lines:

```
% -----
i13  cd opx liq q - g ksp
3.19 841.6 % g = 0ksp = 0
```

```
% -----
u28   cd g liq ksp q  - opx

i12   end

% -----
u29   cd opx liq ksp q  - g

i11   i13

% -----
u30   cd opx liq ksp q  - pl

begin  i11

% -----
u31   cd g opx liq q   - ksp

i13   end
```

there are 2 lines remaining to be calculated that emanate from i13, being:

```
% -----
u32   cd opx liq q   - g

i13   end

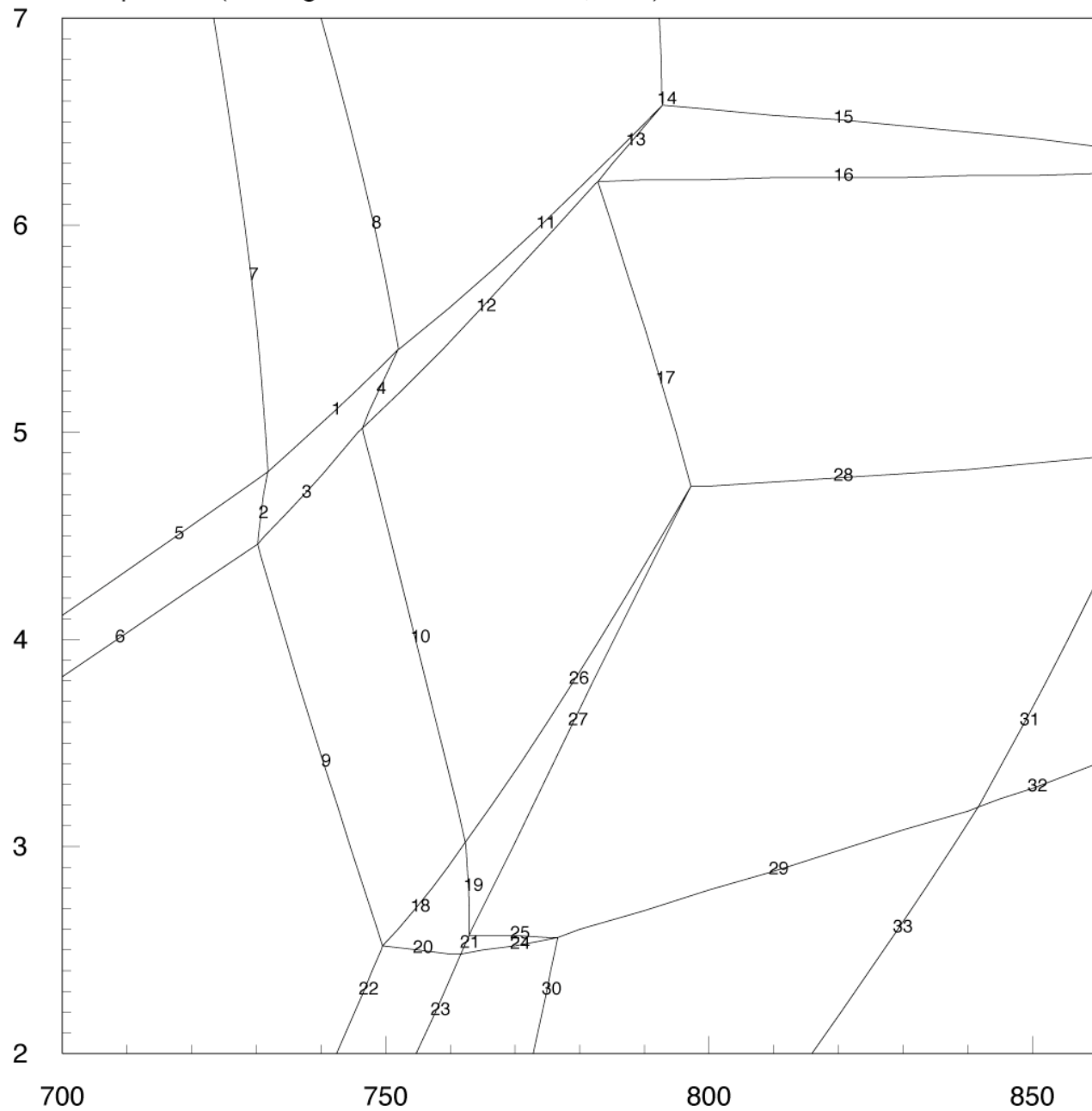
% -----
u33   cd opx liq q   - ksp

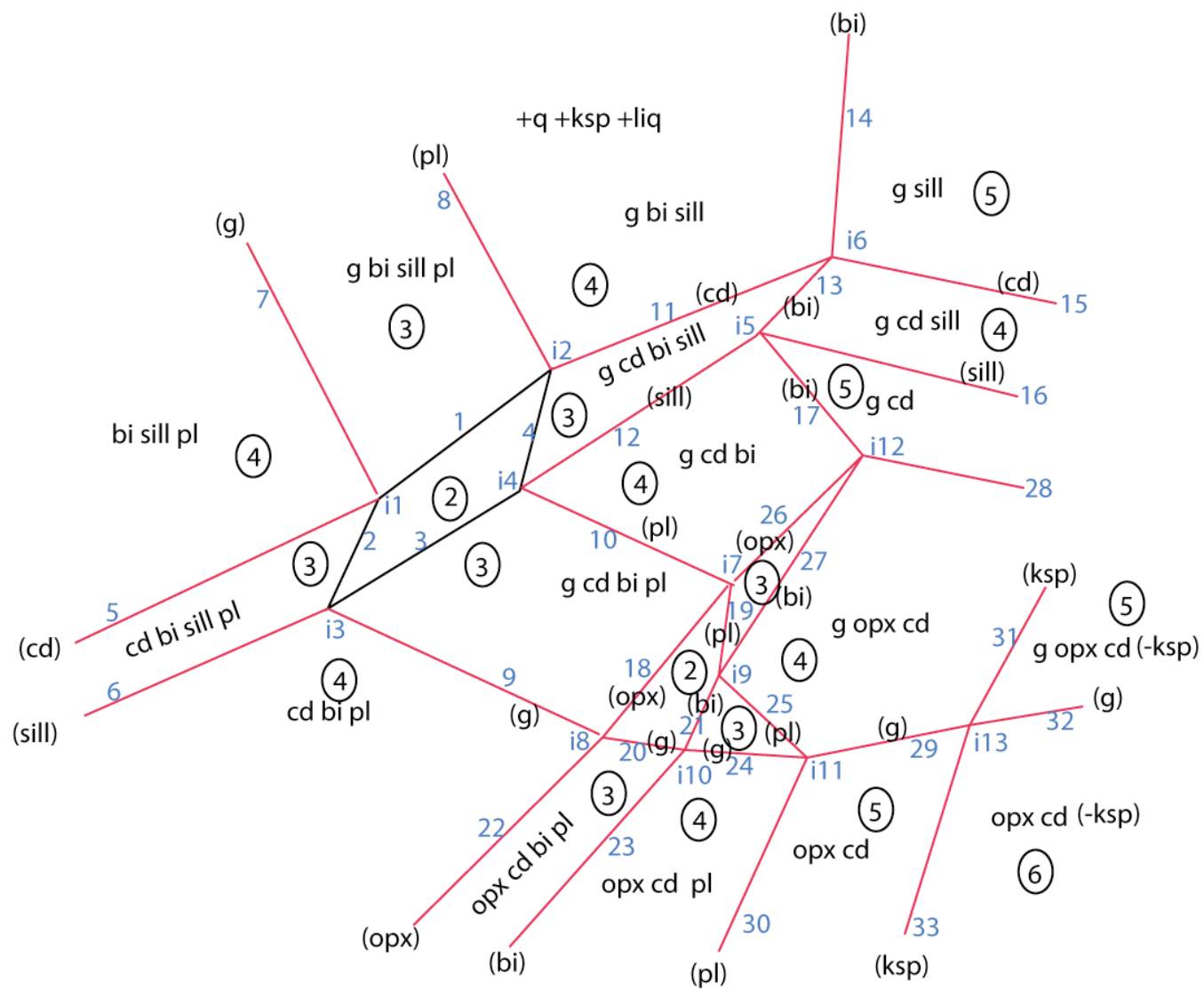
begin  i13
```

and the diagram is now finished (in terms of calculations). You can now fill in each of the areas in the standard way in drawpd.

Below are the finished (but not coloured in) drawpd output and the accompanying sketch

drawpd 1.11 (running at 16.07 on Sat 8 Mar,2008)





the list below is a summary list of each line and point

- i1) bi liq ksp pl sill q (cd g)
- i2) bi g liq ksp sill q (cd pl)
- i3) bi cd liq ksp pl q (g sill)
- i4) bi cd g liq ksp q (pl sill)

i5) cd g liq ksp q (bi sill)  
i6) g liq ksp sill q (bi cd)  
i7) bi cd g liq ksp q (opx pl)  
i8) bi cd liq ksp pl q (g opx)  
i9) cd g opx liq ksp q (bi pl)  
i10) cd opx liq ksp pl q (bi g)  
i11) cd opx liq ksp q (g pl)  
i12) cd g liq ksp q (bi opx)  
i13) cd opx liq q (g ksp)  
u1) bi g liq ksp pl sill q (cd) - 6 data points  
u2) bi cd liq ksp pl sill q (g) - 4 data points  
u3) bi cd g liq ksp pl q (sill) - 6 data points  
u4) bi cd g liq ksp sill q (pl) - 4 data points  
u5) bi liq ksp pl sill q (cd) - 12 data points  
u6) bi cd liq ksp pl q (sill) - 13 data points  
u7) bi liq ksp pl sill q (g) - 21 data points  
u8) bi g liq ksp sill q (pl) - 17 data points  
u9) bi cd liq ksp pl q (g) - 16 data points  
u10) bi cd g liq ksp q (pl) - 21 data points  
u11) bi g liq ksp sill q (cd) - 8 data points  
u12) bi cd g liq ksp q (sill) - 7 data points  
u13) cd g liq ksp sill q (bi) - 3 data points  
u14) g liq ksp sill q (bi) - 11 data points  
u15) g liq ksp sill q (cd) - 10 data points  
u16) cd g liq ksp q (sill) - 13 data points  
u17) cd g liq ksp q (bi) - 17 data points  
u18) bi cd g liq ksp pl q (opx) - 4 data points  
u19) bi cd g opx liq ksp q (pl) - 5 data points  
u20) bi cd opx liq ksp pl q (g) - 2 data points  
u21) cd g opx liq ksp pl q (bi) - connect  
u22) bi cd liq ksp pl q (opx) - 7 data points  
u23) cd opx liq ksp pl q (bi) - 7 data points  
u24) cd opx liq ksp pl q (g) - 6 data points  
u25) cd g opx liq ksp q (pl) - 6 data points  
u26) bi cd g liq ksp q (opx) - 14 data points  
u27) cd g opx liq ksp q (bi) - 12 data points  
u28) cd g liq ksp q (opx) - 7 data points  
u29) cd opx liq ksp q (g) - 8 data points

u30) cd opx liq ksp q (pl) - 11 data points

u31) cd g opx liq q (ksp) - 9 data points

u32) cd opx liq q (g) - 13 data points

u33) cd opx liq q (ksp) - 11 data points

window: x = 700.0 <=> 860.0; y = 2.0 <=> 7.0