

T-x pseudosection tutorial for building a diagram from an existing P-T pseudosection to a new composition

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This tutorial assumes you know how to run THERMOCALC and calculate lines and points. If you don't know how to do this, start with the P-T pseudosection tutorial and then the basic T-x tutorial.

In this tutorial I will go through the process of building a T-x pseudosection from a known bulk (where the P-T pseudo has already been constructed) to a new composition. This is a useful way to start a new diagram. The known bulk composition is that of White et al 2007 Fig 8b. The new composition is one I just made up. The T-x diagram will be constructed at 5 kbar over a T range of 700-860°C, and some additional calculations at 6.4 kbar.

I've tried to keep this tutorial as realistic as possible, having not pre run it before embarking on writing it up. As you will see, the original calculations at 5 kbar are not as fruitful as I had hoped, so I did what I would normally do in this situation and started calculating a second T-x diagram at a different pressure (6.4 kbar).

This tutorial was prepared using THERMOCALC 3.30 and drawpd 1.11 on a mac (input files for using thermocalc 3.33 and drawpd 1.15 are available in the folder "txtute2-333").

A P-T pseudosection for the new composition is covered in P-T pseudo tute 2.

In your THERMOCALC folder you will need the following files

tc-txpstute (this is for the 5kbar example described below)
tc-txpstute2 (this is for the additional 6.4 kbar example)
tc-NCKFMASHP

In your drawpd folder you will need the following files

dr dtxpstute (for mac : blank 5kbar file but with the T-X ranges and axes predefined)
dr dtxpstute2 (for mac : blank 6.4kbar file but with the T-X ranges and axes predefined)
drdtx2 (for PC : blank 5kbar file but with the T-X ranges and axes predefined)
drdtx22 (for PC : blank 6.4kbar file but with the T-X ranges and axes predefined)

dr dtxpstutef (for mac : finished 5kbar file)
dr dtxpstute2f (for mac : incomplete 6.4 kbar file)
drdtx2f (for PC : finished 5kbar file)

drdtx22f (for PC : incomplete 6.4 kbar file)

In your tc-prefs file use the scripts

calcmode 1

scriptfile txpstute

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

From the existing P-T pseudosection (P-T pseudo tute 1: Fig 8b from white et al 2007 JMG) we already know what equilibria the $x=0$ side of the diagram will have. Much of this tute involves tracing those equilibria across the diagram to our new composition. In comparison the new composition is richer in Al_2O_3 and has a lower XFe .

You could just guess which equilibria exist, and in this simple system with pelite compositions this would probably work, but this gets much harder in bigger systems. The main advantage of drawing the T-X pseudosection is that you get a number of equilibria that will be stable that you can work from and, importantly, you get the opportunity for using starting guesses from the $x=1$ side of the diagram that are appropriate for your new bulk. This saves you from the problem of missing an equilibria that exists but could not be calculated because the starting guesses were too far from a solution.

In this example I have defined points simply by running one of the low variance equilibria at small increments and taken the first or last point on that line as the effective invariant point. Ie i1 is the last point on u1 where $p_l=0$ and $g \approx 0$. For steep equilibria you may need very small increments. Obviously if you prefer to define points using a different approach you can.

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 :

The first equilibria encountered at 5kbar in the (g) line from the g-sill-bi equilibria. So we calculate this from $x=0$ to $x=1$

```
% -----  
u<k>  bi liq ksp pl sill q  - g  
  
begin  end  
  
0.0000 5.00 731.4 % g = 0  
0.0500 5.00 733.4 % g = 0  
0.1000 5.00 735.5 % g = 0  
0.1500 5.00 737.6 % g = 0  
0.2000 5.00 739.9 % g = 0  
0.2500 5.00 742.2 % g = 0
```

0.3000	5.00	744.6	% g = 0
0.3500	5.00	747.1	% g = 0
0.4000	5.00	749.7	% g = 0
0.4500	5.00	752.5	% g = 0
0.5000	5.00	755.4	% g = 0
0.5500	5.00	758.4	% g = 0
0.6000	5.00	761.5	% g = 0
0.6500	5.00	764.8	% g = 0
0.7000	5.00	768.3	% g = 0
0.7500	5.00	772.0	% g = 0
0.8000	5.00	775.9	% g = 0
0.8500	5.00	780.0	% g = 0
0.9000	5.00	784.3	% g = 0
0.9500	5.00	788.9	% g = 0
1.0000	5.00	793.7	% g = 0

and see that this line is seen by both compositions so goes right across the diagram unless it intersects a divariant field (which it will). The next line seen at $x=0$ is the (cd) line from the divariant field bi-sill-g-cd. This line only exists at $x<0.1$ before it runs out of garnet

```

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

```

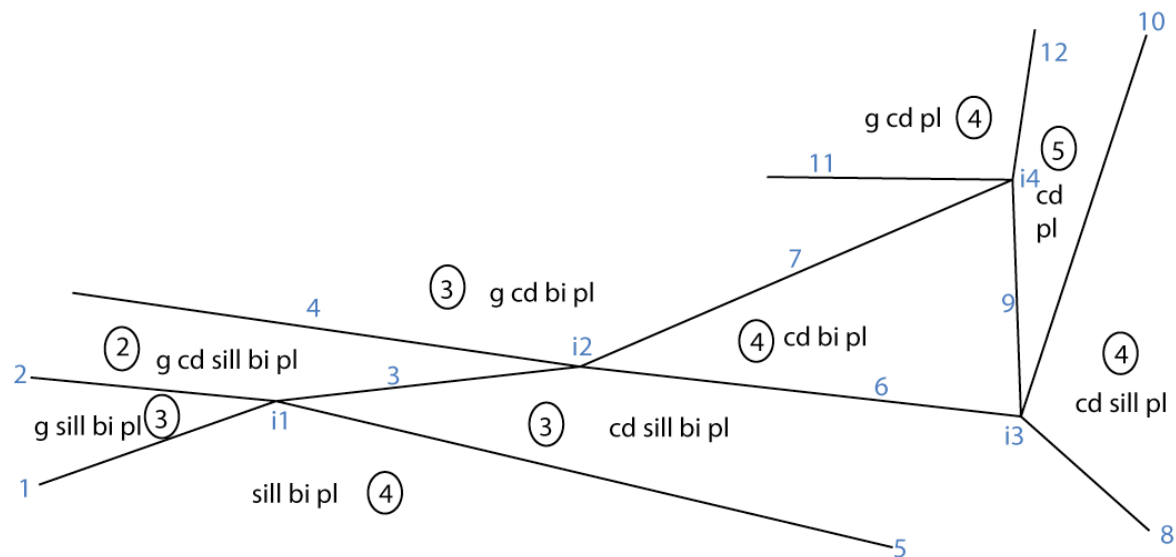
[illegible]

0.040	0.3400	0	0.02651	0.06446	0.04450	0.02845	0.04614	0.4499											
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	736.3	0.6818	0.5574	0.07132	0.4454	0.5995	0.8418	0.01851	0.1670	0.3032	0.4939	0.006844	0.002747	0.8093	0.5044	0.2627	0.01131	0.2917	0.04822
mode	bi	cd	g	liq	ksp	pl	sill	q											
0.050	0.3468	0	0.02074	0.05938	0.04099	0.03072	0.04789	0.4535											
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	735.9	0.6816	0.5572	0.07145	0.4450	0.5997	0.8417	0.01797	0.1662	0.3038	0.4992	0.006627	0.002741	0.8092	0.5050	0.2688	0.01129	0.2798	0.05020
mode	bi	cd	g	liq	ksp	pl	sill	q											
0.060	0.3536	0	0.01497	0.05431	0.03735	0.03310	0.04964	0.4571											
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	735.5	0.6814	0.5570	0.07156	0.4447	0.5999	0.8416	0.01745	0.1654	0.3044	0.5042	0.006416	0.002735	0.8090	0.5055	0.2748	0.01127	0.2682	0.05225
mode	bi	cd	g	liq	ksp	pl	sill	q											
0.070	0.3604	0	0.009174	0.04924	0.03357	0.03561	0.05140	0.4606											
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	735.1	0.6812	0.5568	0.07167	0.4444	0.6000	0.8414	0.01693	0.1647	0.3049	0.5091	0.006211	0.002729	0.8089	0.5060	0.2808	0.01124	0.2569	0.05438
mode	bi	cd	g	liq	ksp	pl	sill	q											
0.080	0.3672	0	0.003369	0.04417	0.02964	0.03825	0.05316	0.4642											

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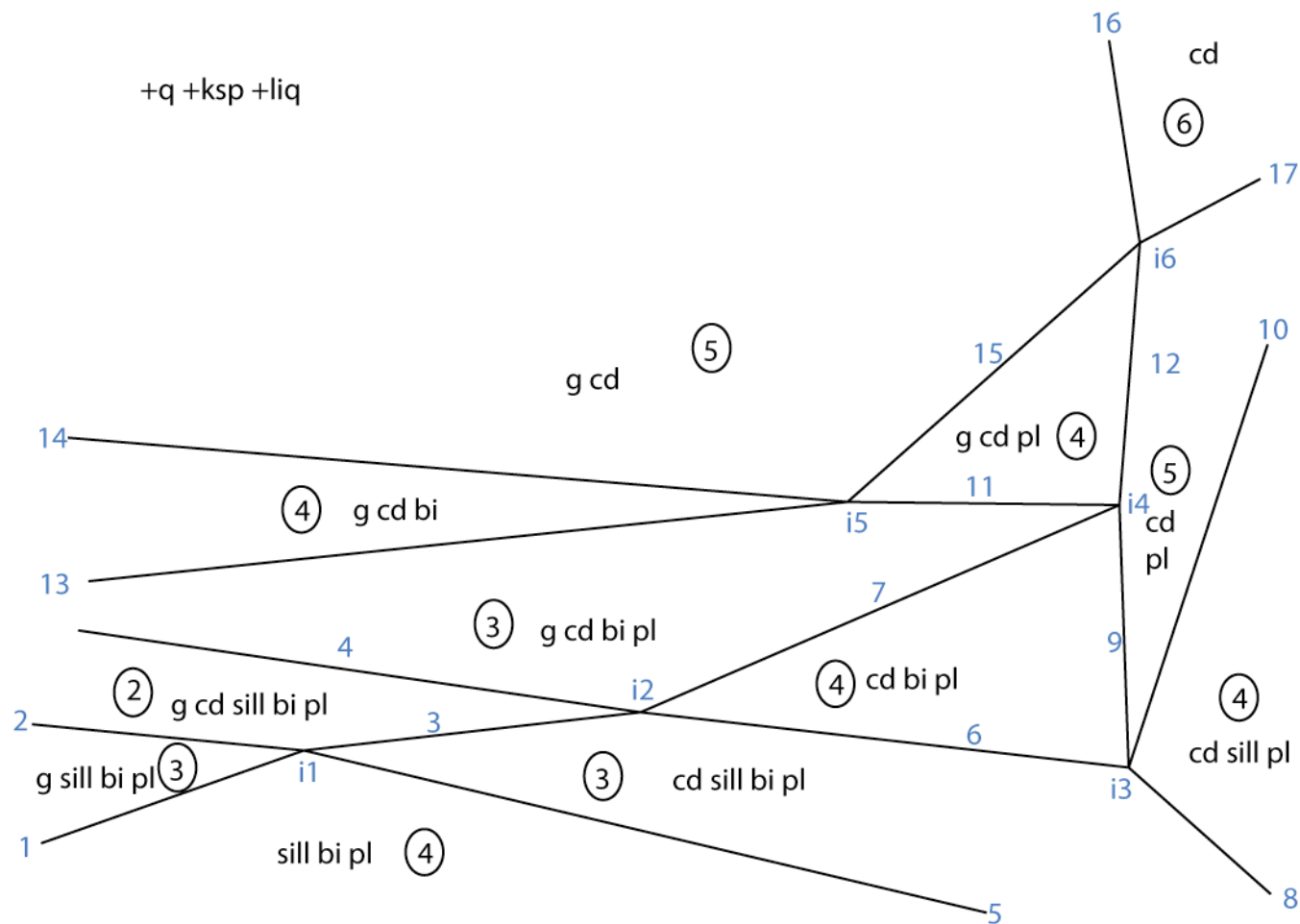
The (g) line extends as far as $x \approx 0.4$ where sill goes to zero. Likewise, the (sill) line goes from $x=0$ to $x \approx 0.4$, thus represents the high T boundary to this field. What this means is that the new composition does not see this divariant field at 5kbar.

Building the diagram across to $x=1$, the diagram should look like



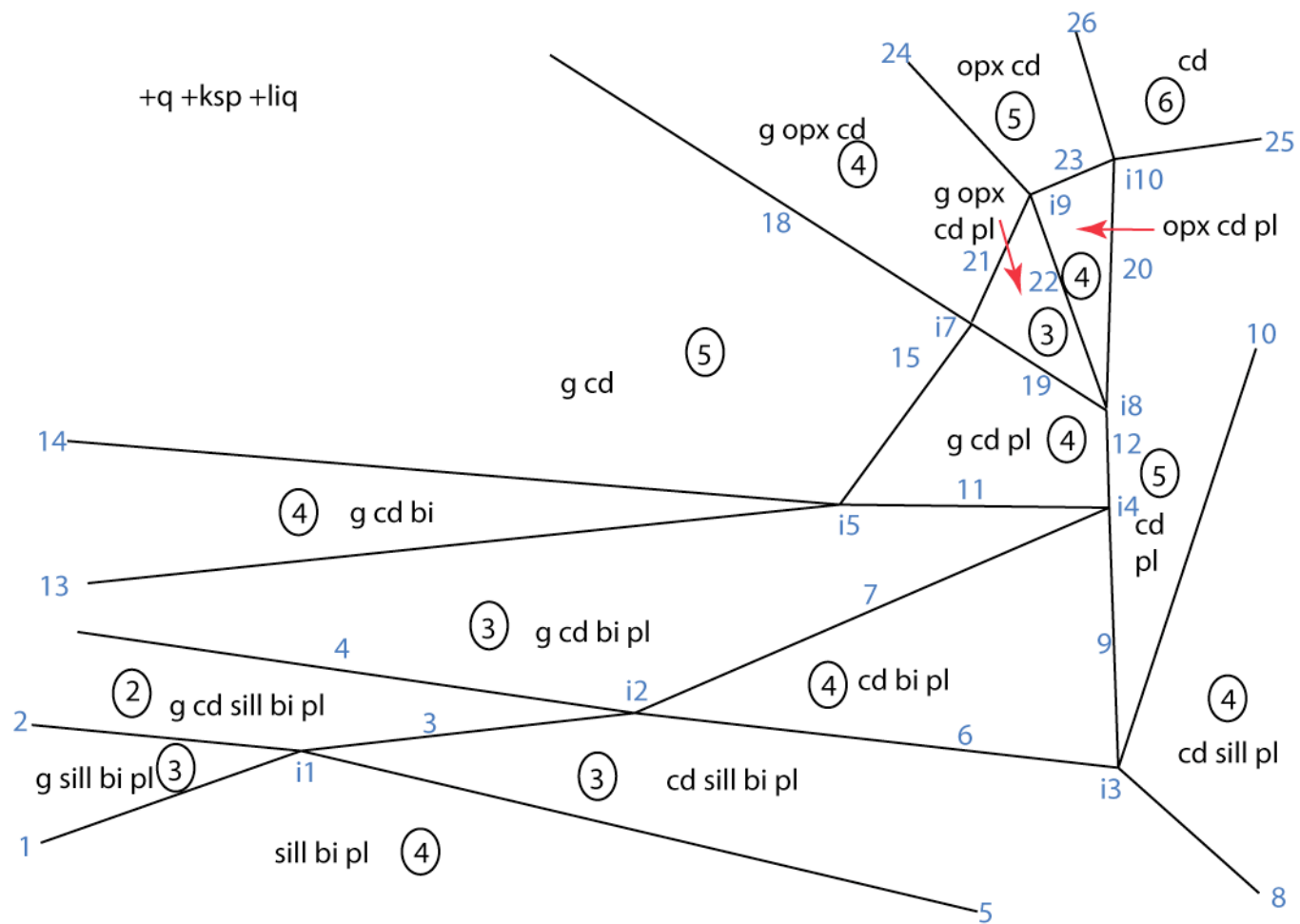
Thus, the key equilibria for the new bulk from this are u8 and u9

There are more equilibria that can be calculated to higher T based on the pseudosection for the x=0 composition, firstly the (pl) line from the g-cd-bi-pl field joints up with u11 and we could calculate the other lines that come from this point. Finishing off these lines and points, the diagram should look like



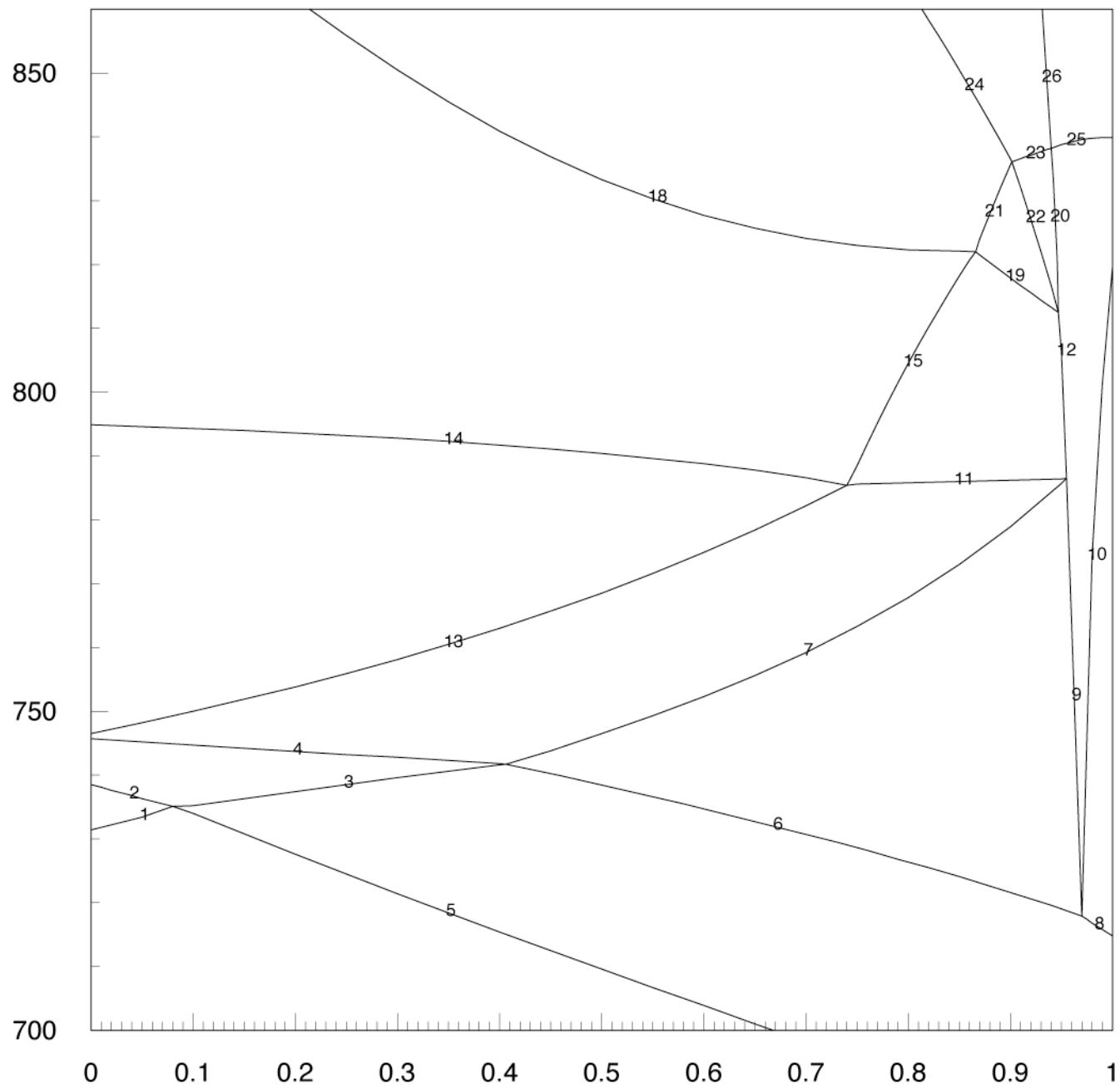
We could assume that the diagram is finished at this point, but we should check to see if any other minerals come in. Looking at the high-T assemblages, it would seem possible, in not likely, that orthopyroxene may become stable. The big g-cd assemblage would be a good place to look for an opx in line, and indeed there is one.

The (opx) line from the g-opx-cd assemblage cuts across the diagram from the top left to lower T on the right where it intersects line u15. What this means is u16, u17 and i6 are metastable relative to opx-bearing equilibria. Calculating the opx bearing equilibria results in a diagram that looks like



Below is the finished drawpd .ps file

drawpd 1.11 (running at 15.31 on Sun 9 Mar,2008)



Now you could build a P-T pseudosection for the $x=1$ composition from the equilibria that intersect the right hand side of the above diagram. However, we only have moderately high variance equilibria to start with and there would be some guess work involved. This is largely due to the two compositions used being rather different. Using a composition closer to your own allows you to have a better chance of some of the low variance equilibria extending right across the diagram. If you have no choice but to use a fairly different composition it is worthwhile calculating a few T-x diagrams. As the new bulk has a lower XFe we would expect the low variance equilibria to occur to higher P-T than in the $x=0$ P-T pseudo

Calculating at 6.4 kbar (rather than 5 kbar used above) I found the divariant assemblage bi-cd-g-liq-ksp-pl-sill-q across to $x=1$ with the low-T boundary being (cd) and the high-T boundary being (bi), so this is a good place to start a new P-T pseudosection- (see tutorial named P-T pseudo tute 2). below is a rough sketch of part of the 6.4 kbar t-x pseudosection

