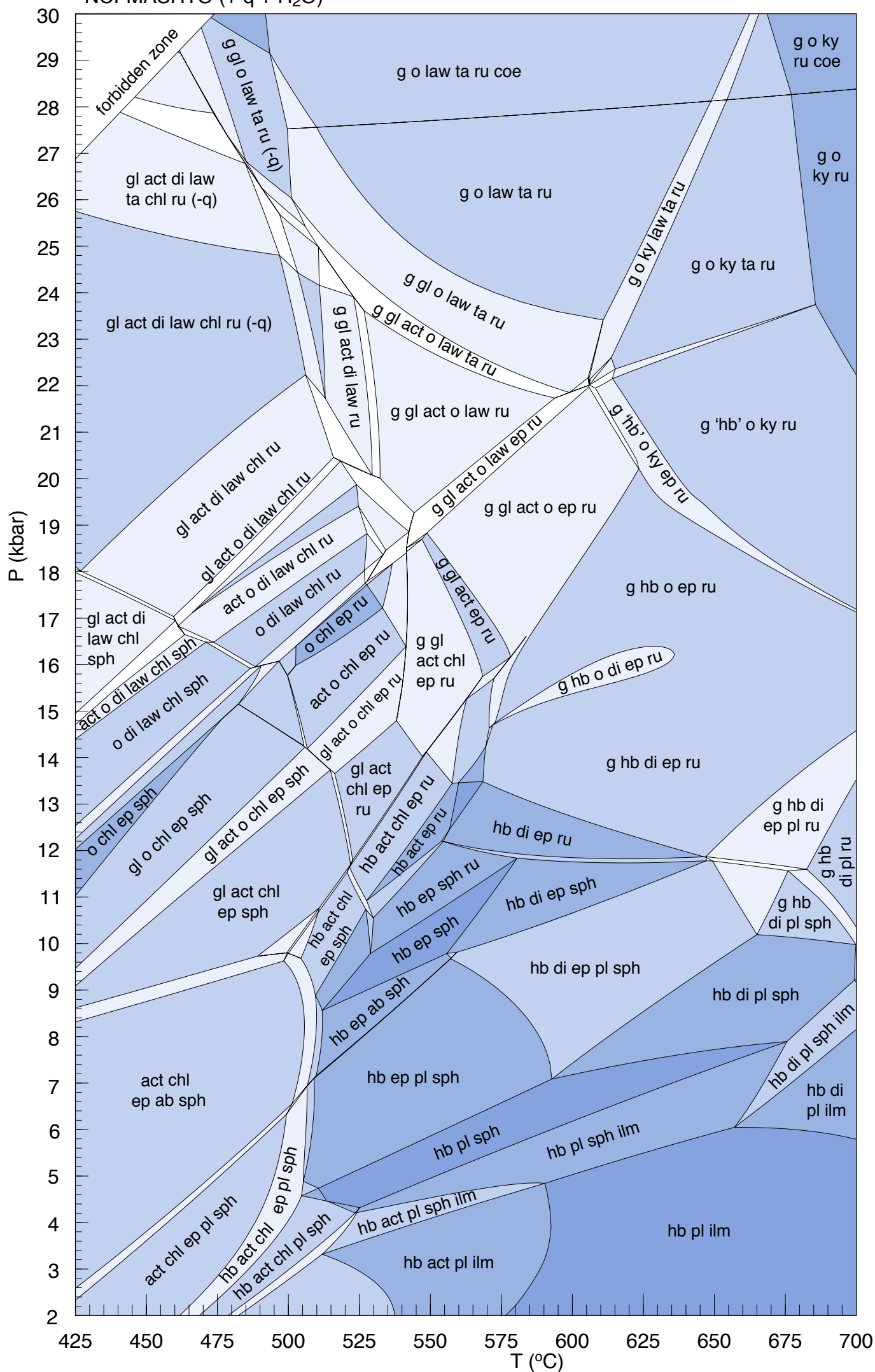


# NCFMASHTO (+ q + H<sub>2</sub>O)



# Some tips to surviving phase diagram calculations for mafic rocks with your sanity relatively intact

by Johann Diener

Doing phase diagram calculations with mafic rocks can be a bit more challenging than for pelites because

(1) the phase relations of pelitic rocks are well-known from petrogenetic grids as well as plenty of pseudosections that have been published for these rocks. This is not the case for mafic rocks, so it's a little harder to anticipate what your pseudosection will look like.

(2) the a-x relations for common mafic minerals (amphibole and clinopyroxene) are more involved and need some getting used to. That's what this tute is for.

## a-x of amphibole and clinopyroxene:

All four clinoamphiboles (actinolite (act), hornblende (hb), glaucophane (gl) and cummingtonite (cu)) have the same a-x code and each amphibole is distinguished from the others by different starting guesses. The compositional range of each amphibole is separated from the other by solvi (more on them later). The same goes for the three clinopyroxenes (diopside (di), omphacite (o) and jadeite (jd)).

So to be able to do calculations with these minerals - and find out what is going on when things go wrong - you need to be able to read the code. A full explanation of what each of the variables are is provided in the tc-NCFMASH or tc-NCFMASHTO datafiles, but the important variables, and the range to expect for the different amphiboles are:

variable	what is it?	gl	hb	act	cu
x	Fe/Fe+Mg	0 - 1	0 - 1	0 - 1	0 - 1
y	octahedral Al	0.9 - 1	0.2 - 0.6	0 - 0.25	0 - 0.2
z	Na on the M4 site	0.8 - 1	0 - 0.6 (typically < 0.3)	0 - 0.25	0 - 0.05
a	A-site Na	0 - 0.2	0.2 - 0.6	0 - 0.25	0 - 0.05
c	Ca	0 - 0.2	0.6 - 0.9	0.7 - 1	0 - 0.05
f	Fe <sup>3+</sup>	0 - 1	0 - 0.5	0 - 0.2	0 - 0.2

So glaucophane has high z and y combined with low a and c, hornblende has high a, y and c, actinolite has high c combined with low y and a, and cummingtonite has low values of all variables.

The clinopyroxenes are simpler in that they can be readily distinguished by j, the proportion of jadeite (NaAl) in the pyroxene.

For diopside,  $0 < j < 0.25$ ; for omphacite  $0.35 < j < 0.6$  and for jadeite  $0.8 < j < 1$ .

For any mineral group that has solvi, it is necessary to routinely check that the calculated mineral composition is the same as that of the mineral you specified, e.g. that your actinolite is actually actinolite and not hornblende or glaucophane. Similarly, when you are doing calculations involving multiple amphiboles or pyroxenes, it is necessary to check that the amphiboles have different compositions, and that each composition matches that of the expected mineral. This is particularly important at higher T as the solvi begin to close and the different amphibole or clinopyroxene compositions approach each other. Using the 'samecoding' script is really useful, because it lines up the variables for minerals with the same a-x relations and makes it easier to spot problems. Here is an extreme example involving actinolite, hornblende and glaucophane, at P-T conditions near the top of the glaucophane-hornblende solvus:

P(kbar)	T(°C)	x(gl)	y(gl)	z(gl)	a(gl)	c(gl)	f(gl)	Q1(gl)	Q2(gl)				
16.701	584.80	0.2233	0.6905	0.7468	0.1360	0.2430	0.05861-0.003754	0.003754	0.04562				
		x(act)	y(act)	z(act)	a(act)	c(act)	f(act)	Q1(act)	Q2(act)				
		0.2123	0.4745	0.4708	0.1675	0.5093	0.04027-0.009125	0.009125	0.05184				
		x(hb)	y(hb)	z(hb)	a(hb)	c(hb)	f(hb)	Q1(hb)	Q2(hb)				
		0.2123	0.4745	0.4708	0.1675	0.5093	0.04027-0.009125	0.009125	0.05184				
		x(o)	j(o)	f(o)	Q(o)	Qaf(o)	Qfm(o)	x(g9)	z(g9)	f(g9)	f(ep)	Q(ep)	
		0.2726	0.4518	0.1234	0.3187	0.01746	-0.04753	0.8152	0.3849	0.01348	0.09289	0.09176	
mode	gl	act	hb	o	g9	ep	ru	q					
	0.1711	0.3740	0	0.02903	0.1744	0.1918	0.01011	0.04955					

Note that even though this appears to be a legitimate result, the composition of actinolite and hornblende are identical. It is also possible for two compositions to be very close, but not quite identical. This is still not a valid result:

P(kbar)	T(°C)	x(gl)	y(gl)	z(gl)	a(gl)	c(gl)	f(gl)	Q1(gl)	Q2(gl)				
16.701	584.38	0.2238	0.6926	0.7517	0.1339	0.2383	0.05909-0.003717	0.003717	0.04539				
		x(act)	y(act)	z(act)	a(act)	c(act)	f(act)	Q1(act)	Q2(act)				
		0.2167	0.5199	0.5095	0.1777	0.4718	0.04435-0.008341	0.008341	0.05337				
		x(hb)	y(hb)	z(hb)	a(hb)	c(hb)	f(hb)	Q1(hb)	Q2(hb)				
		0.2168	0.5203	0.5099	0.1778	0.4715	0.04439-0.008332	0.008332	0.05338				
		x(o)	j(o)	f(o)	Q(o)	Qaf(o)	Qfm(o)	x(g9)	z(g9)	f(g9)	f(ep)	Q(ep)	
		0.2731	0.4514	0.1240	0.3186	0.01760	-0.04769	0.8159	0.3852	0.01356	0.09329	0.09216	
mode	gl	act	hb	o	g9	ep	ru	q					
	0.08008	0.4661	0	0.03216	0.1721	0.1878	0.01011	0.05160					

The real result, involving three amphiboles of different composition is:

P(kbar)	T(°C)	x(gl)	y(gl)	z(gl)	a(gl)	c(gl)	f(gl)	Q1(gl)	Q2(gl)				
16.701	584.94	0.2232	0.6922	0.7481	0.1361	0.2417	0.05820-0.003722	0.003722	0.04555				
		x(act)	y(act)	z(act)	a(act)	c(act)	f(act)	Q1(act)	Q2(act)				
		0.2010	0.3545	0.3806	0.1311	0.5972	0.02980 -0.01079	0.01079	0.04727				
		x(hb)	y(hb)	z(hb)	a(hb)	c(hb)	f(hb)	Q1(hb)	Q2(hb)				
		0.2199	0.5664	0.5504	0.1867	0.4322	0.04762-0.007341	0.007341	0.05441				
		x(o)	j(o)	f(o)	Q(o)	Qaf(o)	Qfm(o)	x(g9)	z(g9)	f(g9)	f(ep)	Q(ep)	
		0.2724	0.4522	0.1221	0.3193	0.01721	-0.04741	0.8150	0.3848	0.01334	0.09217	0.09106	
mode	gl	act	hb	o	g9	ep	ru	q					
	0.2929	0.2515	0	0.02282	0.1777	0.1991	0.01011	0.04595					

Note that, along with the compositions, each of these calculations produces very different results for the modes of the minerals, particularly gl and act. This is often a giveaway - if the modes change abruptly as you are doing calculations along a phase boundary, it flags that something has gone wrong and you need to check the results, and probably change the starting guesses to be able to go further.

Almost all your problems related to phase diagrams for mafic rocks will be related to starting guesses. The number of variables involved in the amphiboles and pyroxenes means that mafic rocks are generally more sensitive and fussy about starting guesses than pelites. Some calculations (like the example above) can be extremely sensitive to starting guesses, so do not be scared to update them regularly.

## Calculations that try to cross a solvus:

Sometimes you might calculate a line that just stops, without running out of a phase. Changing the starting guesses do not help either, and it is impossible to calculate the line further. Here is such an example:

P(kbar) f(ep) 8.001 0.1265	T(?C) Q(ep) 505.59 0.1255	x(act) 0.3320	y(act) 0.1351	z(act) 0.1520	a(act) 0.1000	c(act) 0.8369	f(act) 0.01873	Q1(act) -0.04152	Q2(act) 0.08103	x(hb) 0.4096	y(hb) 0.5627	z(hb) 0.2107	a(hb) 0.4938	c(hb) 0.7768	f(hb) 0.07802	Q1(hb) -0.03116	Q2(hb) 0.1479	x(chl) 0.4007	y(chl) 0.5104	Q(chl) 0.4896
mode	act 0.3537	hb 0	chl 0.1961	ep 0.2327	ab 0.1544	sph 0.02877	q 0.03440													
P(kbar) f(ep) 8.501 0.1246	T(?C) Q(ep) 505.52 0.1236	x(act) 0.3312	y(act) 0.1464	z(act) 0.1719	a(act) 0.1021	c(act) 0.8173	f(act) 0.01973	Q1(act) -0.04063	Q2(act) 0.08050	x(hb) 0.4092	y(hb) 0.5772	z(hb) 0.2486	a(hb) 0.4838	c(hb) 0.7394	f(hb) 0.07779	Q1(hb) -0.02980	Q2(hb) 0.1473	x(chl) 0.4023	y(chl) 0.5102	Q(chl) 0.4897
mode	act 0.3563	hb 0	chl 0.1951	ep 0.2346	ab 0.1503	sph 0.02877	q 0.03500													
P(kbar) f(ep) 9.001 0.1223	T(?C) Q(ep) 504.12 0.1213	x(act) 0.3305	y(act) 0.1613	z(act) 0.1959	a(act) 0.1046	c(act) 0.7936	f(act) 0.02104	Q1(act) -0.03972	Q2(act) 0.08013	x(hb) 0.4091	y(hb) 0.5960	z(hb) 0.3003	a(hb) 0.4665	c(hb) 0.6886	f(hb) 0.07772	Q1(hb) -0.02813	Q2(hb) 0.1466	x(chl) 0.4038	y(chl) 0.5099	Q(chl) 0.4900
mode	act 0.3599	hb 0	chl 0.1937	ep 0.2368	ab 0.1451	sph 0.02877	q 0.03573													
P(kbar) f(ep) 9.501 0.1193	T(?C) Q(ep) 500.23 0.1184	x(act) 0.3300	y(act) 0.1823	z(act) 0.2275	a(act) 0.1076	c(act) 0.7630	f(act) 0.02281	Q1(act) -0.03875	Q2(act) 0.07999	x(hb) 0.4095	y(hb) 0.6231	z(hb) 0.3857	a(hb) 0.4285	c(hb) 0.6050	f(hb) 0.07795	Q1(hb) -0.02573	Q2(hb) 0.1451	x(chl) 0.4052	y(chl) 0.5094	Q(chl) 0.4906
mode	act 0.3652	hb 0	chl 0.1917	ep 0.2395	ab 0.1382	sph 0.02877	q 0.03670													
2222222222222222																				

You can see that there are no phases running out, and updating the starting guesses do not allow the calculation to go any further. The reason that the calculation stopped is that it is up against a solvus. Have a look at the values of y(hb), z(hb) and a(hb) as the point where the calculation stops is approached: the amount of Al is increasing, but more significantly, the amount of Na on M4 (z(hb)) is increasing rapidly and A-site Na (a(hb)) is decreasing rapidly. This implies that the hornblende composition is becoming more glaucophane-like, and the calculation stops because it needs to cross the hornblende-glaucophane solvus to be able to go further. The same change can be seen in the actinolite composition, although it is more subtle. Adding glaucophane to the assemblage stabilises the gl-hb effective invariant at 9.6 kbar, and from there the hb-in line can be followed to higher P.

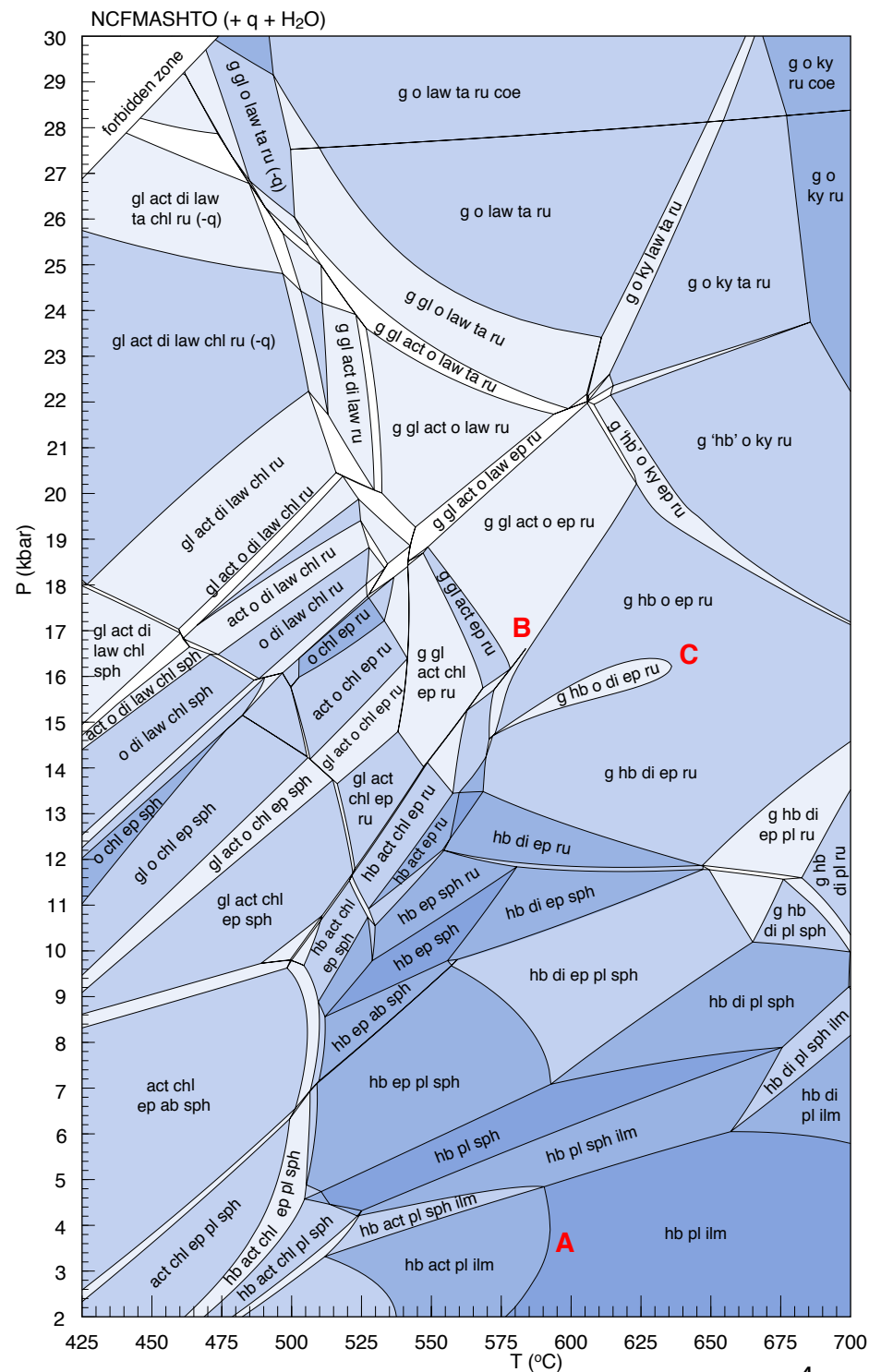
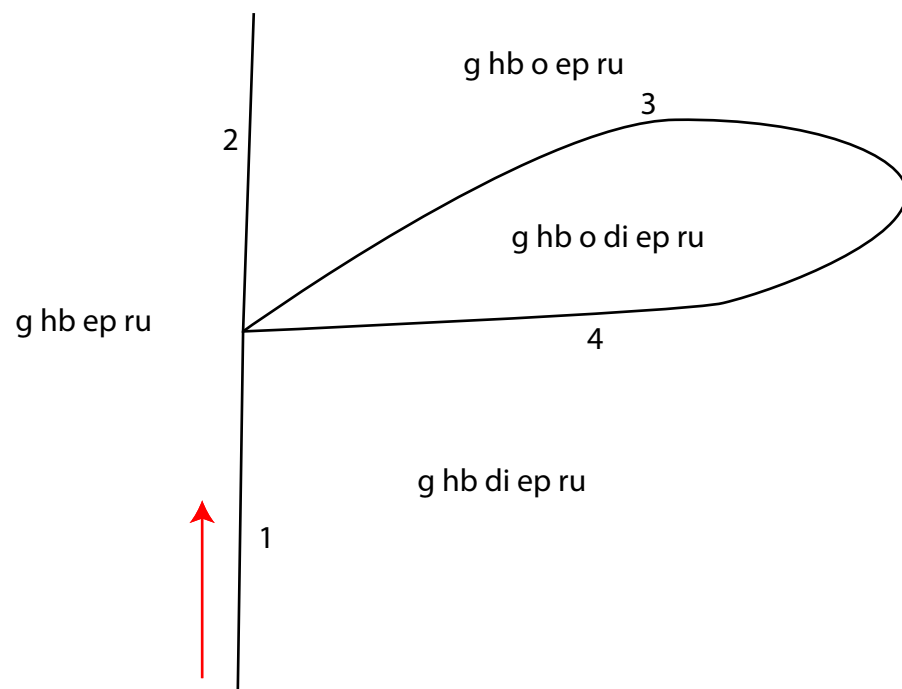
P(kbar) a(hb) 9.627 0.4078	T(?C) c(hb) 498.38 0.5676	x(gl) f(hb) 0.4204 0.07825	y(gl) 0.7632	z(gl) 0.8846	a(gl) 0.1138	c(gl) 0.1134	f(gl) 0.09425	Q1(gl) -0.01035	Q2(gl) 0.1158	x(act) 0.3299	y(act) 0.1891	z(act) 0.2375	a(act) 0.1084	c(act) 0.7533	f(act) 0.02335	Q1(act) -0.03851	Q2(act) 0.08000	x(hb) 0.4098	y(hb) 0.6336	z(hb) 0.4238
		Q1(hb) -0.02475	Q2(hb) 0.1440	x(chl) 0.4056	y(chl) 0.5091	Q(chl) 0.4908	f(ep) 0.1184	Q(ep) 0.1175												
mode	gl 0	act 0.3669	hb 0	chl 0.1911	ep 0.2403	ab 0.1359	sph 0.02877	q 0.03701												

Note that this problem can be encountered for any group of minerals that have solvi, e.g. amphiboles, clinopyroxene, feldspar, white mica, ilmenite-hematite and magnetite-spinel.

## Dealing with closing solvi

The solvi of both the clino- and orthoamphiboles as well as the clinopyroxenes close at crustal metamorphic temperatures, so you are likely to encounter one or more of these sooner or later. For the clinoamphiboles, the solvus between actinolite and hornblende closes at around 600°C at low P of around 3 kbar (point **A**). The hornblende-glaucophane solvus closes at around 17 kbar and 600°C (point **B**). The orthoamphibole solvus - between gedrite and anthophyllite - closes at a little over 600°C at around 4 kbar (not shown). For the clinopyroxenes, the diopside-omphacite solvus closes at around 630°C at 15-16 kbar (point **C**).

Doing calculations around the area where a solvus is closing can be frustrating because you have to deal with two minerals of different composition going to the same composition, which makes the starting guesses all the more sensitive and important. Here is a worked example of how to calculate the closure of the diopside-omphacite solvus in the diagram on the right. The datafile used is 'tc-morb', and the a-x file is tc-NCFMASHTO. Note that for simplicity, I will ignore the appearance and disappearance of actinolite in this example, therefore the diagram will look something like this:



If we approach the area from low P, along the diopside-in boundary (red arrow; reaction 1), our calculation will proceed to a point at 15.2 kbar:

etc etc

P(kbar)	T(?C)	x(hb)	y(hb)	z(hb)	a(hb)	c(hb)	f(hb)	Q1(hb)	Q2(hb)	x(di)	j(di)	f(di)	Q(di)	Qaf(di)	Qfm(di)	x(g)	z(g)	f(g)	f(ep)	Q(ep)
15.001	572.55	0.3130	0.5424	0.4162	0.2806	0.5623	0.04533	-0.01757	0.09269	0.3402	0.2627	0.2405	0.07271	0.01476	-0.1016	0.8684	0.3613	0.009612	0.09042	0.08942
mode	hb	di	g	ep	ru	q														
	0.6673	0	0.05937	0.2042	0.01002	0.05912														
P(kbar)	T(?C)	x(hb)	y(hb)	z(hb)	a(hb)	c(hb)	f(hb)	Q1(hb)	Q2(hb)	x(di)	j(di)	f(di)	Q(di)	Qaf(di)	Qfm(di)	x(g)	z(g)	f(g)	f(ep)	Q(ep)
15.101	572.75	0.3087	0.5413	0.4253	0.2718	0.5535	0.04514	-0.01714	0.09050	0.3380	0.2691	0.2364	0.08011	0.01543	-0.1002	0.8669	0.3604	0.009557	0.09035	0.08935
mode	hb	di	g	ep	ru	q														
	0.6620	0	0.06430	0.2059	0.01002	0.05779														
P(kbar)	T(?C)	x(hb)	y(hb)	z(hb)	a(hb)	c(hb)	f(hb)	Q1(hb)	Q2(hb)	x(di)	j(di)	f(di)	Q(di)	Qaf(di)	Qfm(di)	x(g)	z(g)	f(g)	f(ep)	Q(ep)
15.201	572.95	0.3044	0.5401	0.4346	0.2628	0.5445	0.04494	-0.01669	0.08825	0.3363	0.2782	0.2304	0.09211	0.01643	-0.09834	0.8654	0.3594	0.009501	0.09027	0.08927
mode	hb	di	g	ep	ru	q														
	0.6567	0	0.06922	0.2077	0.01002	0.05644														

11111111222211111  
more phase diagram calculations ?

where it stops because it is up against the diopside-omphacite solvus, as flagged by the increase in j(di) as we approach this point. Adding omphacite to the assem-  
blage stabilises the di-o effective invariant at 14.9 kbar

P(kbar)	T(?C)	x(hb)	y(hb)	z(hb)	a(hb)	c(hb)	f(hb)	Q1(hb)	Q2(hb)	x(di)	j(di)	f(di)	Q(di)	Qaf(di)	Qfm(di)	x(o)	j(o)	f(o)	Q(o)
14.874	572.34	0.3183	0.5437	0.4049	0.2913	0.5731	0.04555	-0.01811	0.09540	0.3433	0.2561	0.2445	0.06583	0.01410	-0.1031	0.3692	0.4153	0.1334	0.2923
		Qaf(o)	Qfm(o)	x(g)	z(g)	f(g)	f(ep)	Q(ep)											
		0.01968	-0.07693	0.8702	0.3625	0.009682	0.09049	0.08950											
mode	hb	di	o	g	ep	ru	q												
	0.6741	0	0	0.05311	0.2020	0.01001	0.06077												

It is a good idea to save this result as starting guesses for further calculations. Emanating from this effective invariant, we'll have a di-absent o-in reaction to higher P, (reaction 2, not calculated here) as well as an o-bearing di-out reaction (reaction 3) and di-bearing o-out reaction (reaction 4). These reactions are relatively flat and are easier to calculate by specifying T. If we calculate the di-out reaction (reaction 3) up-T, we get:

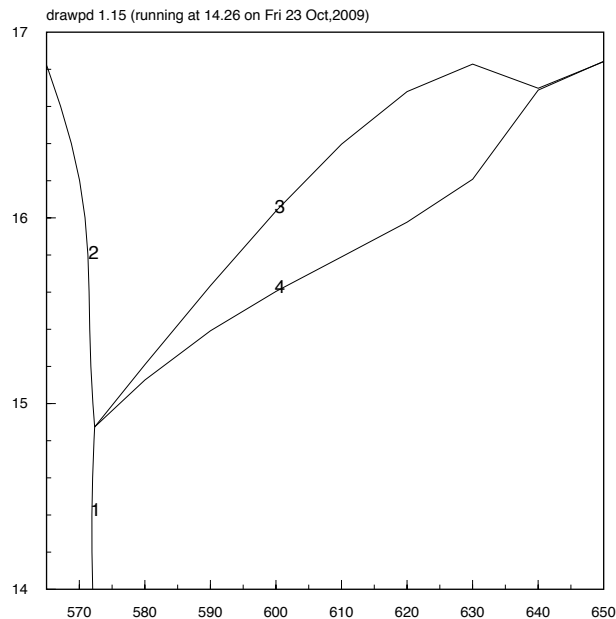
P(kbar)	T(?C)	x(hb)	y(hb)	z(hb)	a(hb)	c(hb)	f(hb)	Q1(hb)	Q2(hb)	x(di)	j(di)	f(di)	Q(di)	Qaf(di)	Qfm(di)	x(o)	j(o)	f(o)	Q(o)
16.397	610.01	0.2289	0.5875	0.3797	0.3546	0.5932	0.05234-0.007096	0.07174	0.2508		0.2952	0.2314	0.08803	0.01632	-0.07348	0.2632	0.3990	0.1589	0.2468
		Qaf(o)	Qfm(o)	x(g)	z(g)	f(g)	f(ep)	Q(ep)											
		0.02111	-0.05599	0.7954	0.3375	0.009996	0.09604	0.09466											
mode	hb	di	o	g	ep	ru	q												
	0.5128	0	0.1107	0.1539	0.1324	0.01018	0.07996												
P(kbar)	T(?C)	x(hb)	y(hb)	z(hb)	a(hb)	c(hb)	f(hb)	Q1(hb)	Q2(hb)	x(di)	j(di)	f(di)	Q(di)	Qaf(di)	Qfm(di)	x(o)	j(o)	f(o)	Q(o)
16.680	620.01	0.2148	0.6039	0.3703	0.3783	0.6012	0.05397-0.005012	0.06862	0.2350		0.3075	0.2239	0.09884	0.01694	-0.06729	0.2445	0.3919	0.1654	0.2302
		Qaf(o)	Qfm(o)	x(g)	z(g)	f(g)	f(ep)	Q(ep)											
		0.02098	-0.05338	0.7753	0.3325	0.01004	0.09642	0.09495											
mode	hb	di	o	g	ep	ru	q												
	0.4808	0	0.1349	0.1717	0.1179	0.01021	0.08447												
P(kbar)	T(?C)	x(hb)	y(hb)	z(hb)	a(hb)	c(hb)	f(hb)	Q1(hb)	Q2(hb)	x(di)	j(di)	f(di)	Q(di)	Qaf(di)	Qfm(di)	x(o)	j(o)	f(o)	Q(o)
16.828	630.01	0.2065	0.6243	0.3580	0.4087	0.6117	0.05572-0.003275	0.06761	0.2253		0.3230	0.2133	0.1156	0.01769	-0.06216	0.2315	0.3812	0.1734	0.2077
		Qaf(o)	Qfm(o)	x(g)	z(g)	f(g)	f(ep)	Q(ep)											
		0.02054	-0.05278	0.7584	0.3294	0.01014	0.09639	0.09483											
mode	hb	di	o	g	ep	ru	q												
	0.4564	0	0.1555	0.1843	0.1043	0.01024	0.08922												
P(kbar)	T(?C)	x(hb)	y(hb)	z(hb)	a(hb)	c(hb)	f(hb)	Q1(hb)	Q2(hb)	x(di)	j(di)	f(di)	Q(di)	Qaf(di)	Qfm(di)	x(o)	j(o)	f(o)	Q(o)
# 16.698	640.01	0.2087	0.6513	0.3405	0.4515	0.6273	0.05781-0.001975	0.07048	0.2282		0.3599	0.1876	0.1672	0.01930	-0.05639	0.2282	0.3599	0.1876	0.1672
		Qaf(o)	Qfm(o)	x(g)	z(g)	f(g)	f(ep)	Q(ep)											
		0.01930	-0.05639	0.7504	0.3307	0.01038	0.09579	0.09417											
mode	hb	di	o	g	ep	ru	q												
	0.4488	0	0.1688	0.1862	0.09106	0.01025	0.09501												
P(kbar)	T(?C)	x(hb)	y(hb)	z(hb)	a(hb)	c(hb)	f(hb)	Q1(hb)	Q2(hb)	x(di)	j(di)	f(di)	Q(di)	Qaf(di)	Qfm(di)	x(o)	j(o)	f(o)	Q(o)
16.841	650.00	0.2007	0.6640	0.3302	0.4726	0.6361	0.05912-0.0005599	0.06876	0.2184		0.3636	0.1866	0.1639	0.01881	-0.05371	0.2184	0.3636	0.1866	0.1639
		Qaf(o)	Qfm(o)	x(g)	z(g)	f(g)	f(ep)	Q(ep)											
		0.01881	-0.05371	0.7337	0.3283	0.01056	0.09612	0.09439											
mode	hb	di	o	g	ep	ru	q												
	0.4261	0	0.1852	0.1991	0.08143	0.01027	0.09788												

If we look at the values of j(di) and j(o), we can see that they approach each other (j(di) increases and j(o) decreases) until they become the same from 640°C onwards. We can do the same for the o-out boundary

P(kbar)	T(?C)	x(hb)	y(hb)	z(hb)	a(hb)	c(hb)	f(hb)	Q1(hb)	Q2(hb)	x(di)	j(di)	f(di)	Q(di)	Qaf(di)	Qfm(di)	x(o)	j(o)	f(o)	Q(o)
15.977	620.01	0.2445	0.6408	0.3540	0.4321	0.6169	0.05594-0.005712	0.08152	0.2612		0.3094	0.2171	0.1036	0.01673	-0.07348	0.2712	0.3886	0.1632	0.2261
		Qaf(o)	Qfm(o)	x(g)	z(g)	f(g)	f(ep)	Q(ep)											
		0.02026	-0.06033	0.7952	0.3419	0.01021	0.09401	0.09260											
mode	hb	di	o	g	ep	ru	q												
	0.5201	0.1258	0	0.1417	0.1111	0.01018	0.09124												
P(kbar)	T(?C)	x(hb)	y(hb)	z(hb)	a(hb)	c(hb)	f(hb)	Q1(hb)	Q2(hb)	x(di)	j(di)	f(di)	Q(di)	Qaf(di)	Qfm(di)	x(o)	j(o)	f(o)	Q(o)
16.208	630.01	0.2313	0.6511	0.3442	0.4502	0.6251	0.05719-0.003892	0.07800	0.2482		0.3264	0.2072	0.1222	0.01763	-0.06726	0.2543	0.3768	0.1731	0.2016
		Qaf(o)	Qfm(o)	x(g)	z(g)	f(g)	f(ep)	Q(ep)											
		0.01997	-0.05903	0.7774	0.3382	0.01034	0.09461	0.09311											
mode	hb	di	o	g	ep	ru	q												
	0.4919	0.1452	0	0.1586	0.09969	0.01021	0.09436												
P(kbar)	T(?C)	x(hb)	y(hb)	z(hb)	a(hb)	c(hb)	f(hb)	Q1(hb)	Q2(hb)	x(di)	j(di)	f(di)	Q(di)	Qaf(di)	Qfm(di)	x(o)	j(o)	f(o)	Q(o)
16.688	640.01	0.2091	0.6517	0.3403	0.4521	0.6276	0.05783-0.001985	0.07064	0.2285		0.3592	0.1880	0.1661	0.01926	-0.05660	0.2285	0.3592	0.1880	0.1661
		Qaf(o)	Qfm(o)	x(g)	z(g)	f(g)	f(ep)	Q(ep)											
		0.01926	-0.05660	0.7507	0.3309	0.01038	0.09577	0.09414											
mode	hb	di	o	g	ep	ru	q												
	0.4494	0.1686	0	0.1857	0.09100	0.01025	0.09509												

6

Both calculations show the composition of omphacite and diopside becoming the same between 630 and 640°C, which indicates the closure of the solvus at these T. Plotting the reactions looks like this:



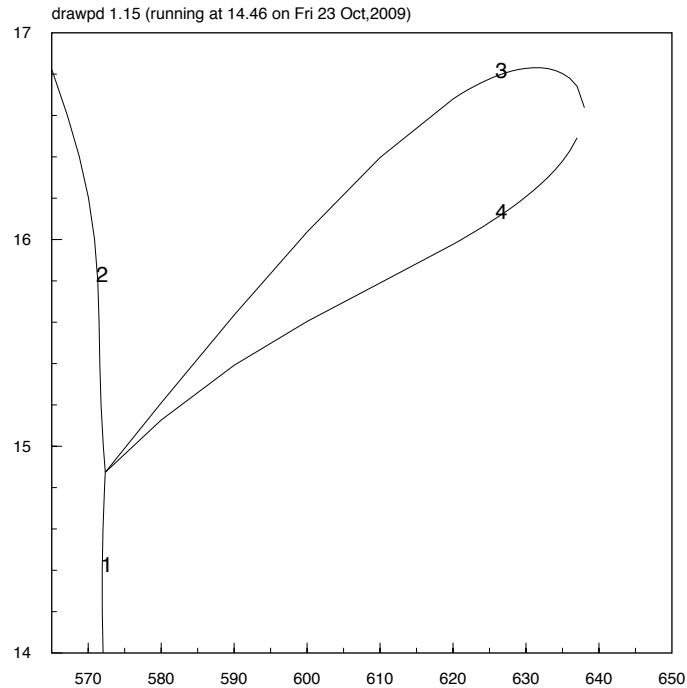
Because both reactions 3 and 4 abruptly change their slope where the solvus closes, the calculation needs to be refined to ensure that these lines are smooth. Re-doing both calculations between 620 and 640°C with an interval of 1°C reveals that the solvus closes between 638 and 639°C.

P(kbar)	T(?C)	x(hb)	y(hb)	z(hb)	a(hb)	c(hb)	f(hb)	Q1(hb)	Q2(hb)	x(di)	j(di)	f(di)	Q(di)	Qaf(di)	Qfm(di)	x(o)	j(o)	f(o)	Q(o)
16.741	637.01	0.2079	0.6438	0.3457	0.4393	0.6228	0.05721-0.002345	0.06962	0.2264	0.3419	0.1998	0.1408	0.01858	-0.05917	0.2289	0.3655	0.1838	0.1785	
		Qaf(o)	Qfm(o)	x(g)	z(g)	f(g)	f(ep)	Q(ep)											
		0.01974	-0.05541	0.7525	0.3302	0.01030	0.09593	0.09433											
mode	hb	di	o	g	ep	ru	q												
	0.4506	0	0.1652	0.1858	0.09476	0.01025	0.09338												
P(kbar)	T(?C)	x(hb)	y(hb)	z(hb)	a(hb)	c(hb)	f(hb)	Q1(hb)	Q2(hb)	x(di)	j(di)	f(di)	Q(di)	Qaf(di)	Qfm(di)	x(o)	j(o)	f(o)	Q(o)
16.638	638.01	0.2116	0.6497	0.3420	0.4489	0.6262	0.05760-0.002305	0.07131	0.2307	0.3527	0.1920	0.1575	0.01908	-0.05828	0.2312	0.3571	0.1890	0.1646	
		Qaf(o)	Qfm(o)	x(g)	z(g)	f(g)	f(ep)	Q(ep)											
		0.01929	-0.05757	0.7547	0.3317	0.01036	0.09565	0.09405											
mode	hb	di	o	g	ep	ru	q												
	0.4552	0	0.1647	0.1823	0.09295	0.01024	0.09460												
P(kbar)	T(?C)	x(hb)	y(hb)	z(hb)	a(hb)	c(hb)	f(hb)	Q1(hb)	Q2(hb)	x(di)	j(di)	f(di)	Q(di)	Qaf(di)	Qfm(di)	x(o)	j(o)	f(o)	Q(o)
16.682	639.01	0.2096	0.6500	0.3416	0.4493	0.6265	0.05768-0.002126	0.07068	0.2293	0.3595	0.1877	0.1675	0.01934	-0.05670	0.2293	0.3595	0.1877	0.1675	
		Qaf(o)	Qfm(o)	x(g)	z(g)	f(g)	f(ep)	Q(ep)											
		0.01934	-0.05670	0.7521	0.3310	0.01036	0.09576	0.09414											
mode	hb	di	o	g	ep	ru	q												
	0.4511	0	0.1670	0.1848	0.09209	0.01025	0.09470												
P(kbar)	T(?C)	x(hb)	y(hb)	z(hb)	a(hb)	c(hb)	f(hb)	Q1(hb)	Q2(hb)	x(di)	j(di)	f(di)	Q(di)	Qaf(di)	Qfm(di)	x(o)	j(o)	f(o)	Q(o)
16.733	640.00	0.2074	0.6500	0.3413	0.4494	0.6266	0.05774-0.001942	0.06995	0.2273	0.3623	0.1862	0.1709	0.01941	-0.05572	0.2273	0.3623	0.1862	0.1709	
		Qaf(o)	Qfm(o)	x(g)	z(g)	f(g)	f(ep)	Q(ep)											
		0.01941	-0.05572	0.7492	0.3302	0.01036	0.09588	0.09425											
mode	hb	di	o	g	ep	ru	q												
	0.4468	0	0.1694	0.1875	0.09128	0.01025	0.09476												

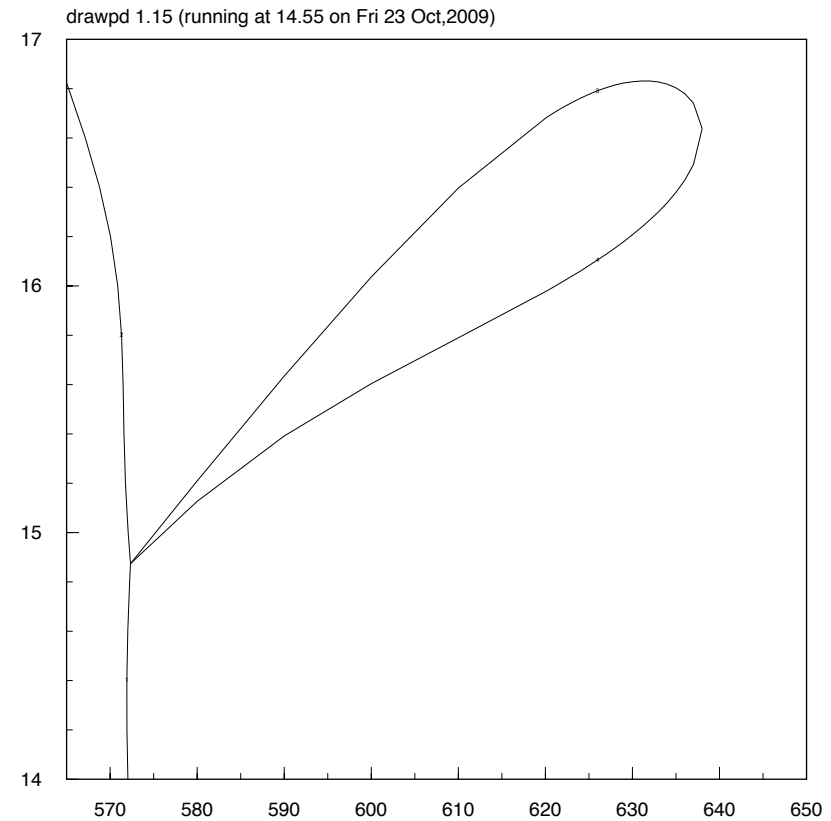
7



Appending the new results to the lines in drawpd and removing the parts calculated above the solvus gives:



The only thing that remains to be done is to connect lines 3 and 4 and close the area so that drawpd can do the colouring. Obviously the lines do not end at an effective invariant point, and therefore the point cannot be calculated by THERMOCALC. The two lines have to be joined manually, and what I usually do is to take the last value of either line and copy it as an invariant point in drawpd. Sometimes it is also necessary to manually add a few points to either of the lines to ensure that the solvus top looks smooth. And the end-result is:



## Getting started with a new composition

Part of the challenge with doing calculations for mafic rocks is that it's not as easy to predict exactly what your diagram will look like because these rocks don't have a strong 'backbone' system, like KFMASH for the pelites. There also aren't too many pseudosections out there for these rocks, so you might not necessarily find one for a composition that is similar to yours.

One relatively foolproof way to start would be to calculate a P-x or T-x section from a composition for which there is a pseudosection to your unknown composition, as already discussed in a separate tutorial. This works well as long as you are able to anticipate any new minerals that might be introduced along the compositional traverse.

Another method that works surprisingly well is to begin your section at greenschist facies conditions and to assume that actinolite, chlorite, epidote, albite and quartz make up the assemblage in NCFMASH, with sphene additionally present in NCFMASHTO and biotite additionally present in NCKFMASHTO. This assemblage is stable in a large variety of broadly mafic bulk compositions, as changes in e.g. bulk rock Al content, Fe/Fe+Mg, Ca/Na ratio or amount of Fe<sup>3+</sup> do not change the assemblage (apart from the introduction of hematite in extremely oxidised compositions), but only the modal abundance of the different minerals. This field is also invariably bounded by the introduction of hornblende and plagioclase to higher T, and by the introduction of glaucophane to higher P, although paragonite can also be introduced in more Al-rich compositions. Once these new minerals are stable, all hell is likely to break loose, and each section will be different but at least you would have the start of a section that you knew was real.