

Calculating isopleths (aka contours) tutorial

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This tutorial involves calculating mode and composition isopleths/ contours on the finished P-T pseudosection from the introductory phase diagram tutorial. So, this tutorial assumes that you have already finished that practical. However, a finished drawpd file for that prac, that also has the fields filled is provided

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))

Mode isopleths are lines of equal mode of any of the phases present and are fairly straightforward to calculate, being done in much the same way as the boundaries between fields which are zero mode isopleths.

Composition isopleths are lines of equal value for compositional variables. These compositional variables are those that are used to define the compositions of phases (i.e. the same variables used as starting guesses being those that are output in each run of thermocalc). They typically have the form x(g), y(opx) etc.

Other than telling thermocalc you want to calculate these, the mechanics of running thermocalc is the same as for most calculations.

This tutorial was prepared using thermocalc 3.33i and drawpd 1.15 on a mac
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)

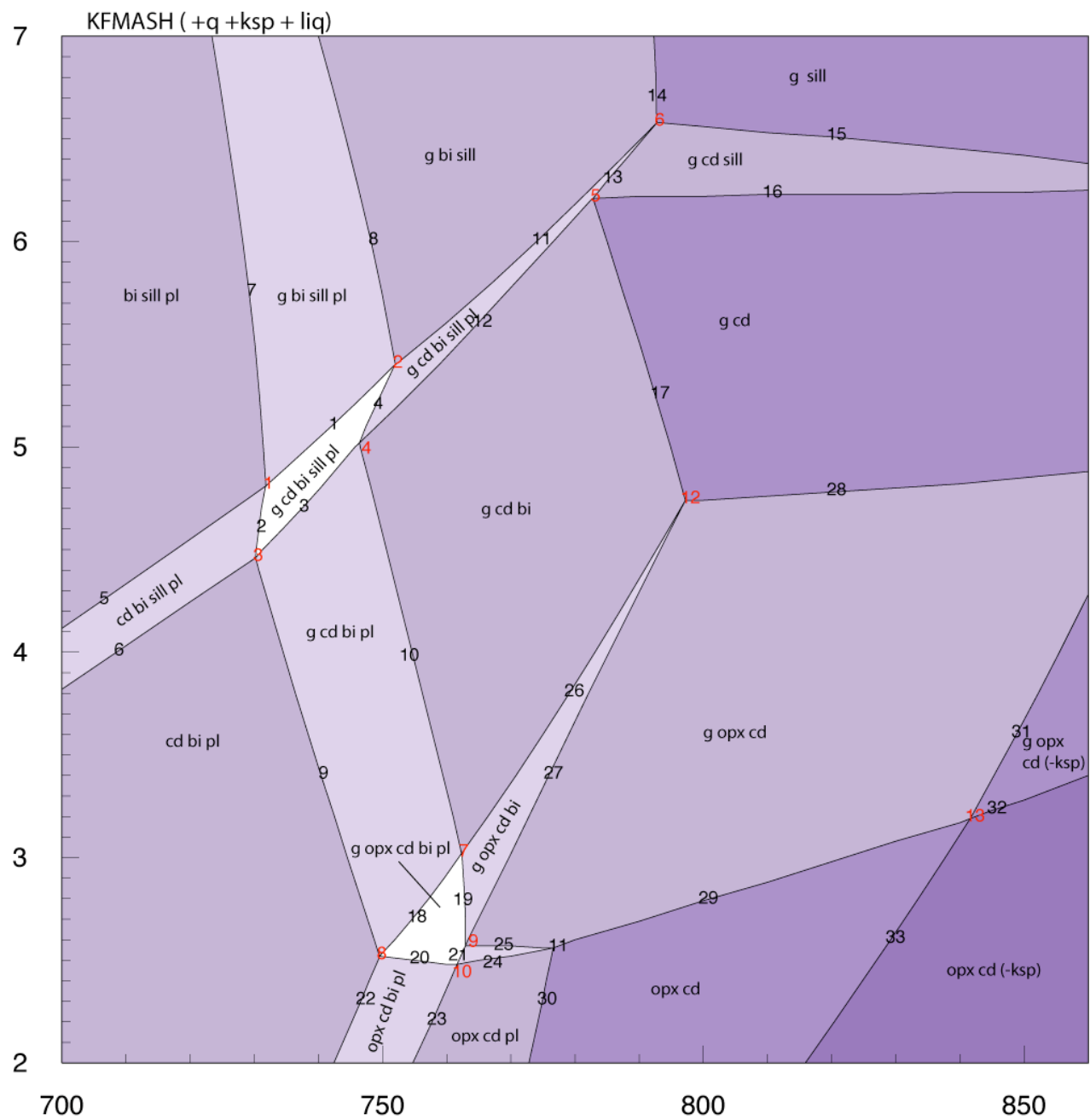
dr-iso For mac and pc drawpd 1.15 (in whatever folder you have drawpd)
 The above files are the base drawpd files for the pseudosection)
dr-fin is the finished drawpd files

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.

Starting with the finished pseudosection below, I will cover doing some mode and composition isopleths for the g-cd-bi-pl and g-cd-bi fields.



Part 1 – Mode isopleths

I will start by contouring for the mode of garnet. Normally, I would calculate around one or two of the field boundaries or the points that terminate them just to get an idea of the range in garnet mode that occurs in the diagram so I can pick an appropriate isopleth interval. For this I will re-run points 4 & 5 from the original tutorial getting:

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)
5.02	746.3	0.6849	0.5613	0.06917	0.4512	0.5982	0.8440	0.03045	0.1865	0.2886	0.3567	0.01209	0.002890
mode	bi	cd	g	liq	ksp	pl	sill	q						
	0.1576	0.1017	0.1210	0.1617	0.1216	0	0	0.3364						

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)
6.21	782.8	0.5270	0.5105	0.1085	0.3378	0.6373	0.7475	0.01390	0.1909	0.2935	0.2348	0.008458	0.004180
mode	bi	cd	g	liq	ksp	sill	q							
	0	0.05441	0.2619	0.2918	0.1450	0	0.2469							

Given that the low-P boundary of the g-cd-bi-pl field is the g=0 line then I will contour these fields for garnet between 0.05 and 0.3 at 0.05 intervals.

To calculate mode isopleths the important scripts in the script file are “setmodeiso” and “zeromodeiso”, so these scripts should be set to:

```
setmodeiso yes
zeromodeiso no
```

though if you are only contouring for one phase at a time then you could also set these to:

```
setmodeiso g
zeromodeiso no
```

to automatically prompt for garnet modes, though for now we will use the first option.

Starting with the g-cd-bi-pl field I will calculate the 0.05 0.1 and 0.15 mode isopleths for garnet. Running thermocalc with these new script codes, is the same as normal until we are prompted for entering the phase we want to contour and then the modes we want to contour for.

```
you may set modal proportions, from:bi cd g liq ksp pl q
which to set : g
```

```
specifying mode isopleths for g:
list of values OR start, finish, interval :
```

The first question is simple you just give the phase abbreviation (ie g). For setting the modes (2nd qn) there are two options, a list of numbers or a start, finish, interval. Thermocalc works out which one you want from the input. For the first method you would answer

```
list of values OR start, finish, interval :0.05 0.1 0.15
```

For the second method:

```
list of values OR start, finish, interval :0.05 0.15 0.05
```

Either method (calculating for 2-5 kbar at 0.25 kbar increments) gives the results for g=0.05 and 0.1 but no result for 0.15 suggesting it does not exist in that field.

Note that the two isopleths are given as a single list (rather than as two lines) in the output files. So for the “–dr” the output looks like:

```
% -----  
u<k>   bi cd liq ksp pl q   - g
```

```
begin  end
```

```
2.000 764.12 % g = 0.05  
2.250 761.49 % g = 0.05  
2.500 758.85 % g = 0.05  
2.750 756.19 % g = 0.05  
3.000 753.53 % g = 0.05  
3.250 750.88 % g = 0.05  
3.500 748.26 % g = 0.05  
3.750 745.66 % g = 0.05  
4.000 743.11 % g = 0.05  
4.250 740.61 % g = 0.05  
4.500 738.16 % g = 0.05  
4.750 735.78 % g = 0.05  
5.000 733.45 % g = 0.05  
3.500 758.03 % g = 0.1  
3.750 755.34 % g = 0.1  
4.000 752.67 % g = 0.1  
4.250 750.05 % g = 0.1  
4.500 747.47 % g = 0.1  
4.750 744.94 % g = 0.1  
5.000 742.46 % g = 0.1
```

When putting this into your drawpd file you will have to make this into two lines manually. When giving lines numbers, you can also use letters. This is useful if you are contouring for lots of minerals as it makes labeling the diagram easier. I’ve used u5ga and u10ga for 5% garnet, field a. These lines in your drawpd file and pseudosection will look like:

% -----
u5ga bi cd liq ksp pl q - g

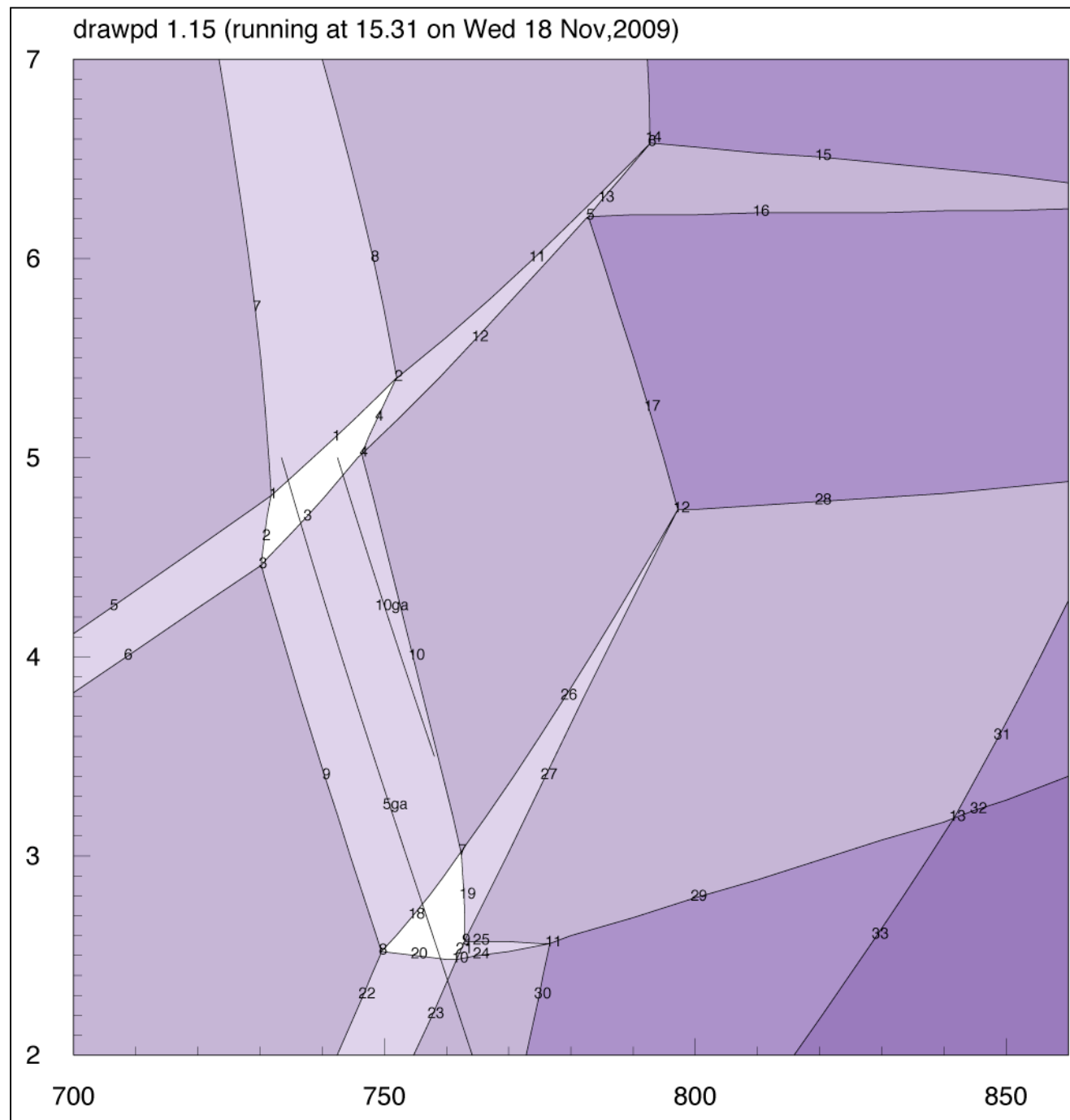
begin end

2.000	764.12	% g = 0.05
2.250	761.49	% g = 0.05
2.500	758.85	% g = 0.05
2.750	756.19	% g = 0.05
3.000	753.53	% g = 0.05
3.250	750.88	% g = 0.05
3.500	748.26	% g = 0.05
3.750	745.66	% g = 0.05
4.000	743.11	% g = 0.05
4.250	740.61	% g = 0.05
4.500	738.16	% g = 0.05
4.750	735.78	% g = 0.05
5.000	733.45	% g = 0.05

% -----
u10ga bi cd liq ksp pl q - g

begin end

3.500	758.03	% g = 0.1
3.750	755.34	% g = 0.1
4.000	752.67	% g = 0.1
4.250	750.05	% g = 0.1
4.500	747.47	% g = 0.1
4.750	744.94	% g = 0.1
5.000	742.46	% g = 0.1



The next step is to calculate the points where an isopleth begins or ends. For the top left points for these lines where they cross line 3, run the divariant assemblage, setting both g and sill as modes. You will be prompted for each mineral, for garnet enter “0.05 0.1” and for sillimanite “0”, getting the result below.

```
which phases : g sill cd bi pl ksp q liq
no phases in excess (from script)
variance of required equilibrium (2?) : 2
you may set modal proportions, from:bi cd g liq ksp pl sill q
which to set : g sill
```

```
specifying mode isopleths for g:
  list of values OR start, finish, interval : 0.05 0.1
```

```
specifying mode isopleths for sill:
  list of values OR start, finish, interval : 0
```

```
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
5.919	69.113	8.819	0.270	3.590	8.799	2.930	0.560

<=====>

```
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)
4.67	736.5	0.7342	0.5754	0.05639	0.4955	0.5824	0.8681	0.02520	0.1827	0.2940	0.4138	0.009351	0.002667	0.8312
mode	bi	cd	g	liq	ksp	pl	sill	q						
	0.2396	0.1165	0.05000	0.1007	0.09662	0.01339	0	0.3831						

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)
4.91	743.3	0.7011	0.5660	0.06494	0.4651	0.5932	0.8520	0.02900	0.1856	0.2899	0.3728	0.01128	0.002821	0.8178
mode	bi	cd	g	liq	ksp	pl	sill	q						
	0.1817	0.1061	0.1000	0.1437	0.1146	0.003725	0	0.3501						

more phase diagram calculations ?

and the “-dr” output

```
% -----
i<k>   bi cd liq ksp pl q  - g sill

4.672 736.52 % g = 0.05, sill = 0
4.912 743.33 % g = 0.1, sill = 0
```

which again has to be manually converted to two separate points (which I’ve numbered i30 & i31) ie:

```
% -----
i30  bi cd liq ksp pl q  - g sill
```

```
4.672 736.52 % g = 0.05, sill = 0
```

```
% -----
i31  bi cd liq ksp pl q  - g sill
```

```
4.912 743.33 % g = 0.1, sill = 0
```

doing the other two points completes this field

```
% -----
i32  bi cd liq ksp q  - g pl
```

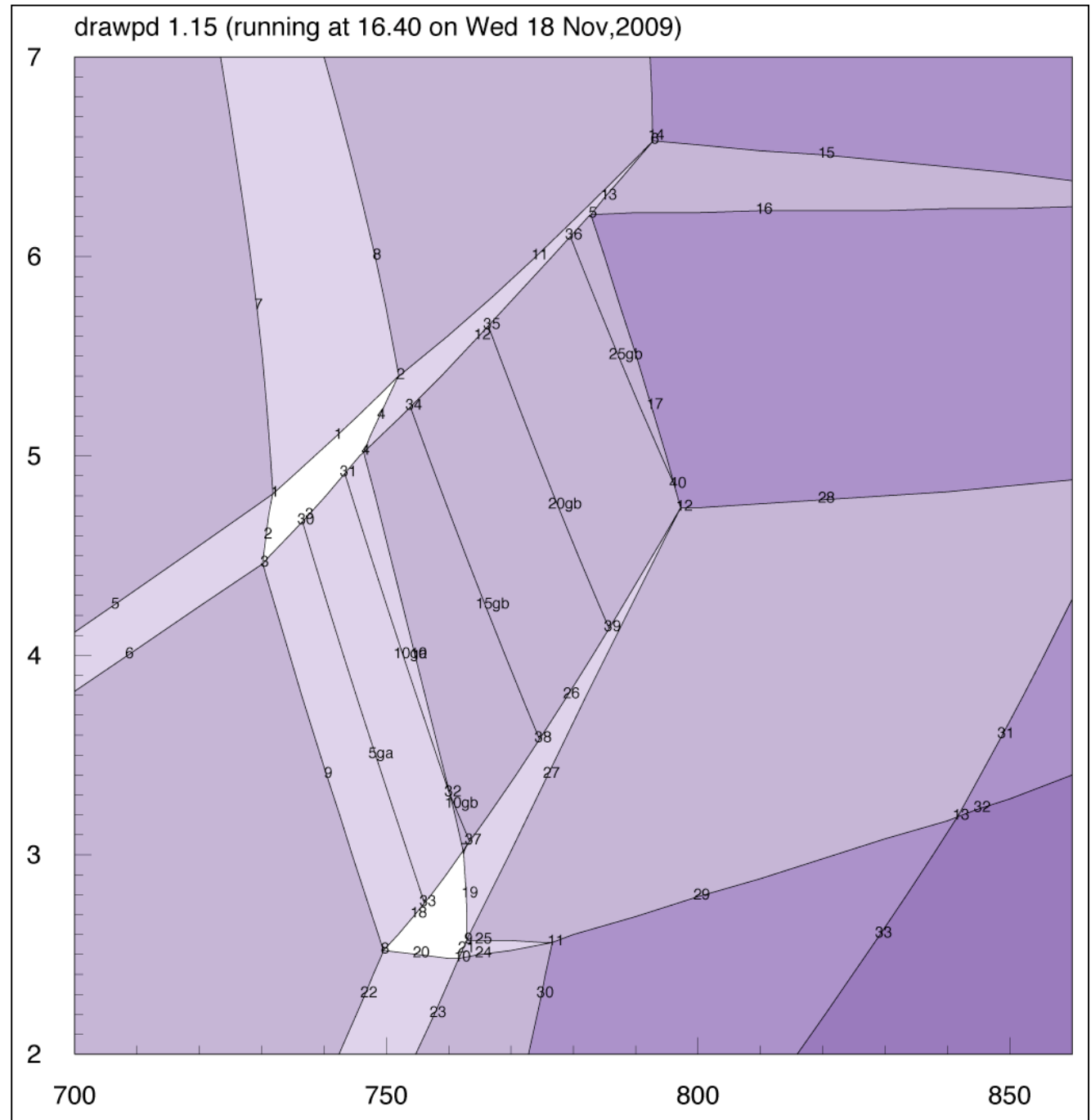
```
3.308 760.11 % g = 0.1, pl = 0
```

```
% -----
i33  bi cd liq ksp pl q  - g opx
```

```
2.758 756.10 % g = 0.05, opx = 0
```

going through the same process for the field g-cd-bi for the 0.1, 0.15, 0.2, 0.25 & 0.3 mode isopleths for garnet, your diagram should look like that to the right. Note that the 0.3 isopleth does not exist for this field.

Hint: if you can't be bothered calculating all the end points for the lines, you can just calculate the lines and use the scissors tool in illustrator to get rid of the unwanted parts. To be honest, this is the way I normally do it.



Part 2 Composition isopleths

I will go through contouring the fields g-cd-bi-pl-ksp-q-liq and g-cd-bi-ksp-q-liq for $x(g)$ where $x(g) = \text{FeO}/(\text{FeO} + \text{MgO})$ in garnet. To get an idea of the $x(g)$ range in that field I've looked at the output for the 0.05 and 0.1 mode contours for the g-cd-bi-pl-ksp-q-liq. You could also look at the boundaries of that field to get an idea. Given that most of you will have overwritten these earlier calculations the first step is to calculate the mode isopleths or boundaries around these fields. What you will discover is that $x(g)$ does not vary that much in the g-cd-bi-pl-ksp-q-liq field (mostly between 0.85 and 0.88), but gets as low as about 0.75 in the higher variance field. So, for this example I'll calculate the 0.76 0.78 0.8 0.82, 0.84 and 0.86 isopleths for $x(g)$

Setting the scripts for the mode isopleths back to

```
setmodeiso yes
zeromodeiso yes
```

you now need to set the script for composition isopleths which is:

```
setiso yes
```

Again, if you want to only do $x(g)$ isopleths, you can use the script

```
setiso x(g)
```

but I will use the first approach here. Running thermocalc, all is normal until you get to

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

where you just hit return to set no zero modes. The next new prompt is

```
you may set compositional variables, from: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)
(maximum number to set = 3
which variables to set :
```

where you input " $x(g)$ ". However you can also input a number to represent the n'th variable from the list. In this case you could enter "6" rather than $x(g)$

so the first run looks like

which phases : g cd bi pl ksp q liq
 no phases in excess (from script)
 variance of required equilibrium (3?) : 3
 you may set zero modal proportions, from:bi cd g liq ksp pl q
 which to set :
 you may set compositional variables, from: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)
 (maximum number to set = 3
 which variables to set : x(g)

specifying isopleths for x(g):
 list of values OR start, finish, interval : 0.86
 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)

H2O	SiO2	Al2O3	CaO	MgO	FeO	K2O	Na2O
5.919	69.113	8.819	0.270	3.590	8.799	2.930	0.560

<=====>

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

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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)
3.00	761.9	0.7097	0.4075	0.09372	0.4998	0.4167	0.86	0.03277	0.2438	0.3217	0.3036	0.01279	0.009257
mode	bi	cd	g	liq	ksp	pl	q							
	0.1578	0.1355	0.09226	0.2268	0.093020	0.005206	0.2942							

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)
3.25	758.9	0.7108	0.4311	0.08867	0.4971	0.4422	0.86	0.03200	0.2349	0.3175	0.3152	0.01246	0.007833
mode	bi	cd	g	liq	ksp	pl	q							
	0.1641	0.1323	0.09111	0.2082	0.09729	0.001407	0.3056							

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)
3.50	755.9	0.7119	0.4545	0.08373	0.4944	0.4673	0.86	0.03124	0.2263	0.3132	0.3270	0.01212	0.006622
mode	bi	cd	g	liq	ksp	pl	q							
	0.1706	0.1291	0.08959	0.1913	0.1007	0.002330	0.3163							

etc

Calculating the other isopleths in the g-cd-bi-ksp-q-liq field, the “-dr” file will look like:

```

% -----
u<k>  bi cd g liq ksp pl q  -

begin  end

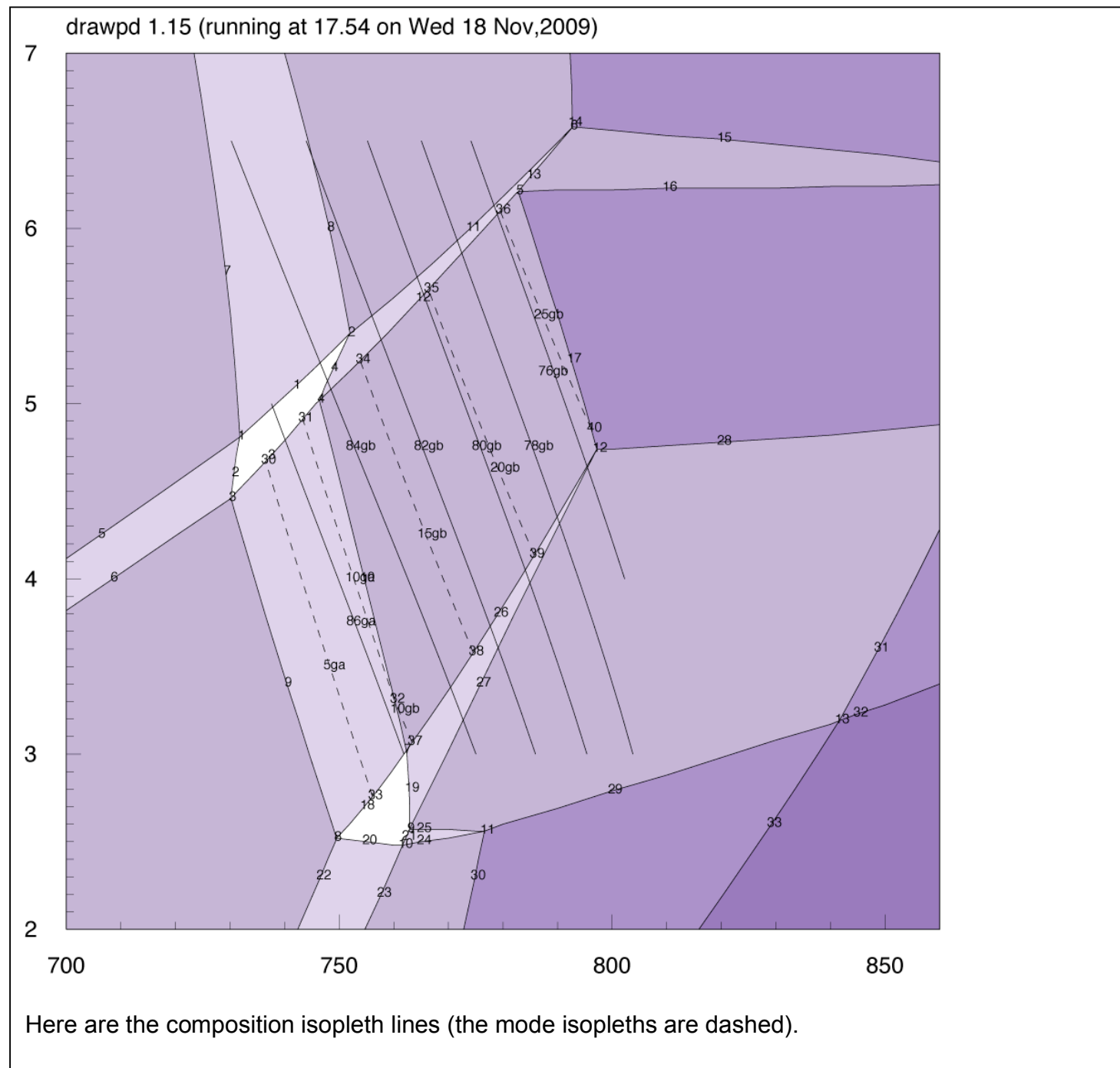
3.000 761.85 % x(g) = 0.86
3.250 758.90 % x(g) = 0.86
3.500 755.90 % x(g) = 0.86
3.750 752.86 % x(g) = 0.86
4.000 749.80 % x(g) = 0.86
4.250 746.73 % x(g) = 0.86
4.500 743.66 % x(g) = 0.86
4.750 740.61 % x(g) = 0.86
5.000 737.59 % x(g) = 0.86

% -----
u<k>  bi cd g liq ksp q  -

begin  end

4.000 802.30 % x(g) = 0.76
4.250 799.68 % x(g) = 0.76
4.500 796.98 % x(g) = 0.76
4.750 794.21 % x(g) = 0.76
5.000 791.39 % x(g) = 0.76
5.250 788.53 % x(g) = 0.76
5.500 785.65 % x(g) = 0.76
5.750 782.76 % x(g) = 0.76
6.000 779.88 % x(g) = 0.76
6.250 776.99 % x(g) = 0.76
6.500 774.13 % x(g) = 0.76
3.000 803.81 % x(g) = 0.78
3.250 801.53 % x(g) = 0.78
3.500 799.09 % x(g) = 0.78
3.750 796.52 % x(g) = 0.78
4.000 793.85 % x(g) = 0.78
4.250 791.10 % x(g) = 0.78
4.500 788.28 % x(g) = 0.78
4.750 785.41 % x(g) = 0.78
5.000 782.51 % x(g) = 0.78
5.250 779.59 % x(g) = 0.78
5.500 776.66 % x(g) = 0.78
5.750 773.73 % x(g) = 0.78
6.000 770.82 % x(g) = 0.78
6.250 767.92 % x(g) = 0.78
6.500 765.05 % x(g) = 0.78
etc
etc

```



To find the start and end points for each line you need to set both a mode to zero and a composition to the required value. So for the end (ie top left) of u86ga enter the divariant assemblage, set the mode of sillimanite to zero and the x(g) value to 0.86

```
which phases : g sill bi cd ksp pl q liq
no phases in excess (from script)
variance of required equilibrium (2?) : 2
you may set zero modal proportions, from:bi cd g liq ksp pl sill q
which to set : sill
you may set compositional variables, from: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)
(maximum number to set = 1
which variables to set : x(g)
```

```
specifying isopleths for x(g):
list of values OR start, finish, interval : 0.86
```

```
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
  5.919 69.113  8.819  0.270  3.590  8.799  2.930  0.560
```

```
<=====>
```

```
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)  ....
  4.79    740.1  0.7175 0.5707 0.06067 0.4799 0.5880 0.86 0.02727 0.1844 0.2917 0.3917 0.01037 0.002747 0.8244 0.4935 ....

mode      bi      cd      g      liq      ksp      pl      sill      q
      0.2089  0.1110 0.07650 0.1235 0.1064 0.008085      0  0.3656
```

for the ends of the other (0.76 – 0.84) isopleths, you can set one mode to zero (again sill) and give a list of x(g) values to get a list of end points, which you need to make into individual points in your drawpd file. The finished pseudosection is shown on the next page.

As you may of noted, plotting isopleths can result in a great number of lines on a pseudosection that can be hard to read or work with. Colouring the lines or turning them into dashed lines can make them more readable. If you use illustrator, you can put different isopleths in different layers which makes them easier to manage. An easy way to do this is to move all the base diagram info to the “storage area” of the drawpd file (ie below the last *), run drawpd just with a given set of isopleths and copy and paste the output diagram into a different layer of your diagram. This also makes it easier to hide or show different isopleths when you print.

What I recommend you do now is calculate the rest of the garnet modes in the other fields, or do the mode isopleths for another phase such as biotite or melt. You could also calculate different compositional isopleths such as y(opx) which is octahedral Al₂O₃.

You can work out what the different composition variables mean by looking at the a-x relationships in the ax file.

drawpd 1.15 (running at 9.20 on Thu 19 Nov,2009)

